

DRAFT REPORT National Landscape of High-Impact Crosscutting **Opportunities for Next Generation Harsh** Environment Materials and Manufacturing Process Research, Development, and Demonstration

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List of Abbreviations

ARB – Accumulative Roll Bonding AEM – Anion Exchange Membrane AFSD – Additive Friction Stir Deposition AHSS – Advanced High Strength Steel AI – Artificial Intelligence AM – Additive Manufacturing AMT – Advanced Manufacturing Technology AMMT – Advanced Materials and Manufacturing Technologies (also, a program in the DOE NE office) AMMTO – Advanced Materials and Manufacturing Technologies Office in EERE ANL – Argonne National Laboratory AOE – Annual Energy Outlook APOLLO – Advanced Projects Offering Low Levelized cost of energy Opportunities ARPA-E – Advanced Research Projects Agency-Energy ART – Advanced Reactor Technologies program of the Office of Nuclear Energy ASME – American Society of Mechanical Engineers A-USC – Advanced Ultra Super Critical Steam BNL – Brookhaven National Laboratory CALPHAD – Calculation of Phase Diagrams CCA – Compositionally Complex Alloy CCGT – Combined Cycle Gas Turbine Plant CEFAS – Continuous Electric Field Assisted Sintering CHADWICK – Creating Hardened And Durable fusion first Wall Incorporating Centralized Knowledge CHP - Combined Heat and Power CHX – Compact Heat Exchanger CMAS – Calcia Magnesia Alumino Silicate (corrosion attack on thermal barrier coatings) CMC - Ceramic Matrix Composite CPU - Central Processing Unit CSAM – Cold Spray Additive Manufacturing CSP - Concentrating/Concentrated Solar Power CST – Concentrating/Concentrated Solar Thermal CTE – Coefficient of Thermal Expansion CVD – Chemical Vapor Deposition CVI – Chemical Vapor Infiltration DED – Directed Energy Deposition DLC - Diamond-like Coatings DLP – Digital Light Processing DoE – Design of Experiments DOE – U.S. Department of Energy EBC – Environmental Barrier Coating EBW – Electron Beam Welding ECAE - Equal Channel Angular Extrusion ECAS – Electric Current–Assisted Sintering EDM – Electrostatic Discharge Machining EEII – Energy and Emissions Intensive Industries (IEDO program) EERE – Office of Energy Efficiency and Renewable Energy EFAS – Electric Field-Assisted Sintering

- EFRC Energy Frontier Research Center
- EGS Enhanced Geothermal System

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EHEA - Eutectic High Entropy Alloy EIA – Energy Information Administration EPRI – Electric Power Research Institute EV – Electric Vehicle FECM – Office of Fossil Energy and Carbon Management FEM - Finite Element Method FGM – Functionally Graded Material FM – Ferritic Martensitic steel FMMAM – Fundamental Measurements for Metal Additive Manufacturing (NIST program) FSAM – Friction Stir Additive Manufacturing FSP/W – Friction Stir Processing/Welding GB – Grain Boundary GDZ – Gadolinium Zirconium Oxide (Gd₂Zr₂O₇) GMAW – Gas Metal Arc Welding GPU - Graphics Processing Unit GTAW – Gas Tungsten Arc Welding GTO – Geothermal Technologies Office HAZ – Heat Affected Zone HEA – High Entropy Alloy (a.k.a. MPEA, CCA) HEDE – Hydrogen-enhanced decohesion HELP - Hydrogen-enhanced Local Plasticity HEM – Harsh Environment Materials HFTO - Hydrogen and Fuel Cell Technologies Office HIP - Hot Isostatic Pressing HPC – High Performance Computing HSLA – High Strength Low Alloy steel HTF – Heat Transfer Fluid HTM – Heat Transfer Media HTTES – High-Temperature Thermal Energy Storage HX – Heat Exchanger ICME – Integrated Computational Materials Engineering ICWE – Integrated Computational Welding Engineering IDZ – Interdiffusion Zone IEDO - Industrial Efficiency and Decarbonization Office INL - Idaho National Laboratory LBW – Laser Beam Welding LCFFES - Low Carbon Fuels, Feedstocks, and Energy Sources LCM – Lithography-based Ceramic Manufacturing LCOE – Levelized Cost of Electricity LFW – Linear Friction Welding LIS – Laser-Induced Slip Casting LPBF – Laser Powder Bed Fusion LSAM – Large-Scale Additive Manufacturing LWR – Light Water Reactor MCHX – Microchannel Heat Exchanger MDF – Manufacturing Demonstration Facility MIC – Microbially-induced Corrosion MIG - Metal Inert Gas MIM – Metal Injection Molding ML - Machine Learning MMC – Metal Matrix Composite

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MPEA - Multi-Principal Element Alloy (a.k.a. HEA) MSEE – Molten Salts in Extreme Environments (DOE EFRC) MSR – Molten Salt Reactor NACE – National Association of Corrosion Engineers NE – Office of Nuclear Energy NETL – National Energy Technology Laboratory NG – Natural Gas NGMP – Next-Generation Materials and Processes (AMMTO program) NIST - National Institute of Standards and Technology NNS - Near Net Shape NRC – Nuclear Regulatory Commission NREL - National Renewable Energy Laboratory ODS – Oxide Dispersion Strengthened OEM – Original Equipment Manufacturer **OES – Ocean Energy Systems** O&M – Operation and Maintenance OPC – Ordinary Portland Cement ORNL - Oak Ridge National Laboratory OT – Operating Temperature OTT – Office of Technology Transitions PBF - Powder Bed Fusion PCHX – Printed Circuit Heat Exchanger PEI – Polyethyleneimine (polymer) PEM – Proton Exchange Membrane (a.k.a. Polymer Electrolyte Membrane) PIP – Polymer Infiltration and Pyrolysis PKA – Primary Knock-on Atom PM – Powder Metallurgy (a.k.a. P/M) PNNL – Pacific Northwest National Laboratory PRF – Permeation Reduction Factor PTA – Plasma Transferred Arc PV - Photovoltaic PVA - Polyvinyl alcohol (polymer) PVD – Physical Vapor Deposition PWR – Pressurized Water Reactor RAFM - Reduced Activation Ferritic Martensitic steel R&D – Research and Development RD&D - Research, Development, and Demonstration RDD&D – Research Development, Demonstration, and Deployment RFW – Rotary Friction Welding RHEA – Refractory High Entropy Alloy RICE – Reach, Impact, Confidence, Effort analysis RISE – RICE analysis + Significance Index **RPV – Reactor Pressure Vessel** sCO₂ – Supercritical Carbon Dioxide SE - Solid Electrolyte SETO – Solar Energy Technologies Office SFR – Sodium-cooled Fast Reactor ShAPE - Shear-Assisted Processing and Extrusion SLA – Stereolithography 3D printing SLM – Selective Laser Melting SLP - Selective Laser Processing

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SLS - Selective Laser Sintering SMR - Small Modular Reactor SOEC – Solid Oxide Electrolyzer Cell SOFC - Sold Oxide Fuel Cell SPD – Severe Plastic Deformation SPS – Spark Plasma Sintering (a.k.a. EFAS) SRZ - Secondary Reaction Zone SS - Stainless steel SSMAM - Solid-State Metal Additive Manufacturing STEP - Supercritical Transformational Electric Power SwRI - Southwest Research Institute T_H – Homologous Temperature TBC – Thermal Barrier Coating TEG – Thermoelectric Generator **TES** – Thermal Energy Storage TIG - Tungsten Inert Gas TMS - The Minerals Metals and Materials Society TPV - Thermophotovoltaic TR – Thermal Runaway TRL – Technology Readiness Level (see Appendix for TRL table with descriptions) UFG - Ultra-Fine Grained ULTIMATE – Ultrahigh Temperature Impervious Materials Advancing Turbine Efficiency (ARPA-E program) UWBG - Ultra-Wide Bandgap Semiconductor VHTR - Very High Temperature Reactor VTO – Vehicle Technology Office WAAM – Wire Arc Additive Manufacturing WBG – Wide Bandgap Semiconductor WEC - Wave Energy Converter WETO – Wind Energy Technologies Office WHP - Waste Heat-to-Power WHR - Waste Heat Recovery WLAM – Wire Laser Additive Manufacturing WPTO - Water Power Technologies Office YSZ - Yttria-Stabilized Zirconia

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Executive Summary

Accelerating harsh environment materials research and development is vital for the United States because these materials are crucial to industries that contribute nearly a half-trillion dollars to the annual U.S. gross domestic product. Even with the widespread adoption of advanced computational tools, the design, development, and deployment of new materials and components for harsh environments remains a slow and often multi-decade process from the conception phase through to commercialization. At the same time, accelerating electrification of the economy is a frontier that has created an urgent demand for new materials with superior performance in increasingly harsh environments.

The goal of this landscape document is to provide a survey of the opportunities to accelerate the design, development, and manufacturing of globally competitive, crosscutting next generation harsh environment material (HEM) components engineered for demanding service applications through capabilities development and transformative research. These advanced, high-performance HEM components are needed to achieve energy efficiency gains, emissions reductions, and lowered overall costs through improvements in energy production/conversion, energy storage, and energy utilization technologies, which constitute the landscape scope. Innovation in the development of advanced materials and manufacturing processes to produce more durable high-performance components intended for service in demanding harsh environments—without an unsupported cost penalty—will help transform America's energy future and build a globally competitive U.S. manufacturing sector that accelerates the adoption of these innovative technologies.

The Advanced Materials and Manufacturing Technologies Office (AMMTO) in the U.S. Department of Energy (DOE) established the vision, mission, framework, and goals of the landscape. However, a large team of subject matter experts from across DOE, its national laboratories, industry, and academia were involved in stakeholder engagement activities to determine the high-impact opportunities, to identify the technical challenges to be addressed, and to establish the current baseline state of the art (the benchmarks), targeted performance metrics, and pathways for technology developments in the field of high-performance harsh environment materials. These developments will leverage the power of modern tools like advanced manufacturing techniques (AMTs), computational-based materials/process development and qualification acceleration approaches, and smart manufacturing methods (e.g., artificial intelligence powered data analysis and process control systems, robotics/automation, digitally connected machines and assets) to improve manufacturing efficiency, adaptability, quality, productivity, and profitability.

One of the difficulties with establishing the various criteria for this topical area is defining a standard for "harsh." Operational requirements for a given technology are critically dependent on not only the environment, but also on the underlying material system and final application. Thus, the relative nature of what is considered harsh in one environment may not meet operational requirements in another. This report proposes the following as a comprehensive description of what constitutes a harsh environment: *an environment consisting of one or more stressors exceeding the current thresholds that can be experienced by a system component in any given application such that its functionality, material attributes, and durability are unduly degraded.* Such stressors include extreme temperatures, thermal cycling, extreme pressures, corrosive chemicals, extreme pH, dust and particulates, mechanical wear, abrasion, erosion, cavitation, neutron irradiation, and hydrogen attack. Individually, these conditions present substantial challenges. However, materials are rarely subjected to a single stressor, as shown in Figure 1.

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Figure 1. Diagram of harsh environment applications with associated stressors and representative components that show the commonalities between various energy generation, storage, transmission, and related technologies. The outer perimeter shows energy applications, while the middle layer shows stressors imposed on representative materials and devices in the center of the figure. Icon descriptions are shown at the bottom and in Appendix Figure 34.

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Though the technical aspects of materials selection, research, and development to achieve specific energy target metrics remain the purview of each DOE office, AMMTO has adopted four strategic goals (SG) for this landscape that involve pathways to:

- Accelerate the exploration, development, and demonstration of structural and functional highperformance materials (including enabling technologies) engineered for harsh service conditions with materials circularity and sustainability considerations. Structural and functional materials families are entire classes or sub-classes of materials that exhibit exceptional properties and have potential crosscutting interests to DOE. Achieving this goal will involve the use of materials development acceleration tools, including physics-based modeling and simulation, as well as artificial intelligence (AI) applications like machine learning (ML).
- 2. Drive improvements to traditional manufacturing technologies as well as develop and de-risk competitive novel advanced manufacturing technologies (AMTs) that promise greater process repeatability, reproducibility, cost savings, and sustainability to produce high-quality HEM components at industrially relevant scales. Similar to the first goal, achieving this goal will leverage the use of computational-based process development acceleration tools.
- 3. Shorten HEM manufacturing qualification and field certification times. This goal will capitalize on the power of modern physics-based modeling and simulation—in concert with accelerated testing and high-throughput materials characterization techniques—as well as AI/ML using the wealth of digital manufacturing data for qualification/certification with minimal required testing validation.
- 4. Support targeted HEM/component development and/or manufacturing for specific high-impact opportunities working in synergy with other DOE offices.

The framework of this landscape is not developed around explicitly categorizing materials needs based on the type of environment or material stressor it is exposed to because, for many applications, material components are exposed to coupled or multiple stressors. Therefore, to better serve the needs of the whole Department. A holistic approach involving five focus areas, or thrusts, has been adapted that originated from an earlier Innovation Impact Report conducted by The Metals, Minerals, and Materials Society (TMS) and Oak Ridge National Laboratory (ORNL), and sponsored by the predecessor of AMMTO, the former Advanced Manufacturing Office (AMO). These focus areas are:

- Focus Area 1: Functional surface technologies
- Focus Area 2: Materials integration into energy systems
- Focus Area 3: High-performance materials
- Focus Area 4: New paradigm materials manufacturing processes
- Focus Area 5: Materials and process development acceleration tools

These five thrusts are scoped for energy production, energy storage, and efficient industrial energy utilization technologies, for which the application-specific material stressors are already well known. By initially focusing on the end-use application requirements across the energy landscape and working backwards toward suitable materials and manufacturing technology solutions—rather than pursuing less directed technology development and subsequently trying to find a market application—means the landscape will better address the R&D needs of domestic industries to remain competitive while producing HEM products that improve energy performance across multiple applications.

The higher impact, crosscutting opportunities identified can be grouped together into the following five grand challenges, with their relevance to the five focus areas (FA), four strategic goals (SG), and application spaces given in brackets and their urgency (i.e., no-later-than timeframe to begin TRL advancement) indicated in boldface parenthesis:

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• Focus Area 1, Functional surface technologies grand challenge:

Develop materials, coatings, cladding, and manufacturing processes for components exhibiting superior molten salt and liquid metal corrosion resistance, validated/qualified under realistic (real world) conditions of temperature, flow, pressure, and irradiation. [*Also relevant to FA 3 & 4; SG 1, 2, 3 & 4; and to thermoelectric power production, energy storage, industrial applications.*] (2030-2035)

• Focus Area 2, Materials integration into energy systems grand challenge:

Improve capabilities to produce FGMs and multi/dissimilar-material integration through advanced joining/bonding techniques, including solid-phase processing like AFSD, FSW, and diffusion bonding (EFAS, HIP) to create systems with superior properties for specific harsh environment applications. [*Also relevant to SG 2 & 4; and all forms of energy production, energy storage, and industrial applications.*] (2030-2035)

• Focus Area 3, High-performance materials grand challenge:

Continue to enhance the performance and lower the manufacturing cost of components made from advanced alloys, ceramics, and coatings with superior high-temperature oxidation-, corrosion-, and/or wear-resistance. This would include near net shape (NNS) monolithic and composite components having complex geometries, large dimensions, textured microstructures, or surface engineering for enhanced properties and performance. [*Also relevant to FA 1 & 4; SG 1 & 2; and to thermoelectric power production, industrial applications.*] (2030-2035)

• Focus Area 4, New paradigm materials manufacturing processes grand challenge:

Evolve domestic manufacturing capability and feedstock/supply chain capacity to competitively produce ultra-large-scale metallic components for service in harsh environment energy and industrial systems, including establishment of community-accepted validation benchmarks to accelerate qualification and certification for AMTs. [*Also relevant to SG 2 & 3; and all forms of energy production, energy storage, and industrial applications.*] (2025-2030)

• Focus Area 5, Materials and process development acceleration tools grand challenge:

Progress and utilize enhanced length- and time-scale bridging methods for physics-based (deterministic) process-informed approaches, as well as probabilistic methods like machine learning, with the compilation of large research community accessible microstructure databases on HEMs to predict, design, and control microstructures, properties, and long-term performance of HEM components. [*Also relevant to SG 1, 2 & 3; and all forms of energy production, energy storage, and industrial applications.*] (2025-2030)

This landscape's broad scope and ambitious goals reflect the urgency with which the R&D community must tackle the HEM challenges and the opportunities facing the energy sector and more electrified industrial economy. Successful implementation of the landscape's recommendations would enable domestic manufacturers to produce competitively priced, advanced high-performance materials and components that promote U.S. leadership in the energy and manufacturing technologies of the future that support the nation's energy goals. The pages that follow outline DOE's HEM landscape and summarize the HEM efforts to date.

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1. Introduction

The U.S. Department of Energy's (DOE) High-Impact, Crosscutting Next Generation Harsh Environment Materials and Manufacturing Process Research, Development, Demonstration, and Deployment Landscape is a comprehensive plan sponsored by the Advanced Materials and Manufacturing Technologies Office (AMMTO). The landscape has been developed by a consortium comprised of Idaho National Laboratory (INL), Oak Ridge National Laboratory (ORNL), the National Renewable Energy Laboratory (NREL), and the Pacific Northwest National Laboratory (PNNL), in consultation with multiple DOE program and technology offices. Since 2019, AMMTO has invested over \$70 million into harsh environment materials research and development. The programs and initiatives have been known by various monikers: Materials for Harsh Environments, Materials for Extreme Environments, and Materials for Harsh Service Conditions. This report will henceforth refer to it as Harsh Environment Materials (HEM). While many independent DOE program offices (e.g., EERE, NE, FECM, ARPA-E, and SC) and technology offices (e.g., AMMTO, IEDO, SETO, HFTO, GTO, WETO, WPTO, VTO, BETO, and BTO) have established individual technical performance and economic targets as well as technology development roadmaps or multi-year program plans for the development of advanced high-performance materials (often involving harsh service environment requirements) in their respective domains, DOE has not, until now, published a comprehensive strategy to unify desired technological advancements of materials for harsh environments, and their manufacturing processes, in a complete crosscutting manner.

The energy mix in the United States is changing. For example, solar photovoltaic (PV) generating capacity will grow by about 325% to 1,019% by 2050 compared to 2022, while wind energy generating capacity will grow by about 138% to 235%. Growth is also expected in installed battery capacity to support the increased deployment of renewables. Nuclear generating capacity is expected to decline by 18% from 2022 to 2050. Acknowledging that these AEO 2023 forecasts are hypothetical predictions that also exclude early-developmental-stage technologies (e.g., hydrogen, enhanced geothermal, concentrating solar power (CSP), and nuclear fusion) as well as some existing technologies (e.g., hydroelectric generation), it is still clear that further advancements are needed in highperformance materials capable of withstanding harsh service conditions over the full spectrum of energy-production methods, including the more-established energy technologies like steam and gas-fired turbomachinery that collectively account for 80% of U.S. electricity production today. Efforts to enhance energy efficiency and power generation require components that must withstand various environmental stressors, including dust, high temperatures, acidic solutions, corrosive chemicals, oxidative and reducing environments, irradiation, mechanical stresses, hydrogen attack, and particulate-laden fluids. Frequently, multiple material stressors are coupled, or simultaneously present. To meet and exceed these harsh environment material challenges, high-performance materials are essential for providing longer service life and resulting in cost savings. DOE has prioritized the development of such materials through federal investments in research and development to address the significant challenges in developing advanced materials for harsh environments.

One funding initiative aims to accelerate the exploration and design of materials to shorten the time from research and development to demonstration. Another focus is on the domestic manufacture of bulk components and coatings/linings/claddings that can withstand harsh environments without experiencing undesired phase changes or microstructural changes. Developing a greater fundamental understanding of extreme and complex conditions is crucial, since material degradation—ranging from gradual performance loss to catastrophic failure—can result from a complex combination of factors that are challenging to replicate experimentally or predict computationally. Additionally, pathways to cost-effective manufacturing are needed, including the production of materials and components, as well as the assembly of parts that require the integration of materials in structures (e.g., welding, joining, bonding, coatings/cladding, sealing) while considering the entire supply chain.

1.1 AMMTO's HEM Portfolio

DOE's efforts to advance materials for harsh environments began in 2007 with the Basic Energy Sciences Workshop for Materials under Extreme Environments. This workshop engaged stakeholders to address specific

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types of extreme environment stressors, such as energetic flux, chemically reactive agents, thermomechanical forces, and electromagnetic fields. By 2011, the concept had evolved into a formal technology portfolio under Next-Generation Materials within the Buildings and Industrial Efficiency Technology Assessments, as described in the First DOE Quadrennial Technology Review. This review characterized materials for harsh environments as high-performance materials—including ceramics, engineered polymers, and metals—capable of operating in extreme conditions. The review also included related categories like high-performance, low-cost heat-transfer materials, functional coatings and interfaces, and thermal and degradation-resistant materials.

In the second DOE Quadrennial Technology Review in 2015, the definition of aggressive service environments was refined to include high temperatures or thermal cycling, high pressures, corrosive chemicals, dust and particulates, mechanical wear, neutron irradiation, and hydrogen attack. That same year, AMO—the predecessor to AMMTO—held a Materials for Harsh Service Conditions Workshop. Since 2015, there have been two additional workshops in 2020 and 2023 for this portfolio. Currently, AMMTO funds projects on harsh environment materials RD&D relevant to various energy production and energy storage technologies, as well as for efficient energy utilization in the manufacturing and industrial sectors, by using diverse design, development, and manufacturing tools.

1.2 Mission

Materials for harsh environments are essential for energy technologies spanning various DOE interest areas, addressing energy challenges with transformative science and technology solutions to ensure America's security and prosperity. AMMTO's mission is to "inspire people and drive innovation to transform materials and manufacturing for America's energy future." Recognizing that advanced materials and manufacturing are critical to all DOE program offices, AMMTO's Next-Generation Materials and Processes (NGMP) program has diversified its harsh environment materials project funding to increasingly sponsor and prioritize RD&D projects that intersect with other DOE program offices.

1.3 Vision

AMMTO envisions a globally competitive U.S. manufacturing sector that accelerates the adoption of innovative materials and manufacturing technologies. In order to maximize energy security, manufacturing competitiveness, and energy equity and environmental justice, the United States must remain the leader in advanced materials and manufacturing innovation for technologies of relevance across the energy sector. The landscape's objective is not to drive technology development under the purview of other DOE offices but to provide a framework fostering collaboration and synergism between these programs and AMMTO. The landscape provides guidance in developing strategies to drive innovation for improvements to traditional manufacturing methods as well as developing competitive advanced materials and manufacturing technologies (AMMTs) for harsh environments of broad interest across DOE. Traditional manufacturing methods and advanced manufacturing technologies (AMTs) for the production/fabrication of components can be grouped into additive manufacturing, subtractive manufacturing, and formative processing (including joining/bonding and surface treatments). Some of the many methods, which will be discussed in strategic goal #2, include various kinds of casting, forging, extrusion, powder metallurgy techniques (e.g., HIP, EFAS, high-energy ball milling, compaction, and densification), 3D printing, convergent/hybrid manufacturing routes, and severe plastic deformation, or SPD using very large plastic strains to produce ultrafine-grained high-strength materials and joints (e.g., shear-assisted processing and extrusion, or ShAPE; friction stir processing/welding, or FSP/W; and accumulative roll bonding, or ARB).

Multiple methods can even be combined into hybrid approaches to yield otherwise unobtainable results consistent with the four facets of the materials tetrahedron paradigm, structure-processing-properties-performance. A comprehensive understanding of material performance requires accurate hierarchal representations of multiscale features, material properties, and their processing and in-service evolution. As a simple example, the materials tetrahedron of Figure 2 illustrates how a refractory alloy might be 3D printed from a powder and then fully densified by hot isostatic pressing (HIP) or electric field assisted sintering (EFAS) to produce a complex geometry part (e.g., compact heat exchanger, turbine blade, etc.) with high-temperature strength that can be used in an application capitalizing on the specific multi-scale structure and properties of this particular component. Acquiring a detailed

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understanding and control of each of the four material facets can be facilitated by materials informatics (modeling & simulation, machine learning, data science), advanced in situ/operando sensors with process automation/closedloop control (digital twins), as well as nondestructive and high throughput synthesis and testing/characterization.



refractory alloy), both aided by digital twin technology

shaped refractory component with desired microstructure

Figure 2. An illustration employing the materials tetrahedron for a strategy to produce a complex geometry net-shaped part from a difficult-to sinter-and-machine refractory alloy for use at high temperatures. In this example, a hybrid approach is used in which the refractory alloy part is 3D printed from a powder and subsequently fully densified by HIP or EFAS. Digital tools (middle of tetrahedron) are central to understanding, designing, and controlling all facets of the material's multiscale structure (from microscopic to macroscopic), processing, properties, and performance.

There also exist manufacturing technologies possessing digitization functionalities supporting business applications to solve business problems—and which can be applied to manufacture multiple products—that are referred to as platform manufacturing technologies. These systems support manufacturing by collecting, storing, processing, and delivering data. Additive manufacturing (AM) platforms are an example of this type of technology, which is digitizing the manufacturing value proposition (i.e., software + material + hardware/printers) by integrating the flow from idea to design to product development and production, potentially on demand. More broadly, smart manufacturing refers to the entire suite of platform technologies that directly support this digital transformation of the manufacturing enterprise across the entire production lifecycle, which includes design, process, production, supply network, and enterprise levels. Platform manufacturing technologies and smart manufacturing technologies are key contributors to increasing production and lowering the manufacturing costs of HEM components. Thus, they are within the landscape scope.

Also included are enabling technologies such as materials and process development acceleration tools like advanced modeling and simulation, including high-performance computing (HPC) and multi-scale physics-based deterministic methods (e.g., integrated computational materials engineering, ICME), data-driven stochastic National Landscape of High-Impact Crosscutting Opportunities for Next Generation Harsh Environment Materials and **20** Manufacturing Process Research, Development, and Demonstration / January 16, 2025

methods (e.g., artificial intelligence, AI, and machine learning, ML), as well as associated hardware such as inline sensors, probes, and instrumentation for implementing smart manufacturing digital twins that can be used for realtime process/quality monitoring and AI-enabled autonomous control. These process-informed science, design, and engineering tools will facilitate improved and new manufacturing approaches for the production of high-performance HEM components satisfying pre-defined criteria and without an unsupported cost penalty by incorporating state-of-the-art as well as new and emerging digital/data-driven techniques. In contrast to ML, a traditional method used in industrial statistics is the Design of Experiments (DoE). It has proved to be one of the most effective when dealing with innovation, especially in product development and process improvement. The key tenet of DoE is that by systematically manipulating the values of several variables of interest while controlling all other variables (by holding them constant or randomizing), statistical models will yield *causal* knowledge of the relationship between the manipulated and dependent variables. If appropriate algorithms are chosen, ML methods can even be applied to DoE data to achieve better predictive performance without necessarily losing much in terms of interpretability with respect to the parametric approaches.¹

Another area of interest in this landscape involves the continued evolution of HEMs with superior properties relevant to many crosscutting energy applications, which we refer to as foundational materials. Examples of foundational materials of interest include high entropy or multi-principal element materials, superalloys (Ni-, Co-, and Fe-based), refractory alloys (e.g., containing Mo, W, Re, Ta, or Nb), ODS alloys (a type of MMC), advanced high strength steel and high strength low alloy steel (AHSS and HSLA), ductile intermetallic phases, bulk metallic glasses, advanced monolithic technical ceramics (e.g., oxides, carbides, nitrides, borides, silicides, various electroceramics, ceramics with room temperature plasticity), particle- and fiber-reinforced composites (e.g., ceramic matrix composites, or CMCs, and metal matrix composites, or MMCs), cermets (i.e., ceramic/metal composites with < 20% metal by volume), certain ordered layered materials (e.g., MAX phases), functionally graded materials, self-healing materials and coatings, and ultra-wide bandgap semiconductors. By pursuing advanced materials and manufacturing technologies that cut across DOE, AMMTO/NGMP can fulfill its mission to focus on funding innovation for novel materials with improved properties and scalable manufacturing processes in a collaborative manner and in synergy with other DOE offices.

1.4 Strategic Goals for the Landscape

The purpose of this landscape is to provide a survey of the highest impact opportunities for AMMTO's future investments in harsh environment materials with superior properties to enable and accelerate DOE's energy goals and reinforce the U.S. supply chain.

This purpose includes three clear and measurable landscape objectives:

- Identify critical, energy-related harsh environment material and manufacturing development technical challenges, associated R&D needs, and a measure of the R&D degree of difficulty—or level of required effort—for high-impact opportunities in the power and industrial sectors for maximum emissions reductions and energy efficiency improvements.
- 2. Determine the sequence of advancements or development pathways to be undertaken this decade to achieve national energy goals.
- 3. Establish a realistically aggressive schedule and visual timeline(s) for the landscape.

Through consultation with other DOE programs and technology offices, AMMTO established four strategic landscape goals for HEM R&D investments over the next decade:

1. Accelerate the exploration, development, and demonstration of structural and functional highperformance materials (including enabling technologies) engineered for harsh service conditions with

¹ Arboretti, R, Ceccato, R, Pegoraro, L, Salmaso, L, Housemekerides, C, Spadoni, L, et al. Machine learning and design of experiments with an application to product innovation in the chemical industry J of App Stats [Internet]. 2022 Jul [cited 2021 Mar 26];49(10):2674-99. Available from: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC9225671/

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materials circularity and sustainability considerations. Structural and functional materials families are entire classes or sub-classes of materials that exhibit outstanding properties and have potential crosscutting interests to DOE.

- 2. Drive improvements to existing manufacturing technologies as well as develop and de-risk competitive novel advanced manufacturing technologies (AMTs) that promise greater process repeatability, reproducibility, cost savings, and sustainability to produce high-quality HEM components at industrially relevant scales. Similar to the first goal, achieving this goal may involve the use of process development acceleration tools.
- 3. Shorten HEM manufacturing qualification and field certification times.
- 4. Support targeted HEM/component development and/or their manufacturing for specific high-impact opportunities.

These goals are designed to position the office to support DOE-wide efforts in harsh environment materials R&D collaboratively while also leading the further development and application of structural and functional foundational material families and platform manufacturing technologies. This approach aims to maximize synergy and avoid duplicative efforts.

Landscape Terminology

It is imperative for the reader to understand certain vocabulary used in this document, which are clarified in Table 1, accompanied by some synonyms and their meaning, as used in this document.

Phrase	Commonly used synonyms	Definition
Scope	-	The breadth or extent of the area of subject matter covered
Goal	-	A desired result or outcome to be achieved over a long term
Roadblock	Obstacle	A barrier (technical or economical) impeding or hindering progress
Challenge	Task, Opportunity	A specific technical objective (perhaps one of many) that needs to be accomplished to overcome a roadblock and ultimately achieve a goal
Maturation	Pathway	The technology development course followed
Innovation	Product, Invention, Idea	A potential solution, created to address a challenge. Innovative solutions are solicited in response to funding opportunities
R&D Need	Problem	A specifically identified capability deficit, without inclusion of a solution

Table 1. Terminology and definitions used throughout this landscape.

To minimize duplicative efforts, a core team of nine members was formed, comprising representatives from AMMTO, INL, NREL, ORNL, PNNL, as well as GTO, HFTO, WETO, and WPTO. Additional consultation was sought from offices such as IEDO, NE, SETO, and VTO. The core team was entrusted with strategic planning, assembling primary and secondary teams (comprising experts from industry and academia), drafting survey questions, organizing a workshop, prioritizing identified pathways, and authoring the landscape report.

Subsequently, the primary team, consisting of 33 representatives—11 from industry, 11 from academia, and 11 from national labs—was selected by the core team. Their role was to provide overarching insights into the R&D landscape of HEM in the U.S., offering expert knowledge on the current state of research and development along with identifying opportunities.

The six key tasks performed by the core team were:

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- 1. Identification of DOE-internal stakeholders
- 2. Planning for stakeholder engagement
- 3. Solicitation of R&D direction
- 4. Engagement and validation with external stakeholders
- 5. Analysis of the portfolio
- 6. Development of the landscape along with the assessment report for portfolio maturation.

Collaborating with the core team, the primary team assisted in assembling a group of specialized experts (the secondary team) to delve deeper into technical aspects, ensuring comprehensive coverage of landscape constraints and addressing any blind spots. Both primary and secondary teams participated in responding to survey questions, attending workshops, and characterizing and voting on the landscape roadblocks requiring attention. These efforts aimed to inform research direction and prioritize crosscutting R&D roadblocks for immediate resolution, thereby accelerating DOE's emissions and energy goals across various application domains such as nuclear, solar, wind/hydro, geothermal, energy storage, and decarbonization. The secondary team comprised 144 members, representing experts from industry, academia, and national labs. 77% of the primary team and 50% of the secondary team actively participated in survey responses and voted on critical crosscutting technical roadblocks within the HEM landscape.

The core team recognized the necessity for a comprehensive approach, which led to the identification of five focus areas:

Focus Area 1: Functional Surface Technologies Focus Area 2: Materials Integration into Energy Systems Focus Area 3: High-Performance Materials Focus Area 4: New Paradigm Materials Manufacturing Processes Focus Area 5: Materials and Process Development Acceleration Tools.

These focus areas were derived from an earlier Innovation Impact Report conducted by The Metals, Minerals, and Materials Society (TMS) and ORNL, sponsored by AMO, the precursor of AMMTO. Applying the focus areas across the four strategic goals (see Table 2) produced a map for goals and areas that have impactful crosscutting capabilities.

	Focus Area 1	Focus Area 2	Focus Area 3	Focus Area 4	Focus Area 5
Strategic Goal 1			\checkmark		\checkmark
Strategic Goal 2	\checkmark	\checkmark		\checkmark	\checkmark
Strategic Goal 3	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Strategic Goal 4	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

Table 2. Description of how the landscape's four strategic goals relate to its five focus areas.

AMMTO's HEM landscape strategic goals are further elucidated below.

Strategic Goal 1: Accelerate the exploration, design, development, and demonstration of advanced highperformance structural and functional materials/components (including enabling technologies like in-situ sensors) engineered for harsh service conditions, with consideration given to materials circularity and sustainability.

Certain structural and functional material families are known, observed, or predicted to exhibit exceptional properties, durability, and performance and thus hold significant crosscutting interest for DOE program offices in achieving their specific technology goals. In some cases, materials having the needed attributes are not available,

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and in other cases they are too costly. Historically, the primary portfolio focus has been on materials with expanded high-temperature functionality. Materials have been sought that are thermally stable and exhibit high strength and corrosion/oxidation/irradiation resistance at the required elevated service temperatures. With the broad energy application space in focus for this landscape, a plethora of material families (i.e., foundational materials) are of interest. These include high entropy or multi-principal element materials, superalloys (Ni-, Co-, and Fe-based), refractory alloys (e.g., containing Mo, W, Re, Ta, or Nb), ODS alloys (a type of MMC), advanced high strength steel (AHSS) and high strength low alloy (HSLA) steel, ductile intermetallic phases, bulk metallic glasses, monolithic technical ceramics (e.g., oxides, carbides, borides, nitrides, silicides, various electroceramics, as well as ceramics with room temperature plasticity), particle- and fiber-reinforced composites (e.g., ceramic matrix composites, or CMCs, and metal matrix composites, or MMCs), cermets (i.e., ceramic/metal composites with < 20% metal by volume), MAX phases, functionally/compositionally graded materials, and ultra-wide bandgap (UWBG) semiconductors that can be used to fabricate in situ sensors (i.e., for operando detection/measurement of strain, pressure, gases, temperature), as well as power electronic and control devices for extreme environments that are beyond the capability of more established semiconductor materials.

Ideally, advanced harsh environment materials would combine properties (e.g., high temperature strength, ductility, and fracture toughness) rarely found together in a single material, which could impart multifunctionality. Additionally, there is a need for advanced self-healing materials and coatings/films/engineered surfaces to protect base materials from mechanical wear, abrasion, erosion, and corrosive environments for solving early detection problems, monitoring real-time conditions, and autonomous repairing. It should be stressed that not all these materials were identified explicitly as high-impact opportunities in the next decade by the various landscape teams but, nonetheless, they all remain in scope; as the various energy technologies progress, so too do the requirements (sometimes in unexpected ways) of the requisite energy system materials/components.

Achieving this strategic goal involves accelerating the research, development, and deployment of advanced materials, coatings, claddings, and components/devices fabricated from these materials. This acceleration will be facilitated through tools such as high-performance computing (HPC), multi-scale physics-based deterministic methods (e.g., integrated computational materials engineering, or ICME), as well as data-driven stochastic methods (e.g., artificial intelligence, machine learning). Coupling deterministic with probabilistic methods is also fruitful for facilitating accelerated modeling by taking advantage of both traditional direct design (i.e., given the material, find its properties) and inverse design (i.e., given the properties, find a suitable material) approaches.

In addition to physics-informed ML approaches for composition – process – property design, data-driven ICME is being used for discovering and optimizing new materials. For example, ML algorithms can be used to screen/purge low-quality data from large computational thermodynamics and kinetic datasets for more efficient and higher-throughput microstructural simulations. Finally, in-situ measurements, characterization methods, and digital twins will also be utilized to facilitate the design, processing optimization, and modeling of in-service performance of advanced components to meet application requirements.

Strategic Goal 2: Drive improvements to traditional manufacturing technologies as well as develop and derisk competitive novel AMTs with the highest possible degree of process repeatability, reproducibility, and sustainability to produce HEM components at industrially relevant scales with consistently high quality in conformance to design specifications. Similar to goal 1, achieving this goal may involve the use of process development acceleration tools.

Harsh environment components can be fabricated (net shaped) by a variety of traditional methods as well as AMTs, including additive manufacturing (e.g., various kinds of 3D printing), subtractive manufacturing (e.g., machining, drilling, cutting), and formative/deformation processing (e.g., casting, forging, rolling, extrusion, powder metallurgy). Generally, materials processing is aimed at achieving multiscale structures that optimize a specific property of interest. The various pertinent length scales correspond to (in decreasing order of visibility): system level, or overall geometrical shape; macroscopic structural features discernable to the unaided eye; microscopic features too small to be viewed by the unaided eye; nanoscopic; and atomic/molecular). For HEMs, the property of most interest is often strength, which microstructure greatly influences as well as hardness, toughness, ductility, and malleability These mechanical properties rely on a material's plasticity, which is rooted in the ease of slip (gliding motion) of

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close-packed planes of atoms across one another, especially dislocation mobility. Dislocations are metastable extended defects containing an abrupt change in the arrangement of atoms, which are introduced in crystalline materials primarily through processing when stress is applied.

Plastic (permanent) deformation processes such as forging are often used to produce HEM components because such parts generally have higher strength (directionally dependent), durability, and hardness than do cast parts. There are many strengthening mechanisms at play in plastic deformation processes. These work by inhibiting the movement of dislocations, for which slip occurs much more readily than it does for close-packed planes in a perfect crystal. In competition with grain refinement, plastic deformation processes (e.g., forging, rolling, extrusion) carried out below the recrystallization temperature increase dislocation density, which hinders dislocation motion, strengthening a material, but lowering ductility. This is referred to as work hardening or strain hardening. By contrast, through a complex interplay between recrystallization, grain growth, and recovery, hot working a metal above its recrystallization temperature will preserve or even enhance ductility while maintaining or increasing strength (if there are inclusion stringers), as well as maintaining or lowering hardness. There are various kinds of processes using plastic deformation, including forging (hammering), rolling, extrusion, drawing, bending, stamping, swaging, and others, all of which produce wrought products, by definition referring to the condition of a material worked into shape.

In the extreme case of severe plastic deformation (SPD), the final product is an ultra-fine grain (UFG) material that equates to a much larger volume fraction of grain boundary which, in turn, offers an even greater resistance to dislocation motion yielding enhanced strength, at the cost of reduced ductility or formability. Still another strengthening mechanism is solid solution strengthening, which works through the creation of strain in the crystal by the substitution of host atoms with those of a different atomic radius, again at the expense of ductility. If fine particles of an insoluble impurity phase (precipitates, dispersions) are present, this too can serve to strengthen an alloy (i.e., precipitation strengthening). However, when a brittle metal is combined with a ductile metal with which there is little or no mutual solid phase solubility nor formation of any intermetallic phases (e.g., silver and bismuth), the alloy so formed has both greater strength and ductility, somewhere in between the two end members.

Unfortunately, cast and wrought products are often heterogenous and can contain pores, voids, microcracks, or other defects that can ultimately result in creep (time dependent plastic deformation at constant stress and temperature) or fatigue (cyclical loading) failures. Powder metallurgical techniques have advanced to the point that they can be capable of producing fully dense (zero porosity) net shaped products suitable for higher temperature and strength applications than those produced by casting (solidification) and wrought methods. Additive manufacturing now offers a significant potential for producing net shaped metallic parts with distinctly localized microstructures and mechanical properties, commonly known as functional grading. The layer-by-layer building concept inherent to AM allows the heat input, thermal gradients, and solidification microstructures that enable this compositional-based functional grading. However, the layer boundaries (in the build direction) in addition to the presence of microstructural defects in common with parts produced by more traditional methods, such as inclusions, pores, columnar-coarse grains, and hot cracks, can result in complex microstructures in AM parts that impart significantly different or anisotropic mechanical properties as compared to cast or wrought products.

The "traditional" methods include various mature and well-established families of net shaping techniques (each with many subsets) like casting, forging, powder processing methods involving uniaxial compaction followed by postforming sintering, cold isostatic powder pressing, as well as welding/joining techniques. Note: we tend to prefer the term "traditional" over "conventional" in the context of manufacturing methods. A traditional method implies one passed down from prior art/generations. By contrast, conventional implies a manufacturing method chosen or expected based on what is commonly used. In some cases, it is conventional/expected to use traditional methods, while in other cases more advanced (i.e., less common) manufacturing techniques would naturally be selected.

Examples of advanced manufacturing technologies include (but are not limited to) laser processing, additive manufacturing, and micro manufacturing (both micro parts and micro features). Lasers are ubiquitous and they are used commercially in manufacturing for cutting, surface texturing, ablation, cleaning, hardening, welding, soldering,

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cladding, marking/engraving, peening, and even forming. In hybrid processes, lasers are used to assist in turning, milling, grinding, machining, chemical etching, tape winding, and friction stir welding. However, although manufacturing with lasers is not "new," developments over the last twenty years with different kinds of lasers, designs, operation, and processes speak of new technology.² Some AMTs are relatively mature, established for some applications, and readily scalable but are nonetheless still considered "advanced technologies" because either they are distinctively different, or they have a high degree of sophistication or innovation but may still lack common/broad industry adoption.

Many AMTs, such as some kinds of powder processes like metal injection molding (MIM), electric field assisted sintering (EFAS) and hot isostatic pressing (HIP), as well as other solid-state processing like severe plastic deformation (SPD), have been commercialized but are not as widely used across industries due to significant cost constraints or technical/process/scale-up limitations. For example, SPD can produce UFG metallic components categorized into three groups based on their suitability for bulk, sheet, and tubular samples. However, some of the main challenges in SPD processing are the limited throughput and sample size including the length and cross-sectional area. There also exist convergent/hybrid manufacturing routes (e.g., additive casting).

Success for this strategic goal equates to improving the capabilities, efficiencies, and cost competitiveness of traditional HEM bulk component fabrication and coating/cladding methods (e.g., arc melting, induction melting, forging, casting, and many other techniques) as well as advancing the technology readiness levels (TRLs) of AMTs and hybrid approaches, characterization techniques, and feedstock materials production routes (e.g., tailorable powders for powder fusion additive manufacturing and powder metallurgy processes, extrusions for wire arc additive manufacturing (WAAM) and solid-state metal additive manufacturing, or SSMAM). A TRL table with descriptions is given in Table 13 of the appendix.

For monolithic technical/engineering ceramics, superior functional properties are often possessed but are not easily exploitable due to low fracture toughness and low plasticity/fabricability. Manufacturing methods to produce ceramic components of complex geometries as well as textured (i.e., grain-aligned) microstructures could enable opportunities to take advantage of enhanced anisotropic properties. This can be done with traditional slip casting to a limited extent, and it has also been explored for more complex geometries with SLA/DLP. Complex geometry technical ceramic parts for harsh service environments include impellors, turbine blades, heat exchangers, fuel nozzles, burners/ignitors, micro-reactors, sensors, catalyst supports, sensible thermal energy storage devices (e.g., honeycomb and other porous ceramic blocks), some CSP components, and geothermal/mining components. The U.S. has outsourced much its manufacturing of technical ceramics fired at high temperatures (> 1,100°C). It is also worth noting that most of the monolithic ceramic products currently available from domestic companies lack the geometric complexity that would be needed for the demanding applications mentioned above. Thus, more advanced high-throughput domestic manufacturing (including AM) of ceramics is needed as well as the capability to make large AM ceramic parts (e.g., build volumes > 1 ft³). A very informative roadmap for additive manufacturing of technical ceramics has been published recently.³

This strategic goal includes seeking improvements in cost competitiveness, manufacturing throughput, build quality, and part size scaleup. Improvements in current benchmarks between 25 to 50% are not unreasonable. AMTs capable of competitively producing fully dense (i.e., zero porosity), high strength, high dimensional precision and shape fidelity, high-performance parts or coatings with lower residual stress or UFG high-strength HEMs from secondary (i.e., scrap) feedstock with lower environmental impacts (e.g., high strength lightweight aluminum alloys with improved corrosion and stress cracking resistance) are of particular interest. Most fabrication processes involving non-uniform plastic deformation, localized variations in thermal contraction due to temperature gradients

² "Design for Advanced Manufacturing: Technologies and Processes," L. K. Gillespie, McGraw Hill Education (2017) ISBN 978-1-259-58745-0.

³ Cramer CL, Ionescu E, Graczyk-Zajac M, Nelson AT, Katoh Y, Haslam JJ, et al. Additive manufacturing of ceramic materials for energy applications: Road map and opportunities. Journal of the European Ceramic Society [Internet]. 2022 Jul [cited 2024 Sep 12];42(7):3049–88. Available from: https://doi.org/10.1016/j.jeurceramsoc.2022.01.058

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within a sample, or volume differences in phase transformations of a sample induce residual (internal) stresses inside manufactured components. Residual stresses can be beneficial or, in many cases, can lead to part distortion and be detrimental to the performance of the component. Residual stress management aims at improving service performance and product life cycle. However, quantifying residual stress through modeling and simulation is difficult. Thus, industry needs fast, efficient, and reliable methods for measuring and controlling the state of residual stresses. The most frequently used methods of minimizing residual stress are pre/post heat treatments, microalloying, and part geometry optimization. In some cases, the simple addition of material in critical regions mitigates the accumulation of residual stresses.

Greater utilization of and advances in process development acceleration tools such as the same multi-scale physics-based deterministic (e.g., ICME) and data-driven stochastic methods (e.g., artificial intelligence, machine learning) called for in Strategic Goal One are sought that can be used together with a suite of smart manufacturing digital tools (e.g., in situ/operando sensors, digital twins) to monitor, optimize, and adjust operational parameters in real time—particularly with self-learning or autonomous closed-loop control systems—in order to more efficiently achieve production of components having the desired properties. Finally, a key challenge with this strategic goal is the re-establishment of not only large-scale production capabilities (tonnage quantities) but also recapturing expertise on fabricability through education and workforce development efforts.

Strategic Goal 3: Work to shorten HEM manufacturing qualification and field certification times.

Validated modeling and reliable simulations are needed as testing methods to shorten the time it takes to qualify materials made by AMTs (to ensure they repeatedly meet the production specifications for the material properties) and certify them as meeting the performance requirements for use in a field application. These processes currently rely on extensive empirical testing that varies widely between applications (e.g., critical aerospace and defense applications as well as non-critical applications) and industries, which can take 5 to 15 or more years and millions of dollars to complete, coupled with re-qualification following minor process changes. Materials need to be qualified more rapidly to support innovation in energy technologies that reduce cost, improve safety, and accelerate commercialization.

AMT process conditions tend to be much less well-defined than traditional manufacturing processes. Moreover, many AMTs can have significant process-induced localized (e.g., layer-by-layer) compositional, microstructural, and property variations requiring a thorough understanding of processing-structure-property-performance correlations. An AMT-produced qualification framework must consider the large number of variables involved in feedstock preparation/properties, forming processes, and post-processing. The inhomogeneous nature of AMT-produced components can result in uncertainties in material performance and challenges at the component scale that make the qualification and certification process more complex, time consuming, and expensive. Different microstructures and properties throughout the volume of a component cannot be easily handled by traditional qualification methods. In addition, these conditions vary as a function of geometry. Even components with different geometries made using the same feedstock and the same process can have different defects, properties, and performance.⁴

Several manufacturing qualification/field certification pathways are possible, such as statistical based empirical exsitu testing, in-situ manufacturing data-based qualification, as well as model-based qualification with minimal testing validation. A multi-scale ICME-based qualification using predictive tools that can accurately simulate accelerated aging and provide uncertainty quantification on material evolution and lifetime will be greatly beneficial for components produced by AMTs as well as for HEMs where materials are exposed to coupled materials stressors.

⁴ Englert L, Czink S, Dietrich S, Schulze V. How defects depend on geometry and scanning strategy in additively manufactured AlSi10Mg. Journal of Materials Processing Technology [Internet]. 2021 Aug 18 [cited 2024 Jul 24];299:117331. Available from: <u>https://doi.org/10.1016/j.jmatprotec.2021.117331</u>

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The DOE Office of Nuclear Energy similarly identified rapid qualification of materials for service in nuclear reactors as part of their 5-year AMMT roadmap in 2022.⁵ AMMTO will work with the NE AMMT program to collaborate on and achieve these capability developments.

In the NE AMMT roadmap, which we propose to emulate for non-nuclear materials, a rapid qualification framework will be developed and prototyped using a LPBF 316 SS test case (for use with the ASME Section III, Division 5 rules covering the design and construction of high-temperature nuclear reactors) with combined experimental and computational efforts. It will be further supported by developing a multidimensional data correlation (MDCC) platform to handle multi-length scale data needed for informed qualification and certification of nuclear components. Major planned milestones for the rapid qualification effort include (1) demonstrating process-informed qualification for AM, (2) demonstrating NDE techniques capable of detecting defects and various microstructural features, (3) establishing the MDDC framework and demonstrating its application to the qualification of LPBF 316 SS, and (4) completing the ASME Code qualification experiments and initial demonstration of accelerated model-based qualification.

Additionally, the National Institute of Standards and Technology (NIST) has an ongoing Fundamental Measurements for Metal Additive Manufacturing (FMMAM) program, which will be leveraged to develop the metrology needed to enable qualification of AM parts, the processes, and the feedstocks to reduce the need for complete re-qualification.⁶ As with NE's program, new accelerated qualification/certification frameworks could be demonstrated for non-nuclear applications initially through establishing a code case for a selected material and advanced manufacturing process. This would involve process-informed material processing/property correlation studies, in situ data collection, post-process nondestructive evaluation, modeling for time extrapolation for longterm material performance evaluation, component manufacturing and demonstration, and ASME engagement for qualification. Argonne National Laboratory also has a program that can support accelerated material qualification by using ML to automatically collect the relevant test condition data to reduce uncertainty and train predictive models (i.e., ML-enhanced physics-based methods) for key engineering material properties that bound the long-term performance of materials operating in challenging service conditions. Lessons learned and experience gained in qualifying/certifying a selected system will facilitate expansion/application of the framework to other manufacturing technologies and materials systems. Success for this strategic goal is measured in time reductions for qualification and certification, as well as in reductions in the total burden on manufacturers and research centers by enabling a more competitive materials development environment that promotes higher innovative throughput.

Strategic Goal 4: Collaboratively support targeted development of HEMs, components and/or their manufacturing for specific high-impact opportunities, which have been identified/selected by other DOE offices that cut across DOE for specific applications.

AMMTO is consistently eager to engage in collaborative efforts with other DOE technology offices to support their respective missions (Figure 3). By identifying promising areas of high-impact, crosscutting materials and manufacturing research, development, demonstration, and deployment for harsh environments, AMMTO aims to prevent the duplication of efforts and ensure efficient allocation of resources. Staying abreast of current materials research, development, and demonstration, (RD&D) is essential to drive rapid innovation in materials science.

 ⁵ Li M, Andersson D, Dehoff R, Jokisaari A, Van Rooyen I, Cairns-Gallimore D. Advanced materials and manufacturing technologies (AMMT) 2022 roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 24]. Available from: <u>https://www.energy.gov/sites/default/files/2023-03/ne-ammt-roadmap-030823.pdf</u>
 ⁶ Fox J. Fundamental measurements for metal additive manufacturing [Internet]. NIST 2024 Apr 17 [updated: 2024 Apr 25, cited 2024 Sep 12]. Available from: <u>https://www.nist.gov/programs-projects/fundamentalmeasurements-metal-additive-manufacturing</u>

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Energy Space	Harsh Enviror Technology	nment Energ	y s	Structural Materials	S Fun	econ ctiona	dary I al Pro	Req. perties
	Cold section Hot section	Steam turbine			*		ß	e state
B	Well/Casing Drilling/Hammer	Motors/Sensors Steam turbine			*	()E	re B	
H2	Fuel cells & Elez. H2 infrastructure	H ₂ ICE / turbine					1 1	
*	WHR / TES/ HX Refractories	Heating element Steam turbine			熱		10 ²	
	Primary System Secondary Sys.	Steam turbine			*		10 10	
	Solar Receiver TES	HTF Steam turbine			*	ΞŒ	ß	<u>ر است</u> ل
	Bearings/gears	_					r B	
	Francis Runner						ß	
	Batteries Capacitors	TES]		絷		re E	<u>ر المعالم</u>
	Energy Spaces			Structural Materials		Secondary	Req. Fun	ct. Properties
Symbol Meanin Gas Turb	ng Symbol Meaning ine Industrial Decarbonization	Symbol Meaning Wind Power	Symbol	Meaning Metals/Alloys Intermetallics		Symbol	Mean Coupled T Electrically	ning Fransport Conductive
Geothermal	Power Nuclear Power Power Concentrated Solar Power	Hydro Power Energy Storage	- - - -	Metalloids Ceramics olymers, plastics, & fibe Composites & Cerme Amorphous solids/Glas	rglass As	#A ₩	Electrically Opti Thermally Thermally Semicon	Insulating ical Conductive Insulating iducting

Figure 3. Diagram showing the connections between AMMTO's HEM portfolio and other DOE programs. Tabulated in the figure are typical structural materials (including those providing for oxidation/corrosion/wear/hydrogen/irradiation resistance and other protection from failure mechanisms that degrade structural integrity) currently in use or anticipated for future use in each energy technology. Also shown are representative harsh environment sub-systems and frequently encountered critical secondary functional material property requirements of components. This is not meant to be an exhaustive list. Sub systems operating under what are not normally considered harsh environments (e.g., generators) are omitted. Coupled transport refers to transport properties involving two fluxes and two forces, such as thermoelectric, thermodiffusion, thermomechanical, or magnetotransport properties.

The success of this strategic goal will be evaluated based on the outcomes of synergistic projects with long-term technological implications that pose research challenges beyond the scope of any single program office. By undertaking developmental projects that align with the nation's strategic goal of maintaining competitiveness in the materials sector, AMMTO positions itself as a collaborative partner not only within DOE, but also with other federal agencies and private enterprises. Figure 4 shows a selection of various opportunities that AMMTO is pursuing that crosscut multiple DOE offices.

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HEM Projects by Material Type



FY19-21 HEM Project Crosscuts with DOE Offices



FY22 HEM Project Crosscuts with DOE Offices



Figure 4. Breakdown of % of AMMTO HEM budget by a) application and b) material type as well as HEM project crosscuts between AMMTO and other DOE offices for c) FY19-21 and for d) FY22.

d)

1.5 Prioritization Methodology

a)

Together, the core, primary, and secondary teams conducted a deep dive assessment of the HEM landscape to uncover the technical challenges limiting advancement toward strategic goals for each focus area. Resolving these challenges would also accelerate the four DOE strategy goals. The research identified technical challenges needing immediate resolution if DOE strategy goals are to be achieved. Furthermore, the experts characterized 70 technical challenges through surveys and a virtual workshop and follow-on meetings. Technical challenges were validated by the core, primary and secondary teams through a voting process. Tabulated votes ranked the relative importance of each challenge for a **RICE+Significance Index (RISE)** prioritization analysis, a particular framework tailored for the needs of this landscape. Components of the RICE framework include:⁷

- Reach: This assessment reviewed the crosscutting characteristics of each challenge across the application spaces and focus areas. It objectively assessed the ability of R&D to address diverse needs and challenges while reaching a wide range of users or beneficiaries. The Reach score was determined using expert survey results and votes to evaluate the reach of the technology based on the number of crosscutting applications technology advancements would have.
- Impact: Refers to the anticipated effects, outcomes, or consequences resulting from the adoption, implementation, or use of a particular R&D effort. The impact of technology could be positive, negative, or neutral. In our model, weight was assigned based on the allocation of votes subjectively determined for each challenge by the insights from the expert respondents. Generally, high performance materials with a higher degree of crosscut or lowered cost correlated with a larger impact score. High-temperature functionality (e.g., irradiation/oxidation/creep resistance) of materials relevant to various energy

⁷ Microsoft. Understanding the RICE model and its framework [Internet]. Microsoft 365; 2024 [cited 2024 Sep 12]. Available from: <u>https://www.microsoft.com/en-us/microsoft-365-life-hacks/organization/understanding-the-rice-model-and-its-framework</u>

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production technologies, smart manufacturing methodologies (e.g., insitu sensors), and material or manufacturing/process performance improvements without a substantial cost penalty (e.g., advanced joining techniques) serves as examples of opportunities that garnered high impact scores. For the first, higher temperature processes are more efficient and therefore more impactful form a resource perspective. For the second, smart/platform manufacturing is highly applicable and impactful across the product life cycle. With the third, removing price constraints for high performance materials and advanced processes opens up the potential application space, particularly with the more cost sensitive sectors

- Confidence: Addresses the uncertainty in the other three scores (R, I, and E). In our analysis, a blanket value of 85%T (medium confidence) was used for every challenge.
- Effort: Pertains to the resources of time, money, manpower, and expertise required for the development, implementation, and maintenance of a particular opportunity or innovation. It encompassed the collective exertion and activities undertaken to research, design, prototype, test, refine, and deploy a technology to achieve desired outcomes or objectives. In our model, current TRL assessments (determined from exhaustive literature surveys) provide an objective measure of the level of effort required to move R&D forward through attainment of a completed TRL 7 state (i.e., entering TRL 8) by the end of the next decade. Higher TRL advancements would be handed off to other DOE program offices such as the Office of Technology Transitions (OTT) or directly to the private sector to drive commercialization further. A TRL table is given with descriptions in the appendix. AMMTO generally funds R&D in the TRL 3 to TRL 7 range.

For example, a high impact/reach opportunity requiring a high degree of effort (i.e., one currently at a low TRL) will need to be pursued more aggressively than one with the same impact/reach potential requiring less effort (i.e., one already at a high TRL) in order to enter a state of TRL 8 by the end of the next decade. Most AMMTO projects seek to advance the TRL by a one-to-two step increase over a three-year period of performance. Thus, R&D should begin around 2025 for any high impact opportunity currently at a TRL 3 or lower in order for it to enter TRL 8 by 2035. High impact opportunities currently at TRL 5 or higher could begin as late as 2030 in order for it to enter TRL 8 by 2035.

The RICE Score is computed as $(R \times I \times C)/E$. Lastly, the Significance Index represents the relative importance of each challenge from a schedule or timeline perspective, clarifying the earliest possible time when impact could be expected. This was calculated from program and activity durations and slack times.

Experts reviewed, characterized, and voted on the reach, impact, TRL maturity, and target timelines of 70 technical challenges over the course of a month. Independent peer-review of TRL maturity for each technical challenge validated and baselined the current state of research for each challenge, which was used to assess RD&D progress to date. Data output from survey analysis and expert votes was critical to the semi-quantitative RISE analysis which evaluated each technical challenge or research opportunity.

It is important to remember that the RISE Score Framework is just one tool for prioritizing initiatives. Firstly, it should be used in conjunction with other decision-making frameworks and strategies, such as cost-benefit analysis, to ensure a comprehensive approach. Secondly, it is important to consider the trade-offs between the different components of the analysis. For example, an initiative to address a challenge with a high impact factor may also require a significant amount of effort to implement. In this case, it is important to consider whether the potential impact is worth the resources required. This is the reason the effort/opportunity plot is also given below in Figure 5.

Applying the RISE analysis across the technical challenges produced a semi-quantitative analysis (i.e., based on the subjective information/perspectives from a limited number of subject matter experts) that was used for prioritization. Beyond simply identifying the investment priorities for DOE, the size of the circle for each challenge represents its relative weight (i.e., Impact score). The larger the circle, the greater the Impact score.

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Figure 5. Opportunity potential based on reach vs. effort (objective measures) required for all 70 identified challenges. This plot is helpful when considering whether pursuing challenges with high impact and reach scores are worth the resources and effort required. The overall impact potential (subjective) is indicated by the size of the circles. Larger diameters signify higher expected impact. See each FA section table for associated challenge codes.

The results represent the culmination of expert insights gathered through surveys, workshops, meetings, roundtables, and expert voting rounds. This analysis reviews the crosscutting characteristics of each technical challenge across the application spaces (e.g., wind, solar, hydro, nuclear, geothermal, decarbonization, hydrogen) and the focus areas described above. Challenges with the highest Significant Index scores (Table 1) should be considered for prioritization.

The spectrum of RD&D opportunities that address diverse HEM needs and challenges across application spaces are found in Figure 5 along the High-Impact Opportunity Potential axis in. Opportunities on the left present limited potential for RD&D gains, while those on the right represent a greater potential for results.

Upper Right (UR) Quadrant:

The UR Quadrant represents research areas where DOE investments would make a significant difference. This is mostly due to the level of effort and resources required to advance research. From a research and development perspective, industry may not have the resources and/or capability to resolve these technical roadblocks. It is recommended that research investments in this quadrant would be advantageous to the United States for the reasons cited.

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Ignoring RD&D opportunities in this quadrant would impact U.S. competitive advantage in the future. Research dollars in this area now would minimize the level of effort required in the future and increase industry engagement and potential adoption of new solutions in the future. Research in this quadrant would lower the level of effort barrier and widen the net to include research communities across industry and academia.

Lower Right (LR) Quadrant:

The LR Quadrant represents research areas where DOE investments would achieve the quickest results, mostly due to the high-impact opportunity potential and the minimal effort required to advance research compared to the UR quadrant. Given the quick gains to be expected, it is highly likely that collaboration with industry in these research areas would accelerate technology adoption.

From an accelerated technology adoption perspective, research opportunities in this quadrant should be pursued concurrently with those in the UL quadrant, given that both quadrants represent the high-impact opportunity potential for industry and DOE. It is recommended that DOE dollars in this quadrant should be pursued with the goal of maturing RD&D efforts towards commercialization and industry adoption. Industry cost share arrangements would be strategic to assure continued industry engagement through commercialization.

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2. State of Harsh Environment Landscape

The landscape of harsh environment materials for energy-relevant applications is vast. One of the difficulties with establishing the various criteria for this topical area is defining a standard for "harsh." Operational requirements for a given technology are critically dependent on not only the environment, but also on the underlying material system and final application. Thus, the relative nature of what is considered harsh in one environment may not meet operational requirements in another.

This report proposes the following as a comprehensive description of what constitutes a harsh environment: *an environment consisting of one or more stressors exceeding the current thresholds that can be experienced by a system component in any given application such that its functionality, material attributes, and durability are unduly degraded*. Such stressors include extreme temperatures, thermal cycling, extreme pressures, corrosive chemicals, extreme pH, dust and particulates, mechanical wear, abrasion, erosion, cavitation, neutron irradiation, and hydrogen attack. Individually, these conditions present substantial challenges. However, materials are rarely subjected to a single stressor, as shown by Figure 1 in the executive summary.

This section of the landscape introduces and explores critical challenges in HEM Technologies alongside the necessary advancements in specific industries, sectors, and materials in order to achieve the HEM strategic goals. Key Takeaway boxes in each section indicate the most critical needs.

2.1 Critical Challenges in HEM Technologies

Practitioners in materials science and engineering are well acquainted with the materials science tetrahedron (or, more simply, the materials tetrahedron), a paradigm that graphically illustrates the dependencies between materials structure, processing, properties, and performance. Recently, the materials science tetrahedron has gained a digital twin, integrating materials science with information science. In a prototype implementation of this framework, materials systems provide data to information systems, which then generate insights to guide further improvements in materials design.⁸ The digital analogue of the materials tetrahedron provides a pedagogical framework for cross-disciplinary communication pertaining to information infrastructure built around materials data. It will provide various different stakeholders (from suppliers to end users) with a platform to jointly contextualize, translate, and guide design, development, and deployment efforts in the pursuit of advanced materials and manufacturing technologies (AMMTs). In turn, that will allow us to direct researcher attention and computational resources around extraction of the high-value information that leads to the ultimate translation of tangible solutions for AMMTs. Facilitated by the capabilities of digital tools like this, the enhanced understanding of both traditional and advanced manufacturing technologies and how they influence material properties is expected to drive innovation at an accelerated pace. These innovations encompass situ/operando sensors for data-capturing, real-time analysis/control techniques during manufacturing, as well as the final characterization of application performance.

When applied to competitively producing near net shape (NNS) components (i.e., those very close to their final shape with reduced need for post processing) at an industrially relevant scale, advanced manufacturing technologies, e.g., 3D printing, PM-HIP, and EFAS, require a comprehensive understanding of how processing parameters influence microstructures and properties, which will lead to significant advances in component geometrical design (NNS) flexibilities, as well as potential opportunities for greater microstructural design and control, including the engineering of grain morphology, grain size distribution, grain orientation distribution (texture), and grain boundary (GB) orientation (high and low GB angles/energies) to achieve optimized products.

⁸ Deagen ME, Brinson LC, Vaia RA, Schadler LS. The materials tetrahedron has a "digital twin." MRS Bulletin [Internet]. 2022 Feb 1 [cited: 2024 Jul 31]; 47(4):379-388. Available from: <u>https://doi.org/10.1557/s43577-021-00214-0</u>

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Key Takeaway

While AMTs are capable of producing complex geometry parts with reduced waste unobtainable by traditional means, to increase the competitiveness of AMTs for HEM components relevant to energy applications, R&D must focus on improving process throughput (e.g., parts produced per unit time), reducing feedstock and tooling costs, enhancing the use of secondary feedstock, minimizing process-induced defects, scaling up for production of larger-sized components, attaining a minimum of cost parity with traditional processes, and establishing performance testing standards.

High throughput strategies for materials synthesis and testing can be integrated with physics-driven computational tools, ranging from semi-empirical approaches (e.g., CALPHAD and FEM) to multi-scale modeling and simulation (mod-sim) frameworks like integrated computational materials engineering (ICME). ICME can be coupled with machine learning (supervised or unsupervised) to connect various material and process facets, leading to more accurate predictions of microstructure, properties, and behavior under harsh environments. Using process information in a manufacturing control system could enable precise, autonomous real-time control of both the process and the materials produced. For instance, it has been particularly challenging to 3D print robust components for harsh environments with high repeatability and reproducibility. However, recent advances have demonstrated success, such as a 3D-printed 2-ton part for a hydro lock component that exceeded the base material's strength by almost 30%.⁹

Utilizing realistic, time-resolved in-situ or operando monitoring of material or component aspects (such as geometric dimensions, microstructural evolution, chemical composition, and crystal structure) during manufacturing or service can provide valuable real-time data for process monitoring and quality control, as well as service life indicators. The shift from automation to autonomy could further expand manufacturing capabilities, allowing AI systems to make real-time decisions and adapt fabrication processes in a self-learning fashion. Despite formidable barriers such as small-scale phenomena during solidification, crystallization, microstructural evolution, and defect formation, materials and process development acceleration tools like high throughput processing, physics-informed multi-scale mod-sim, in-situ measurement devices, digital twins, AI/ML-driven data mining, automation, and other smart manufacturing techniques are key focus areas of the landscape.

2.2 Advanced Materials for Electric Energy Production

In this landscape, we are concerned with the harsh environment materials and manufacturing needs for electricity production, utilization, and storage. In 2023, the electric power sector consumed 32 quadrillion btu (quads) of the 93.6 quads (or 34%) of the total primary energy produced in the U.S. Of these 32 quads, electricity net generation accounted for 13.7 quads (electricity sales totaled 13.2 quads) while conversion losses, plant use, and useful thermal output was 18.3 quads. Electrical system energy losses accounted for 18.91 quads. Primary energy sources include fossil fuels (e.g., coal, petroleum, and natural gas), solar radiation, nuclear fuels, wind, falling/flowing water, and other raw, unprocessed inputs into the energy system. These primary energy sources can be converted to other energy forms, such as more refined fuels (e.g., gasoline and hydrogen), or directly to electricity or to heat, which are more useful. All energy that has been subjected to human-made transformation, or converted to other forms (like electricity), are termed energy carriers, or secondary energy.

This section outlines only material advances needed for electric energy production/conversion systems. Advanced material technologies for energy transmission and distribution (grid) applications are under the purview of the Office of Electricity but are briefly discussed here. Transmission and distribution cause a small loss of electricity, around 5% on average in the U.S., according to the EIA. Although occasional adverse weather conditions do not constitute continuous harsh/extreme service environments, grid components (generators, transformers, conductors,

⁹ Fox C. Infrastructure Innovation: New Poe lock arrestor arm is the largest U.S. civil works component produced by 3D printer [Internet]. Sault Ste. Marie (USA): DVIDS; 2024 Apr 1 [updated 2024 Apr 1, cited 2024 Jul 23]. Available from: <u>https://www.dvidshub.net/news/467497/infrastructure-innovation-new-poe-lock-arrestor-armlargest-us-civil-works-component-produced-3d-printer</u>

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insulators, poles, guy wires, clamps, bushings, switches, terminals, meters, etc.) can be affected not only by sporadic harsh/adverse atmospheric and other weather-related phenomena, but also high voltage and electric field stresses, and/or corrosion. The National Association of Corrosion Engineers (NACE) in its 2002 comprehensive report (the most recent available data) on corrosion estimated the annual corrosion of steel transmission towers and poles due to soil content and electrolytes at \$0.6 billion.¹⁰ Hot-dip galvanizing is the most common mitigation strategy, but it is a costly up-front initial expense and does not entirely eliminate corrosion, though it does lower the whole-life cost. The zinc serves the dual function of providing a zinc patina barrier layer to protect the underlying steel, and it also acts as a sacrificial anode in the event the galvanized coating is physically damaged. If individual areas of underlying steel become exposed, the surrounding zinc will provide sacrificial cathodic protection by corroding preferentially. However, even though it does an excellent job of protecting steel when the structure is located in moderately corrosive environments, even galvanized steel will eventually corrode over time in certain atmospheric or in-ground conditions. Marine environments with salt-laden air, as well as industrial environments (e.g., acid rain), are particularly harsh. In soil, corrosion activity can be accelerated by the soil's chemistry (i.e., the presence of moisture, corrosive ions, anerobic bacteria), and stray currents.

It is also worth noting that as far back as the Quadrennial Technology Review of 2015,¹¹ it was recognized that enabling modernization of the electric power system (specifically the transmission and distribution components) will require next-generation technologies based on innovations in material science, such as nano-composites, wide bandgap (WBG) semiconductors, advanced magnetics, new insulators and dielectrics, and high temperature superconductors—which can unleash new capabilities for the grid and improve the performance and lifetimes of current designs. New component technology requirements will need to balance improved functionalities that support greater consumer self-generation, improve resilience, and increase flexibility while managing total costs.

Approximately 96% of electricity production in the U.S. relies on turbomachinery (steam, gas-fired, wind, hydro) for generating electricity through electromagnetic induction. Most of these facilities (~80%) are thermoelectric (a.k.a. thermal power plants and stations) that convert heat from the combustion of fuel (fossil-based or waste/biomass), nuclear reactions, geothermal fluids, or concentrated solar energy into mechanical energy and, ultimately, into electricity. Traditional thermal power plants lose most of the energy going into them; the majority of the energy that goes into a thermal power plant is vented off as waste heat. Other sources of electricity come from non-thermal electric power generation methods, which do not use heat engines. Those include wind turbines, hydroelectric facilities, marine energy (driven by waves, currents, tides, or temperature differences), and solar photovoltaic panels. Non-thermal processes can still be assessed thermodynamically from both resource and technology perspectives through careful consideration of what constitutes the thermodynamic system and its surroundings (e.g., from a resource perspective, wind energy can be modeled as a solar-driven heat engine; likewise, there are thermodynamic models and limitations of solar cells relating their device efficiency to Carnot efficiency in terms of global entropy generation). Each type of electric power generation presents unique challenges related to the specific stressors impacting the material requirements discussed in the following sections.

2.2.1 Thermal Power Generation Systems

When discussing thermal [electric] power plants, it is helpful to analyze them within the context of their thermodynamic subsystems, the heat reservoirs and the heat engines. Each type of thermal power station possesses distinct harsh environment conditions dictated by these subsystems (e.g., irradiation, corrosivity), which in turn determine component materials requirements. This section begins with a focus on the material needs of the

¹⁰ Koch GH, Brongers MPH, Thompson NG, Virmani YP, Payer JH. Corrosion costs and preventative strategies in the United States [Internet]. NACE International; 2002 [cited: 2024 Sept 30]FHWA-RD-01-156. Available from: <u>http://impact.nace.org/documents/ccsupp.pdf</u>

¹¹ Department of Energy. Quadrennial technology review: an assessment of energy technologies and research opportunities [Internet]. Department of Energy; 2015 Sep [updated 2015 Sep; cited 2024 Jul 23]. Available from: <u>https://www.energy.gov/quadrennial-technology-review-2015</u>

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heat engine energy conversion device and follows this with a discussion of the material aspects of the high-temperature heat reservoir, specific to the different technologies.

2.2.1.1 High-performance Materials for Advanced Steam and Gas-fired Turbomachinery

Many thermal power stations function as steam plants, employing steam as a working fluid akin to large steam engines. This process starts with the heat generated from the combustion of a fuel (e.g., coal), a nuclear reaction, geothermal heat, or solar energy being directed to a steam generator (boiler) to produce high pressure steam. A turbine uses the kinetic energy of a moving fluid (i.e., steam or gas) to generate rotational motion, which is then converted to electricity with an electromagnetic generator—either a dynamo for direct current electricity or an alternator for alternating current electricity. While some consider the steam generator/boiler integral to the steam engine, this document treats the steam generator separately from the steam engine (steam turbine), which together constitute a complete steam plant. Steam and gas-fired turbines coupled to two-pole generators for 60 Hz electric power generation rotate at speeds of 3,600 revolutions per minute (rpm), while those driving four pole generators rotate at 1,800 rpm, both of which are much faster than wind and water turbines requiring gear boxes to drive generators at sufficient speeds. Steam turbines used to drive mechanical equipment operate at variable rotational speeds, typically between 3,000 to 8,000 rpm.

Various models describe the work accomplished by the working fluid within the turbine. The Rankine cycle is best suited for steam turbines, reflecting their thermodynamics. For gas-fired turbines (e.g., natural gas), the Brayton cycle aligns closely with the thermodynamics of hot combustion gas and supercritical CO₂ (sCO₂) work. Simple cycle gas-fired turbines often exhibit lower thermal efficiency (typically, up to 40%) than steam turbines but offer higher overall efficiencies in combined cycle configurations (45–60%, with goals of achieving > 65%), along with greater fuel flexibility.¹² Additionally, carbon dioxide emissions from natural gas combustion are approximately half that of coal combustion.¹³ There are combined cycle power plants using both gas and steam turbines, which are known as combined cycle gas turbines (CCGT) or combined gas-steam cycles. They further enhance efficiency by integrating gas turbines with heat recovery steam generators to drive steam turbines. A primary benefit is that power is generated from both the gas turbine and the steam turbine when burning gaseous fuel since the hot exhaust gases from the gas turbines collectively contribute almost 80% of U.S. electric power generation today, with CCGT accounting for about 34%. Cogeneration or combined heat and power (CHP) plants also play a significant role, producing heat for industrial purposes alongside generating electric power. Typical total system energy efficiencies of CHP systems range between 60 and 80%.¹⁴

2.2.1.1.1 Steam Turbine Materials

Despite the differences in power generation methods, all thermal power schemes currently require materials and components for either steam or gas turbines, or both. Steam turbine can be very large. For example, the casing (usually made from two halves of low-alloy steel castings) may be up to 6 meters in length, 3 to 4 meters in diameter, and weigh 100 tons. A number of metallic alloys are needed (e.g., from high-grade alloy steels to nickel superalloys) that are capable of withstanding high rotational speeds (e.g., 3,600 rpm) and temperature gradients, as well as various steam conditions, from saturated (wet) steam (e.g., steam temperatures less than 120°C), superheated (dry) steam (steam temperature that is above the saturation temperature with reduced moisture to minimize turbine blade erosion), supercritical steam (temperatures higher than 374°C—most typically, 566° to 593°C —and pressures higher than 22 MPa), to advanced ultra-supercritical steam (steam temperatures higher than 700°C and

¹³ American Geosciences Institute. How much carbon dioxide is produced when different fuels are burned? [Internet]. AGI. 2014 [cited 2024 Sep 12]. Available from: <u>https://www.americangeosciences.org/critical-issues/faq/how-much-carbon-dioxide-produced-when-different-fuels-are-burned</u>

¹⁴ Environmental Protection Agency. Methods for calculating CHP efficiency. [Internet] EPA [updated: 2024 May 30; cited: 2024 Sep 12]. Available from: <u>https://www.epa.gov/chp/methods-calculating-chp-</u>efficiencyhttps://www.epa.gov/chp/methods-calculating-chp-

¹² Soares CM. Gas turbines in simple cycle & combined cycle applications [Internet]. NETL [cited: 2024 Sep 12]. Available from: <u>https://netl.doe.gov/sites/default/files/gas-turbine-handbook/1-1.pdf</u>
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pressures higher than 30 MPa). It should be noted that compared to coal-fired or flame power plants, pressurized water reactor (PWR) nuclear power plant steam turbines run at lower speeds (1,800 rpm) and lower steam temperatures (rarely exceeding 275°C at 6 MPa for safety reasons).¹⁵ Most PWRs use multi-stage condensing steam turbines and require higher mass flow rates and much larger turbine blades to avoid water erosion.

There are a number of rotating parts (e.g., rotors, discs, blades, pins, shrouds), stationary parts (e.g., blades, nozzles, vanes), and other parts (e.g., seals, pedestals, casings, hoods) to a steam turbine. Numerous metals are used in their construction. These include alloy steels, carbon steel, stainless steels, cobalt alloys, nickel superalloys, and titanium alloys. The rotating parts are subjected to high centrifugal forces, cyclical loading, and temperature gradients, which leads to fatigue failures over time. Other major steam turbine problems include stress corrosion cracking of rotors and discs, corrosion fatigue of blades, pitting, and flow accelerated corrosion. There are several corrosion mechanisms active in steam turbines, which can be mitigated (but not eliminated) through design considerations and corrosion management practices. These mechanisms include fretting, intergranular attack, erosion, crevice, galvanic, exfoliation, and leaching. Important factors contributing to the corrosiveness of the environment are the steam impurity levels, pH control, flow, and velocity control.¹⁶ EPRI has estimated that corrosion in steam turbines costs the U.S. economy over \$1 billion annually.¹⁷

Carnot's theorem indicates that the efficiency (η) of a steam or gas turbine increases with rising inlet temperature and inlet pressure. However, there are physical limits due to the thermal and structural constraints of blades and their materials. While it is feasible to enhance the efficiency of a steam turbine by increasing the short blade heights in high pressure and intermediate-pressure stages—typically employing stainless steel or nickel superalloys—the predominant losses in typical steam turbines are attributed to the low-pressure blade loss and low-pressure exhaust loss, respectively. The last-stage blades, which are crucial components, have been lengthened significantly (up to 60 inches) with the escalating output of steam power stations. The centrifugal and aerodynamic forces acting on these blades are substantial, while their rigidity is comparatively low, leading to blade vibration. Consequently, less dense (and more corrosion-resistant) titanium alloys are occasionally utilized in this stage to elevate allowable stress design levels. Additional considerations, such as intricate internal cooling passages within the blades to enhance turbine efficiency, present opportunities for improved performance but also introduce further challenges in advanced steam turbine blade manufacturing.

The efficiencies of small steam turbines for industrial applications are typically 20 to 40%, while medium steam turbines for power plants achieve between and 45%, and large steam turbines for large-scale power generation are approaching 50%.¹⁸ Utilizing materials that can withstand higher steam temperatures and pressures enable higher efficiency mediums such as (in order of increasing efficiency): superheated (subcritical) steam, supercritical steam, and advanced ultra-supercritical steam (A-USC) conditions. While the cost of an A-USC plant is approximately 20% higher than a non-USC plant because of the need for high-Ni-based alloys (e.g., Inconel 740H, Haynes 282), A-USC plants can yield more than 10% efficiency gains and emissions reductions of up to 30% compared to the current coal-fired boiler fleet.¹⁹ There has been a techno-economic analysis published for a supercritical combined gas-steam cycle, as well, indicating that the increased capital expenditure investment needed to achieve supercritical steam parameters (temperatures up to 800°C) will be balanced out by increased profits from the higher

turbomach symposium [Internet]. 2008 [cited: 2024 Sept 30]. Available from:

https://oaktrust.library.tamu.edu/server/api/core/bitstreams/98edb563-853d-4afb-b20b-a1fd26926067/content ¹⁷ EPRI. Shutdown protection of steam turbines using dehumidified air [Internet]. EPRI, 2008 Mar 26 [cited: 2024 Sept 30]1014195. Available from: https://www.epri.com/research/products/1014195

 ¹⁵ Gicquel R. Pressurized water nuclear power plants (PWR) [Internet]. Mines Paris Tech; 2024 Mar [cited: 2024 Sep 12]. Available from: <u>https://direns.mines-paristech.fr/Sites/Thopt/en/co/centrales-nucleaires-eau.html</u>
 ¹⁶ Jonas O, Machemer L. Steam turbine corrosion and deposits problems and solutions. Proc. Of thirty-seventh

¹⁸ Erguavan A. Efficiency of a steam turbine [Internet]. EMS Power Machines; 2023 Mar 5 [cited: 2024 Sep 12]. Available from: <u>https://ems-powermachines.com/efficiency-of-a-steam-turbine/</u>

¹⁹ Purget R, Hack H, Purdy D, Tanzosh J, Weitzel P, DeBarbadillo J, et al. Materials for advanced ultrasupercritical (A-USC) steam turbines--- A-USC component demonstration [Internet]. Department of Energy; 2022 Jul 7. [updated 2022 Jul 7, cited 2024 Jul 23]. Available from: <u>https://www.osti.gov/biblio/1875111</u>

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efficiencies obtained.²⁰ Note, however, that geothermal power and PWR nuclear plants cannot use supercritical or A-USC steam turbines due to their lower steam temperatures.

The Department has also made significant investments in research, development, and demonstration (RD&D) of Brayton cycle sCO₂ power systems over the past decade, wherein the conventional working fluid in a steam engine is replaced with sCO₂, which does not condense as steam does. Nevertheless, the partial pressure of oxygen in sCO₂ is similar to that of steam and carburization of Fe-based structural alloys is also a major concern.²¹ It has been discovered that Ni-based superalloys and, to a lesser extent, advanced austenitic stainless steels seem to perform well at temperatures between 600° and 800°C in sCO₂. One notable outcome of this investment in sCO₂ power generation is the establishment of the 10 MWe Supercritical Transformational Electric Power (STEP) pilot plant at the Southwest Research Institute (SwRI) in San Antonio, Texas, in collaboration with project partner the Gas Technology Institute. This pilot power plant project has several objectives, but a key goal is the demonstration of at least a 700°C turbine inlet temperature.²² Operating at a turbine inlet temperature of 760°C, sCO₂ systems boast efficiencies 8 to 10% higher than those utilizing steam as the working fluid while occupying a significantly smaller footprint, typically 10x-20x smaller. The STEP project received support from the National Energy Technology Laboratory (NETL) and builds upon the groundwork laid by the APOLLO program (Advanced Projects Offering Low Levelized Cost of Energy Opportunities), which was initiated by the Solar Energy Technologies Office (SETO), aimed at enhancing the performance and reducing the cost of electricity generated from CSP plants. Note that, unlike with A-USC, sCO₂ power systems could also be utilized with PWR nuclear power plants since the supercritical sCO₂ temperature and pressure threshold conditions (31°C, 7.4MPa) are easily achieved. In fact, sCO₂ offers benefits in a range of other power generation technologies, as well, including fossil, biomass, and waste heat.

Critical components in sCO₂ power systems requiring careful material selection include the gas supply system, high pressure CO₂ pumping system, preheater, autoclave, precooler, turbomachinery (housings, disks, blades), as well as nonmetallic seals, elastomers, and thermoplastics. However, the increased cost associated with sCO₂ power systems—primarily due to the necessity for high-performance Ni-based superalloys at T > 700°C—to some extent offsets the techno-economic advantages and the assessment still suffers from a lack of long-term studies on corrosion and mechanical degradation under more realistic conditions of temperature, flow, stress, and impurity levels.

2.2.1.1.2 Gas-fired Turbine Materials

In contrast to steam turbines, current generation natural gas-fired turbines require hot corrosion resistant metallic alloys that can withstand oxidative gases at turbine inlet temperatures between 1,400 to 1,600°C. Nickel-based superalloys are frequently used because of their high-temperature strength. Pure titanium and titanium-based solid-solution alloys are not used because of the drop in titanium's creep resistance and surface oxidation at temperatures greater than ~500°C, as well as the possibility of ignition at oxidative flame temperatures greater than ~1,600°C. However, a titanium aluminide (TiAI) intermetallic phase, was introduced in the late 1990s for use in aero-jet gas turbines due to its favorable strength to density ratio compared with nickel alloys and it has been used in blades in the last two stages of multi-stage low-pressure turbines. However, as with most intermetallic compounds, TiAI is brittle and difficult to work with. Hence, more cost-effective and material-efficient processes are needed for titanium

²⁰ Jamroz M, Piwowarski M, Ziemiański P, Pawlak G. Technical and economic analysis of the supercritical gassteam cycle. Energies. [Internet] 2021 May 21 [cited: 2024 Sep 12];14(11):2985. Available from: <u>https://doi.org/10.3390/en14112985</u>

²¹ Pint BA. High temperature compatibility of structural alloys with supercritical and subcritical CO₂ [Internet] ElectroChem Soc Interface; 2021 Mar [cited: 2024 Sep 12];30(67). Available from: <u>https://doi.org/10.1149/2.F07212IF</u>

²² Marion J. 10 Mwe supercritical carbon dioxide (sCO₂) pilot power plant [Internet] GTI; 2018 Dec [cited: 2024 Sep 12]. Available from: <u>https://www.gti.energy/wp-content/uploads/2019/01/STEP-Project-Detailed-Description-Dec2018.pdf</u>

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aluminide to establish long term use in aerospace applications.²³ More recently, TiAl has found interest in landbased industrial gas turbines.

Other materials are being developed for gas turbines. The Department's ARPA-E office funds the Ultrahigh Temperature Impervious Materials Advancing Turbine Efficiency (ULTIMATE) program targeting advanced alloys, intermetallic phases, and other materials and coatings capable of withstanding gas turbine inlet temperatures up to 1,800°C and blade operating temperatures of 1,300°C.²⁴ Such an initiative poses a challenge for traditional Nibased superalloys as they soften and melt between 1,200 and 1,500°C. Cobalt-based superalloys potentially possess superior hot-corrosion/oxidation and wear resistance compared to Ni-based superalloys, but the cobalt superalloys typically have a lower strength at high temperatures than Ni-based superalloys. Some oxidation-resistant, precipitation strengthened Co-Re based alloys have shown promising behavior at temperatures up to 100°C higher than the limit for single crystal nickel superalloys, such as maraging steel (17-18% nickel, with <0.03% carbon), can have excellent strength but only at moderately high-temperatures (up to 400°C) and less corrosion/oxidation resistance, unless they are of the stainless variety.

Nickel superalloys are more expensive than many other alloys because the same properties that make them attractive for harsh environments (e.g., high strength, corrosion resistance, and hardness at high temperatures) make it difficult to fabricate components from them using traditional formative methods (anecdotally, requiring twice the machine power compared to low alloy steel). Despite the presence of a ductile face-centered-cubic solid solution matrix (γ phase), Ni-based superalloy castings with large volumes of the precipitation-strengthening aluminum and titanium intermetallic γ ' phase Ni₃(Al,Ti) for high-temperature strength have a tendency to crack during processing. Heat treated parts tend to chip and break under shear forces. Further challenges include severe wear and shortened lifespans of ceramic cutting/machining tools, as the cutting temperature for high-speed machining (600 m min⁻¹) of Ni-based superalloys can exceed 1,200°C.²⁵

Advanced superalloy fabrication methods like additive manufacturing (e.g., laser powder bed fusion, LPBF, with subsequent thermomechanical treatment involving cold rolling and annealing) as well as processes using entirely solid-state transformations, such as severe plastic deformation (SPD) techniques (e.g., friction stir deposition/welding or FSP/W, equal channel angular extrusion or ECAE, accumulative roll bonding or ARB, and shear assisted processing and extrusion or ShAPE) or discontinuous precipitation to create a highly entangled grain boundary network, could possibly lead to easier fabrication of components with complex geometries and fewer defects, as well as less rework, machining, and scrap. For certain alloys, SPD can produce grain refinement resulting in both improved strength and ductility. Some of these methods have already been explored specifically for fossil energy power plant applications.²⁶

Other factors that drive up the price of nickel superalloys are due to simple supply/demand factors (about 12% of the nickel consumed is in superalloys, while 65% is in austenitic stainless steel²⁷), and the critical nature/supply risk

²³ Bünck M, Salber R, Stoyanov T. Resource-efficient manufacturing technology for titanium aluminide aerospace components. Transactions of the Indian Nat Acad of Eng [Internet]. 2023 Nov 18 [cited 2024 Sep 30];9(1):141–54. Available from: https://doi.org/10.1007/s41403-023-00436-5

 ²⁴ Jackson H. ULTIMATE: T2M update for phase 2 kickoff & annual program review [Internet]. ARPA-E; 2024 Mar 28 [cited: 2024 Sep 12]. Available from: <u>https://arpa-e.energy.gov/sites/default/files/2024-04/Heather_ARPAE.pdf</u>
 ²⁵ Kitagawa T, Kubo A, Maekawa K. Temperature and wear of cutting tools in high-speed machining of Inconel 718 and Ti 6AI 6V 2Sn. Wear [Internet]. 1997 Jan [cited 2024 Sep 12];202(2):142–8. Available from: <u>https://doi.org/10.1016/S0043-1648(96)07255-9</u>

²⁶ Smith C, Grant G. Integrated process improvement using laser processing and friction stir processing for nickel alloys used in fossil energy power plant applications [Internet]. Department of Energy; 2023 Apr 19. [cited 2024 Jul 23]. Available from: <u>https://netl.doe.gov/sites/default/files/netl-file/23FECM_19_Smith.pdf</u>

²⁷ Stewart AA. Nickel statistics and information [Internet]. United States Geological Survey [cited: 2024 Sept 30]. Available from: <u>https://www.usgs.gov/centers/national-minerals-information-center/nickel-statistics-and-information</u>

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of nickel (a critical material/mineral²⁸) and some superalloy constituents. The benefits of recycling superalloys are undeniable, although recycling them is difficult because of their complex assortments of chemical and physical properties (to be discussed in the FA4 section on C7). Alternative approaches to lowering their overall lifetime costs involve coating the superalloys to extend their useful life (even the most advanced alloys are susceptible to corrosion in some aggressive environments), but this faces challenges of its own, namely, interdiffusion between the coating and underlying superalloy. Interdiffusion results in formation of an interdiffusion zone (IDZ) and an underlying secondary reaction zone (SRZ) containing large amounts of refractory and brittle phases, which tends to induce cracking under stress and ultimately reduces the mechanical properties of the alloys.

Key Takeaway

Imperative to achieving energy goals, is developing the capability for fabricating superalloy components of larger size and/or having more complex geometries and fewer defects, as well as lower rework, machining, scrap, and cost.

Powder metallurgical routes for Ni-based superalloys are considered capable of producing load bearing and structural parts (rotating and static parts) with excellent characteristics and for this reason PM is widely used for gas turbine disks in the aerospace sector (e.g., René 88DT, which has no macro-segregation, high yield strength, good fatigue tolerance, and excellent microstructural stability up to 700°C for extended periods). PM-based nickel superalloys are typically fabricated at temperatures of 1100°C and pressures of 100 MPa for 4 h. Unfortunately, the effects of manufacturing conditions on the microstructural evolution are not well understood for wrought or PM nickel superalloys. For typical conditions used in industry, work hardening will be more dominant than dynamic recovery (during deformation) and this results in an increase in dislocation density. At critical dislocation densities, the nucleation of new grains is observed through recrystallisation. The recrystallized grain size in a component can be controlled to tailor the material properties for a specific application. Larger grains have greater creep strength and improved resistance to fatigue crack growth but reduced tensile strength. Focus should thus be directed to analyze whether dynamic recovery can outcompete recrystallisation mechanisms within typical industrial processing realms to provide the most relevant insight for the superalloy manufacturing industry.²⁹

It is critical to minimize defects in PM produced parts, such as prior particle boundary precipitation, porosity, and nonmetallic inclusions. Simple powder pressing to form green powder compacts followed by sintering is not sufficient to obtain full density consolidation. Thus, most PM routes to fully dense consolidated components typically consists of master alloy melting, gas atomization to produce pre-alloyed powder, which is then compacted, shaped, or formed in some fashion through processes like hot extrusion, hot isothermal forging, hot pressing, hot isostatic pressing, sinter-HIP, or spark plasma sintering (SPS), as well as secondary post-processing like sizing, coining, machining, surface treatments, and heat treatments. However, PM superalloy performance is highly influenced not only by the processing but also by the feedstock powder. Innovative technologies for producing nickel-based superalloy powders could help ensure powder particles with higher sphericity, smoother surfaces, more uniform particle size, and fewer inclusions in order that next generation Ni-based superalloys can meet the performance requirements for turbine disks at higher temperatures and pressures.³⁰ Other challenges associated with PM-HIP, specifically, are discussed in the nuclear energy section, as components used in that industry have some of the highest performance standards making cost premiums more easily tolerated. Although PM processing costs can be cheaper than wrought processes (depending on material), ^{Capex}/acquisition investments can be much higher.

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https://doi.org/10.1080/02670836.2022.2069332
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 ²⁸ Department of Energy. What are critical materials and critical minerals? [Internet]. Department of Energy [cited: 2024 Sept 30]. Available from: <u>https://www.energy.gov/cmm/what-are-critical-materials-and-critical-minerals</u>
 ²⁹ Galpin SJ. A review of microstructure phenomena during manufacture of polycrystalline Ni-based superalloys. Mat Sci and Tech [Internet]. 2022 Nov 16 [cited 2024 Oct 10];38(16). Available from:

³⁰ Yang L, Ren X, Ge C, Yan Q. Status and development of powder metallurgy nickel-based disk superalloys. Int Journal of Mat Res [Internet]. 2019 Oct 16 [cited 2024 Sep 12];110(10):901–10. Available from: <u>https://doi.org/10.3139/146.111820</u>

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For natural gas-fired turbines, smaller components like blades are also crafted from nickel-based superalloys, which are best suited to withstand the high-temperature oxidative conditions encountered in this application The initial stage gas turbine blades are often single-crystalline to augment fracture, fatigue, creep, and corrosion resistance in this demanding section. Presently, these single-crystal blades are manufactured through grain selection during directional solidification, a time- and energy-intensive process. Recent advancements in directed energy deposition additive manufacturing methods, such as electron beam powder bed fusion (EB-PBF) and selective laser melting (SLM), hold promise to produce single-crystalline nickel superalloy parts more affordably, albeit some technical hurdles persist. Powder metallurgy and additively manufactured Ni-Co based superalloys have also been developed for the rim/hub section (near the gas flow path) of high-pressure gas turbine disks. However, as mentioned above, for PM (and AM) routes to advanced superalloy parts it is generally necessary to achieve more cost-efficient powder feedstock production, which requires the preparation of compositionally homogeneous spherical powders with narrow particle size distributions in high yield and at industrial scale. Large gas atomizers are commonly used for this type of purpose. However, optimization of the various gas atomization process parameters (e.g., inert gas-tometal ratio, gas pressure, gas velocity, and temperature) is time consuming and costly and could benefit from machine learning facilitated data mining to reduce the cost as well as hasten practical, large-scale manufacturing of superalloy powders.³¹

SiC fiber-reinforced SiC ceramic matrix composites (SiC(f)/SiC(m) CMCs) are also under development for utilization as blades in land-based natural gas-fired turbines and have already been commercialized for the combustion zone and turbine in aerospace jet engines. SiC CMCs exhibit the capability to withstand turbine inlet temperatures 200 to 300°C higher than Inconel nickel superalloys (i.e., up to 1,400°C), potentially resulting in at least a 2% energy efficiency gain. However, substantial reductions in manufacturing and materials costs of SiC(f)/SiC(m) CMCs are imperative to ensure cost competitiveness in land-based gas turbine blade applications. All the SiC fiber used in these high-temperature applications is currently produced in Japan and costs roughly \$10,000 per kilogram. For non-rotating gas turbine components not requiring the same level of high strength performance, particle reinforced (as opposed to fiber reinforced) SiC/SiC CMCs produced by low-cost additive manufacturing routes are currently being explored. There are also oxide-oxide CMCs (e.g., alumina) gaining momentum as an option for components in the post combustion and post turbine exhaust zone of aerospace and energy gas turbine engines (oxide-based CMCs are not typically used above 1,200°C due to degradation in strength) but like with non-oxide CMCs the oxide CMCs also suffer from high fiber costs.³²

In addition to these high-temperature non-oxide and oxide CMCs, some ultra-high temperature non-oxide CMCs made from borides and nitrides are under increased interest along with certain monolithic ceramics (e.g., MAX phases) for yet more severe environments with temperatures between $1,500^{\circ}$ and $2,000^{\circ}$ C. These include aerospace heat shields, rocket nozzles, and even some CSP/CST applications (see FA3 C109). Finally, other types of gas-fired turbines under development that operate on ammonia (NH₃) and hydrogen (H₂) fuel present challenges due to 1) the reactive and corrosive nature of NH₃ and H₂, as well as water vapor combustion product, towards turbine components at elevated temperatures, and 2) existing supply chain constraints associated with the production of NH₃ and H₂ at the scale required for these applications.

Given the prevalence and resilience of steam and gas-fired turbines, coupled with their significance across various forms of electricity generation (e.g., fossil fuel, waste incineration, CCGT, CSP, nuclear, and geothermal), further advancements in steam and gas turbine technologies to enhance their thermal efficiencies by enabling their operation at higher temperatures carry national significance. These advancements can be accelerated by developing more cost-competitive and high-performing components for steam and gas turbines, crafted from materials that can operate at elevated temperatures and/or are compatible with alternative working fluids (e.g.,

³¹ Tamura R, Osada T, Minagawa K, Kohata T, Hirosawa M, Tsuda K, et al. Machine learning-driven optimization in powder manufacturing of Ni co based superalloy. Materials & Design [Internet]. 2020 Nov [cited 2024 Sep 12];198(15):109290. Available from: <u>https://doi.org/10.1016/j.matdes.2020.109290</u>

³² Karadimas G, Salonitis K. Ceramic matrix composites for aero engine applications—a review. Applied Sciences [Internet]. 2023 Feb 26 [cited 2024 Sep 12];13(5):3017. Available from: <u>https://doi.org/10.3390/app13053017</u>

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sCO₂, hydrogen, ammonia), which can be corrosive. Examples of these types of more corrosion-resistant materials include superalloys, oxide dispersion strengthened (ODS) alloys, and CMCs.

Key Takeaway

Funding the further development of more competitive advanced manufacturing techniques (including post-forming densification steps) for components made from advanced alloys, monolithic technical ceramics, and ceramic matrix composites (CMCs)—which demonstrate superior resistance to high-temperature oxidation, corrosion, wear, creep, and fatigue—as well as coatings to further bolster protection against these materials stressors, remain key focus areas for the Department.

In addition to high temperature oxidation (hot corrosion) of gas turbine engine components (in the turbine section and combustion section), high temperature sulfidation can also occur (nickel readily reacts with sulfur to form nickel sulfides), which causes rapid degradation. Ingested contaminants through the air inlet, water (wash, NO_x control injection, evaporative ucooler), and fuel systems can cause aqueous/acidic corrosion of components in these sections, as well as to components in the compressor section.³³ Other types of corrosion commonly encountered in the fossil fuel industry, on the whole, include, low temperature sulfidation (T < 260°C), hydrogen cracking, hydrogen attack, stress corrosion cracking, fatigue cracking, and crevice corrosion. Galvanic corrosion can also occur with buried storage tanks and underground piping systems when dissimilar materials are improperly joined. According to the 2002 NACE report, the annual cost of corrosion for oil and gas transmission pipelines has been estimated at \$7 billion, while gas utilities corrosion costs are \$5 billion and fossil fuel electricity generation corrosion costs are \$1.9 billion. For the U.S. electricity generating sector as a whole the total annual cost of corrosion is \$6.9 billion, compared to the largest category, drinking water and sewage systems, at \$36 billion. For all sectors across the entire U.S. economy, total corrosion costs are estimated to be \$276 billion, and a staggering \$2.5 trillion globally³⁴

Well established and long-practiced corrosion management, prevention, and mitigation strategies include the use of inspections, testing, and performance validation of corrosion-resistant alloys, plastics, polymers, corrosion inhibitors, cathodic protection with sacrificial anodes (for underground and submerged tanks, pipelines, and offshore structures), anodic protection (for very aggressive environments), and many types of anti-corrosion coatings (including galvanizing, anodizing, cladding, electro deposition/plating, vapor deposition, paints, etc.), which have continued to advance through the years. Further improvements in coating bond/adhesion strength, wear/erosion resistance to turbulent liquids and gases, chemical resistance to more aggressive environments, and higher temperature oxidation resistance would be beneficial.

2.2.1.1.3 Material Supply Chain Needs for Advanced Steam and Gas-fired Turbines

With increased renewable utilization, U.S. coal-fired generation capacity is projected to decline 50% by 2030 (about 200 GW) with a more gradual decline thereafter, to between 23 GW and 103 GW of coal-fired capacity operating in 2050. Incentives for wind and solar power generation are accelerating the near-term decline of coal-fired generating capacity and the retirement in the U.S. coal fleet.³⁵ Nevertheless, single-cycle coal-fired boiler fed steam turbines still accounted for almost 20% of annual U.S. electricity generation in 2022. Furthermore, because steam turbines

³³ Turbomachinery International. Gas turbine corrosion mechanisms [Internet]. Turbomachinery International, 2017 Jan 20 [cited 2024 Sept 30]. Available from: <u>https://www.turbomachinerymag.com/view/gas-turbine-corrosion-mechanisms</u>

³⁴ Koch GH, Brongers MPH, Thompson NG, Virmani YP, Payer JH. Corrosion costs and preventative strategies in the United States [Internet]. NACE International; 2002 [cited: 2024 Sept 30]FHWA-RD-01-156. Available from: <u>http://impact.nace.org/documents/ccsupp.pdf</u>

³⁵ U.S. Energy Information Administration. Electric power annual 2022 [Internet]. Energy Information Administration; 2023 Oct [cited 2024 Jul 23]. Available from: <u>https://www.eia.gov/electricity/annual/pdf/epa.pdf</u>

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are also used in NG-fired and biomass-fired boiler fed steam turbine systems, as well as CCGT, nuclear energy production, CSP plants, and geothermal systems, continued improvement in turbomachinery efficiencies will greatly benefit the power production sector. Many such turbine components can be quite large (10+ tonnes) and subjected to a variety of harsh service conditions, including high pressures, mechanical forces, or corrosive environments. These parts include steam turbine rotor forgings, casings, carrier nozzle turbine castings, superheater and reheater header and tube assemblies, large-diameter pipe extrusions, and forgings.

Supply chain assessments for traditional steam turbine components are sparse. However, anecdotal evidence suggests lead times are typically six to twelve months. The situation is similar for gas turbines. Castings and forgings have incredibly long lead times, in some cases, as long as 1–2 years for critical components. Energy supply chains can be complex, containing many global supply chain steps, while both steam and gas turbines can contain thousands of precision parts.

Key Takeaway

Although the energy sector is subject to the laws of supply and demand, due to its critical importance to the economy and national security, supply chains for materials and components in energy systems need to be more resilient to meet the dynamic demand for energy services; these energy supply chains need to foster transitions to emergent technologies (e.g., large-scale additive manufacturing, LSAM) while also serving and maintaining long-lived infrastructure.³⁶

A-USC installations capable of at least 800 megawatts electrical generation capacity with efficiencies 10% higher than their conventional steam turbine counterparts will require large components to be fabricated from nickel-based superalloys that would operate at a steam temperature up to 760°C and pressure of 7 MPa. These include pipe headers with 56 to 71 cm outer diameter and nozzle carrier/inner shells around 9,000 kg. Age-hardened nickel alloys are generally produced in the form of small ingots of 51 to 61 cm diameter with weight less than 4536 kg. The one major exception is the gas turbine rotor alloy 706 (UNS N07706), which is commercially produced in ingots as large as 91 cm in diameter and 11,340 kg.³⁷ Furthermore, the design and lifetime prediction methodologies, which ensure reliable operation of these nickel superalloy components under steady-state and variable loads, require validation and qualification. Finally, Brayton cycle sCO₂ power blocks are being considered for CSP as well as Gen-IV (e.g., molten salt reactors), and small modular reactor (SMR) systems.

Key Takeaway

Not only are nickel-based superalloys currently cost-prohibitive (due primarily to processing requirements) for some applications, but the fabrication of large-scale high-nickel superalloy components of the needed scale for some energy production applications (e.g., A-USC) is outside the proven capabilities of existing domestic supply chains utilizing traditional manufacturing methods.³⁸

2.2.1.2 Nuclear Energy

Now moving the discussion away from the heat engine (e.g., turbine), when examining a thermal power plant's high temperature heat reservoir (e.g., a combustion chamber, a nuclear reactor, a geothermal well, or a CSP plant solar receiver), the material demands vary based on the characteristics of the heat source. In the nuclear energy space,

³⁶ Graziano DJ, Alonso E, Fields F, Bauer D. Energy supply chains and change. Journal of Critical Infrastructure Policy [Internet]. 2020 [cited 2024 Jul 23];1(1). Available from: <u>https://www.jcip1.org/grazianoalonsofieldsbauer.html</u>

 ³⁷ Purget R, Hack H, Purdy D, Tanzosh J, Weitzel P, DeBarbadillo J, et al. Materials for advanced ultra-supercritical (A-USC) steam turbines--- A-USC component demonstration [Internet]. Department of Energy; 2022 Jul 7. [updated 2022 Jul 7, cited 2024 Jul 23]. Available from: <u>https://www.osti.gov/biblio/1875111</u>
 ³⁸ Purget R, Hack H, Purdy D, Tanzosh J, Weitzel P, DeBarbadillo J, et al. Materials for advanced ultra-

supercritical (A-USC) steam turbines---a-USC component Demonstration [Internet]. Department of Energy; 2022 Jul 7. [updated 2022 Jul 7, cited 2024 Jul 23]. Available from: <u>https://www.osti.gov/biblio/1875111</u>

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advanced structural materials, functional materials (e.g., moderator materials, reflector materials, shielding materials, and sensor materials), and construction materials (e.g., concrete) are needed for next-generation systems. These research gaps are being addressed by various Office of Nuclear Energy (NE) programs (e.g., AMMT, ART, and LWRS). Nuclear power plants currently contribute approximately 18% of U.S. electricity. The United States is part of a multinational declaration to triple nuclear energy capacity by 2050, which would mean increasing the country's nuclear energy from 100 GWe to 300 GWe. Much of this is expected to come from the implementation of SMRs, which are fission-based reactors (with a PWR type of design being the most common) capable of producing up to 300 MWe per module.

The nuclear industry deals with the most aggressive environments due to radiation exposure, causing aging and degradation of even advanced materials like Zircaloy.³⁹ Annual corrosion costs for the nuclear energy sector have been estimated by the NACE report of 2002 to be at \$4.2 billion.⁴⁰ Key degradation modes encompass thermomechanical aging and fatigue, irradiation-induced failures (e.g., segregation and phase transformation, swelling, creep, hardening, and embrittlement), radiation- and stress-modified/assisted corrosion and cracking, and water corrosion with PWRs at temperatures up to 360°C and without pressure up to 320°C.

The temperature within nuclear fuel rods can surge to 1,400°C at their core. Alloys commonly employed in LWRs include zirconium alloys, austenitic stainless steel, nickel alloys, and low alloy steels. For advanced Gen-IV fission reactors—such as liquid sodium-cooled fast reactors (SFRs) with operating temperatures > 500°C, molten salt reactors (MSRs), with operating temperatures > 700°C, and very high temperature reactors (VHTRs) with operating temperatures > 1,000°C—materials within the reactor vessel or containment structure must resist degradation from various agents, typically accelerated at high temperatures. Note that with VHTRs, electricity production based on high temperature steam (700-850°C) could theoretically take advantage of A-USC steam turbines, unlike with today's PWRs.

For SFRs, austenitic stainless steels (SS) 304 and 316 will likely be used for fuel cladding while ferritic steels and ferritic martensitic (FM) steels may be chosen for the reactor vessels, heat exchangers, and steam generator systems. Nickel alloys such as Hastelloy N, GH3535, and Ni-Cr-Mo (MONICR) with lower carbon and chromium contents will likely fare better in MSRs as they have a lower propensity to leach chromium from the alloy (especially at the grain boundaries when coupled with stress) through precipitation of chromium carbides by the molten salt media. Oxide dispersion strengthened (ODS) nickel alloys are also being explored to minimize helium swelling/bubbles in the grain boundaries observed with Hastelloy N. Additionally, SS316 and SS321 austenitic stainless steels are being considered for fluoride salt cooled high-temperature reactors. In fact, in December 2023, the Nuclear Regulatory Commission (NRC) approved the construction of a 35-megawatt demonstration scale molten fluoride cooled reactor that will produce only heat. The so-called Hermes reactor will be built at the Oak Ridge Heritage Center Industrial Park in Tennessee by Kairos Power and is expected to be operational in 2027.⁴¹ The reactor vessel shell, top head, bottom head, and internal systems (defining the flow path of the coolant) will be constructed from 316H SS. Because these alloys have a relatively high chromium content, they could be more prone to molten fluoride salt corrosion (i.e., due to the ready formation of chromium fluoride, CrF₃). Therefore, ASME code requirements have placed new emphasis on further investigation of 316 SS for molten salt facing applications.⁴² Lastly, VHTRs are appealing for Gen-IV reactors due to their simultaneous electricity and hydrogen

³⁹ Cole K. Prevention reduces corrosion costs in power industry [Internet]. Materials Performance, 2024 Oct 1 [cited: 2024 Sept 30]. Available from: <u>https://www.materialsperformance.com/articles/material-selection-design/2023/10/prevention-reduces-corrosion-costs-in-power-industry</u>

⁴⁰ Koch GH, Brongers MPH, Thompson NG, Virmani YP, Payer JH. Corrosion costs and preventative strategies in the United States [Internet]. NACE International; 2002 [cited: 2024 Sept 30]FHWA-RD-01-156. Available from: <u>http://impact.nace.org/documents/ccsupp.pdf</u>

⁴¹ Office of Nuclear Energy. Kairos power starts construction of Hermes reactor. [Internet] Department of Energy; 2024 Jul 30 [cited: 2024 Sep 12]. Available from: <u>https://www.energy.gov/ne/articles/kairos-power-starts-</u> <u>construction-hermes-reactor</u>

⁴² Doniger W, Falconer C, Couet A, Sridharan K. Corrosion of 316L & 316H stainless steel in molten LiF-NaF-KF (FLiNaK). J of Nucl Mat [Internet]. 2023 Jun 1 [cited 2024 Sep 12];579:154383–3. Available from: https://doi.org/10.1016/j.jnucmat.2023.154383

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cogeneration capabilities. Nickel-based superalloys will likely be used in these reactors for heat exchangers, core barrel, and control rod sleeves. There are also composite material and joining technologies relevant to the nuclear space, which will be discussed later in the materials integration into energy systems focus area.

In future nuclear fusion environments (at this time, nuclear fusion technology R&D is under the purview of the Office of Science), temperatures akin to those in VHTRs are expected, along with heightened steady-state heat fluxes and higher first wall primary knock-on atom (PKA) average energies (48 keV compared to 10 keV for LWRs) due to 14.1 MeV neutron energies from the deuterium-tritium fusion reaction. A global fusion materials development strategy has emerged that incorporates Fe-Cr based alloys, reduced activation ferritic-martensitic (RAFM) and ODS steels, nanostructured ferritic alloys, V-Cr-Ti alloys, SiC composites, and W alloys.

If the remaining technical challenges can be successfully addressed, AMTs could be made capable of producing thermal stress-free near-net shape (NNS) parts with high dimensional precision and shape fidelity, high purity, high density, and high strength. These AMTs include various 3D printing approaches, such as directed energy deposition (DED) and powder bed fusion techniques (e.g., selective laser melting/sintering (SLM/S); lithography-based ceramic manufacturing (LCM), (i.e., stereolithography (SLA) and digital light processing (DLP)); laser processing (e.g., laser-induced slip casting, LIS); and/or advanced post-forming densification techniques such as electric fieldassisted sintering (EFAS), melt infiltration, chemical vapor infiltration (CVI), polymer infiltration and pyrolysis (PIP), and advanced electron beam welding (EBW, see Section 2.5). PM-HIP is seen as a potential game changer to compete (fabricate) or supplement (densify) large castings and forgings for nuclear energy production, but it needs to be scaled for larger part production. There already exists PM-HIP machines in the world that can produce parts at least half the volumetric size of those needed for nuclear and other energy production methods, and HIPing costs have dropped by 65% over the last twenty years. However, there are challenges that must be addressed with: 1) industry acceptance, i.e., establishing materials codes, standards, nondestructive evaluation techniques, and performance specifications (e.g., creep and fatigue resistance), especially for critical applications/components; 2) shape limitations associated with canister/capsule design and preparation; as well as 3) micro- and macro-scale modeling and simulation of the powder densification mechanisms and the anisotropic shrinkage, or prediction of the canister distortion occurring in the HIP process. Generally, AMTs hold promise for reducing costs by delivering superior components faster and cheaper than more traditional metal formative manufacturing technologies like extrusion, casting, forging, welding, and ceramic forming techniques (e.g., extrusion, tape casting, freeze casting, slip casting, injection molding, dry pressing, and hot pressing), all of which usually must be followed by densification, machining, or other post-processing.

In anticipation of near-future nuclear components manufactured through AMTs entering the supply chain, the United States Nuclear Regulatory Commission issued a two-volume report in 2020 evaluating the capabilities of state-of-the-art modeling and simulation techniques for AMTs in predicting materials microstructures and properties.⁴³

Key Takeaway

There is a vital need for enhanced length- and time-scale bridging methods for physics-based approaches; microstructural modeling for predicting structural material properties tailored to AMTs; the anticipation of long-term properties like creep, thermal aging, irradiation damage, and creep-fatigue; the prediction of material degradation due to environmental effects like corrosion or radiation damage; the aggregation or creation of larger microstructural databases for data-driven methods; and the development of community-accepted validation benchmarks for the various AMTs of interest.

⁴³ Schneider A, Hiser M, Audrain M, Hull A. NRC workshop on advanced manufacturing technologies for nuclear applications part I -workshop summary [Internet]. Nuclear Regulatory Commission; 2021 Apr [cited 2024 Jul 29]. Available from: https://www.nrc.gov/docs/ML2111/ML21113A081.pdf

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2.2.1.3 Concentrating Solar Power

For emerging thermal power generation technologies like CSP and geothermal energy, distinct and challenging service conditions are intricately tied to each type of heat source, often overlapping with other technologies. CSP plants produce electric power by converting the sun's energy into high-temperature heat in a solar receiver using various mirror configurations. Materials currently used or under investigation as solar receivers include stainless steels, nickel-based superalloys, silicon carbide, and MAX phases with cermets, and transition metal oxides or nitrides as solar receiver absorber coatings. The sun's energy is concentrated in the receiver by various reflectors, and this concentrated energy functions as the heat source for a heat engine (e.g., steam turbine) that drives an electric generator. Take, for instance, current Generation 2 CSP tower plants with integrated thermal energy storage (TES), facilitating dispatchable generation as needed. Here, molten salts (e.g., sodium or potassium nitrates) act as the heat-transfer fluid between the solar receiver (the heat source) and both low-temperature (~260°C) and high-temperature (> 565°C) thermal energy storage tanks. Instead of being temporarily stored thermally in the hot tank, the heat contained in the high-temperature molten salt can also be instantly utilized on-demand in the power block for electricity generation, using steam turbines, even with supercritical steam.

Power cycle inlet temperatures could soar to as high as 720°C, presenting significant corrosion challenges for storage tanks, lines, and heat exchangers at such elevated temperatures. To mitigate risks associated with commercial CSP systems operating under these conditions, SETO is now developing Generation 3 CSP plants. These newer plants will utilize gas-phase or supercritical systems (sCO₂), advanced higher temperature molten salt phase systems (e.g., ternary chlorides), liquid metal (sodium) systems, or solid particles in a flowable powder form to replace current generation molten salts as the heat-transfer medium.⁴⁴ Particle-based systems offer simpler operation with fewer components compared to liquid- and gas-based alternatives. Moreover, they require relatively few high-cost materials for thermal energy collection and transport. These advantages have the potential to enhance plant availability and reliability while streamlining construction and commissioning processes. SETO has established a cost target of 0.05/kWh by 2030 for baseload configurations of CSP equipped with twelve or more hours of thermal energy storage, aiming to drive affordability and accessibility in this evolving sector.⁴⁵ As discussed earlier, the integration of sCO₂ power cycles with CSP thermal energy storage has shown significant potential to meet the needs of the current and future grid.

There are currently 27 CSP projects in the United States.⁴⁶ The Department of the Interior's Bureau of Land Management has recently announced plans to open up to 31 million acres of public land for alternative solar photovoltaic (PV) development. PV panel technologies are not covered in this landscape as they are expected to be capable of serving in adverse weather conditions, including hail, for example, which falls outside of our definition of a harsh environment. Notwithstanding this formality, there has been a rise in the number of reported cases of spontaneous solar panel cover glass breakage believed to be due to the trend in the cover glass becoming thinner (< 3 mm), allowing for easier crack propagation with temperature cycles.⁴⁷ Similarly, the metallic racking and mounting systems in solar farms can experience galvanic corrosion if the different metals are not properly chosen, but this issue is solved through traditional engineering materials selection rather than novel materials innovation.

⁴⁴ Solar Energy Technologies Office. Generation 3 concentrating solar power systems (Gen3 CSP) [Internet]. Department of Energy [cited: 2024 Sep 12]. Available from: <u>https://www.energy.gov/eere/solar/generation-3-concentrating-solar-power-systems-gen3-csp</u>

⁴⁵ Silverman T, Huang H. Solar energy technologies office multi-year program plan [Internet]. Department of Energy; 2021 May [cited 2024 Jul 30]. Available from: Solar Energy Technologies <u>https://www.energy.gov/sites/default/files/2021-</u>

^{06/}Solar%20Energy%20Technologies%20Office%202021%20Multi-Year%20Program%20Plan%2006-21.pdf ⁴⁶ National Renewable Energy Laboratory. Concentrating solar power projects in United States [Internet]. NREL

[[]cited: 2024 Sept 30]. Available from: <u>https://solarpaces.nrel.gov/by-country/US</u>

⁴⁷ Kennedy R. Spontaneous glass breakage on solar panels on the rise [Internet]. pv magazine (USA); 2024 Jun 21 [cited 2024 Jul 23]. Available from: <u>https://pv-magazine-usa.com/2024/06/21/spontaneous-glass-breakage-on-solar-panels-on-the-rise/</u>

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2.2.1.4 Geothermal Energy

For geothermal energy technologies, there are parallels with and distinctions from the environments encountered in oil and gas well drilling. These variances primarily revolve around subsurface conditions such as reservoir and fluid temperatures, rock heterogeneity and fluid permeability, and pressure. Geothermal well drilling often navigates through harsher subsurface environments compared to oil and gas drilling, coupled with more demanding surface conditions like steeper slopes and varied terrain.

The geothermal industry faces a significant challenge in reducing drilling costs, which can represent 50% or more of the total capital outlay for a geothermal energy project. Economically viable geothermal energy production hinges on overcoming this obstacle. In areas with naturally convective hydrothermal resources, extracting geothermal energy for electricity generation is relatively straightforward. As with other kinds of thermal-based electric power production, hot geothermal fluids (which can be supercritical if deep enough) are converted to steam to drive turbomachinery. Alternatively, the heat from the geothermal fluid could be transferred to CO₂, which could then be used as the turbine working fluid in binary-cycle power plants.

Currently, geothermal energy contributes 0.4% of electricity generation in the United States, which amounts to around 17 billion kWh annually,⁴⁸ a figure projected to rise to 37.2 billion kWh by 2050. The continental U.S. possesses over 100 GW of geothermal electric capacity and is theoretically capable of supplying nearly 10% of current U.S. electricity generation—a 26x increase from its current utilization share.⁴⁹ However, accessing geothermal energy is not always feasible due to factors such as excessive depth, rock with minimal fluid permeability (such as igneous or metamorphic formations), or the absence of a hot fluid reservoir. Enhanced geothermal systems (EGS) present a solution in such cases. EGS utilize controlled hydraulic stimulation techniques, such as hydro shearing, to expand existing fractures and create viable flow paths. Unlike hydraulic fracturing in the oil and gas sector, which generates new fractures, EGS enhance existing ones. At a Geothermal Technologies Office summit, five technical pathways for EGS were introduced, highlighting the need for sensing technologies capable of mapping stress, strain, and fractures; drilling tools resistant to extreme temperatures (up to 430°C), corrosive fluids, and mechanical wear; and robust geothermal well construction materials. Key challenges also encompass developing high-temperature capping materials and environmentally inert proppants. The Geothermal Technologies Office aims to halve drilling costs by 2030, aligning with the ideal cost curves outlined in their GeoVision roadmap analysis. The overarching objective is to slash EGS costs by 90%, aiming for a target of \$5 per megawatt-hour by 2035.⁵⁰

2.2.2 Non-Thermal Power Generation Systems

There is a pressing need for research and development in high-impact AMMT advancements for non-thermal power generation, such as wind and hydropower turbines, which convert fluid flow kinetic energy directly into electricity via electromagnetic induction. Unlike with heat engines, the power output of a wind or water turbine is proportional to the fluid density and cube of the fluid velocity (the Betz limit).⁵¹ The coefficient of power is the energy produced by the turbine divided by the total energy available in the fluid. Hence, the efficiency of a wind or water turbine exhibits the reverse trend of a heat engine and slightly decreases at higher temperatures in proportion to the small

 ⁴⁸ U.S. Energy Information Administration. Electric power annual 2022 [Internet]. Energy Information Administration; 2023 Oct [cited 2024 Jul 23]. Available from: <u>https://www.eia.gov/electricity/annual/pdf/epa.pdf</u>
 ⁴⁹ Augustine C, Fisher S, Ho J, Warren I, Witter E. Enhanced geothermal shot analysis for the geothermal technologies office [Internet]. Department of Energy; 2023 Jan [cited 2024 Jul 23]. Available from: <u>https://www.nrel.gov/docs/fy23osti/84822.pdf</u>

⁵⁰ Blankenship D, Gertler C, Kamaludeen M, O'Connor M, Porse S. Pathways to commercial liftoff: nextgeneration geothermal power [Internet]. Department of Energy; 2024 Mar [cited: 2024 Jul 30]. Available from: Pathways to Commercial Liftoff: <u>https://liftoff.energy.gov/wp-</u>

content/uploads/2024/03/LIFTOFF_DOE_NextGen_Geothermal_v14.pdf ⁵¹ Office of Energy Effiency & Renewable Energy. Small wind guidebook [Internet]. Department of Energy [cited: 2024 Sep 12]. Available from: https://windexchange.energy.gov/small-wind-guidebook

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decrease in the fluid density. These non-thermal power generation systems each have their own unique set of harsh environment challenges.

2.2.2.1 Marine Energy

Separate from hydropower, marine energy systems face unique material challenges, including exposure to varying water salinity levels, temperatures ranging from 4–27°C, speeds from 0.1 to 10 knots (0.05 to 5.1 meters per second), corrosive splash zones, fouling, and intensified UV exposure. Similar to offshore oil and gas platforms, conventional floating wave energy converters (WECs) and their associated mooring lines must withstand a large number of high-tension load cycles and high bending fatigue cycles, in addition to possessing high resistance to wear, corrosion and biofouling. Despite these challenges, marine energy systems are attractive for several reasons. The energy density of ocean waves is very high. WECs can capture energy up to 90% of the time compared to 20–30% for wind and solar power device and waves can travel large distances with little energy loss.⁵² The international Ocean Energy Systems (OES) agency has outlined a roadmap to develop 300 GW of ocean energy by 2050, which could create 680,000 jobs and yield \$340 billion in gross value added (GVA).⁵³

2.2.2.2 Hydropower

Hydropower turbines in hydroelectric facilities endure significant stresses from water pressure, leading to severe fatigue, erosion, and cavitation, often resulting in premature failure. Austenitic stainless steel alloys containing 17% to 20% chromium and carbon steel are commonly used in these applications to manage costs. A major challenge identified in the Advanced Manufacturing and Materials for Hydropower report by ORNL is the growing maintenance and repair demands due to the aging of major hydropower components like turbine runners, blades, and hubs. Fatigue from cyclic loading and variations in operating conditions, as well as corrosion of unprotected metal surfaces exposed to water, pose additional challenges. Biofouling by organisms like bacteria, mussels, and freshwater sponges further impedes capacity by causing blockages and increased pipe wall roughness, resulting in reduced efficiency. According to the 2002 NACE report, metallic corrosion costs the hydroelectric industry about \$0.15 billion annually.⁵⁴

To overcome these obstacles, the ORNL report suggests exploring novel structural and functional material families, such as advanced alloys, fiber-reinforced polymer composites, functionally graded materials, and self-lubricating bearings. Advanced coatings to combat fouling, erosion, and cavitation are also recommended to enhance part longevity and operational efficiency. Additionally, advanced manufacturing techniques like additive manufacturing can reduce lead times for replacement or upgrade of large-scale metallic hydropower parts, potentially minimizing downtime. Recent initiatives by entities like the U.S. Army Corps of Engineers demonstrate the feasibility of additive manufacturing for fabricating complex components.⁵⁵ Overall, investing in superior-performing materials and advanced manufacturing processes for the production of superior-performing components with more complex geometric designs—which allow for efficient lightweight components with additional functionality—could

⁵² Hillis AJ, Courtney CRP, Brask A. Wave energy converter platform stabilisation and mooring load reduction through power take-off control. IET Renewable Power Generation [Internet]. 2021 Jul 11 [cited 2024 Jul 23];15. Available from: <u>https://ietresearch.onlinelibrary.wiley.com/doi/full/10.1049/rpg2.12242</u>

⁵³ Ocean Energy Systems. Ocean energy and net zero: an international roadmap to develop 300GW of ocean energy by 2050 [Internet]. Ocean Energy Systems; 2023 [cited: 2024 Jul 31]. Available from: <u>https://www.ocean-energy-systems.org/publications/oes-documents/market-policy/document/ocean-energy-and-net-zero-an-international-roadmap-to-develop-300gw-of-ocean-energy-by-2050/</u>

⁵⁴ Koch GH, Brongers MPH, Thompson NG, Virmani YP, Payer JH. Corrosion costs and preventative strategies in the United States [Internet]. NACE International; 2002 [cited: 2024 Sept 30]FHWA-RD-01-156. Available from: http://impact.nace.org/documents/ccsupp.pdf

⁵⁵ Fox C. Infrastructure Innovation: New Poe lock arrestor arm is the largest U.S. civil works component produced by 3D printer [Internet]. Sault Ste. Marie (USA): DVIDS; 2024 Apr 1; [updated 2024 Apr 1, cited 2024 Jul 23]. Available from: <u>https://www.dvidshub.net/news/467497/infrastructure-innovation-new-poe-lock-arrestor-armlargest-us-civil-works-component-produced-3d-printer</u>

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revolutionize non-thermal power generation technologies, making them more robust, efficient, and environmentally friendly.

2.2.2.3 Wind Energy

For wind energy technologies, the focus of AMMTO's HEM portfolio primarily centers on the drivetrain components of wind turbines. Other DOE programs address challenges related to wind blades, towers, and platforms. Offshore wind turbines pose unique materials challenges compared to their land-based counterparts due to increased exposure to abrasive, erosive, and corrosive seawater elements. Failures in multi-stage gearboxes—encompassing various components like bearings, gears, pinions, and shafts—contribute significantly to unplanned maintenance and early replacement, accounting for up to 60% of operational and maintenance costs in wind energy. Such failures often occur well before the turbines reach their designed lifespan of 20–25 years. The wind and hydro industries also experience corrosion fatigue, stress corrosion cacking, and micro-biologically induced corrosion.

Wind turbine bearings operate in harsh conditions with the environment, temperature, and load continuously changing, making it easy for the bearings to malfunction. Wind turbine gearbox bearings, including planetary and journal bearings, frequently experience premature failure modes (observable failure events, manifestations) attributed to tribological issues such as spalling (a.k.a. flaking, peeling, pitting), which involves the removal of material from contact surfaces due to high loads. The main types of bearing wear mechanisms (underlying causes of failure) are abrasive, adhesive, corrosive, erosive, fatigue, as well as synergistic combinations like fretting. There are different kinds of bearing failure mechanisms and modes besides those due to wear, such as cracks and fractures, and even electric erosion. One type of wind turbine gear box bearing failure that has been studied for decades is called white etching cracks (named after the appearance of a polished and etched sample). This type is believed to be a forced failure created by excessive tensile stresses causing microstructural changes such as phase transformations involving ultra-fine, nano-recrystallized, carbide-free ferrite, or ferrite with a very fine distribution of carbide particles. Another failure mode is rolling contact failure, which occurs after a long period of fatigue cycles, and it is often associated with surface or subsurface cracking of the material.

Finally, one noteworthy failure mode for wind turbine gearbox bearings relates to the use of pulse-width modulated power electronic converters in variable speed wind turbines. This scenario can induce a common-mode voltage that generates stray currents through a parasitic circuit in the generator structure.⁵⁶ Consequently, the bearing lubricant may experience electric stress surpassing its dielectric strength, leading to electrostatic discharge machining (EDM) of the bearing. Mitigation strategies involve proper insulation arrangement for the bearing and shaft grounding, although insulation alone may not suffice and could potentially exacerbate the issue.

2.2.2.4 Established Energy Production (Hydro, Wind, Nuclear) Material Supply Chain Needs

To meet the anticipated expansion in hydropower, wind energy, and nuclear energy sectors, there's a pressing demand for innovation to reduce costs and lead times associated with manufacturing ultra-large-scale metal components. These components—such as wind turbine bed plates, rotor hubs, hydropower runners, and pressure vessels—operate under high loads or pressures. Often weighing over 10 tonnes and with dimensions measured in meters, these parts are typically crafted from conventional materials like ductile cast iron, stainless steel, or mild steel using traditional methods like sand casting and forging.

Key Takeaway

⁵⁶ Robles E, Fernandez M, Andreu J, Ibarra E, Zaragoza J, Ugalde U. Common-mode voltage mitigation in multiphase electric motor drive systems. Renew and Sustain Energ Rev [Internet]. 2022 Apr 1 [cited 2024 Sep 12];157:111971. Available from: <u>https://doi.org/10.1016/j.rser.2021.111971</u>

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Currently, many large-scale metallic components cannot be obtained cost-competitively from domestic foundries and forging houses, leading to reliance on foreign sources.^{57,58,59,60,61,62} Innovation through advanced and hybrid manufacturing approaches and tools (e.g., LSAM, additive casting, large-scale PM-HIP, SSMAM, AM-enhanced forging, robotics/automation, and smart manufacturing) offers promising avenues to bolster the industry, lower production costs, and establish a robust domestic supply chain for large parts needed in energy and various industrial applications, including process industries, heavy machinery, mining, aerospace, defense, and agriculture.

Lead times for producing ultra-large metal castings and forgings usually range from 12 to 18 months, regardless of their source. The urgent necessity to enhance domestic manufacturing capacity for such components and vessels has been underscored in workshops and supply chain assessments across the nation's nuclear energy, wind energy, hydropower energy, defense, and industrial sectors.

2.2.2.5 Hydrogen

Hydrogen, through electrochemical-based fuel cells or combustion-based technologies, can enable reduced emissions in transportation, stationary or remote power, and portable power applications. Specifically, the utilization of hydrogen in fuel cells or low-NO_x H₂ gas turbines emerges as a leading solution to facilitate multi-day storage and dispatchable power generation to the grid. This solution is particularly crucial in scenarios with high integration of variable renewable energy generation. Introducing hydrogen co-firing in current power plants holds the potential to significantly reduce emissions from the power sector. Hydrogen fuel cells offer a viable alternative (for long-duration, dispatchable power) to diesel generators, which cater to the needs of critical facilities such as hospitals, data centers, and remote locations where microgrids and telecom towers demand uninterrupted power supply round the clock. Operating on hydrogen, fuel cells offer quieter operation, enhanced reliability, and improved air quality compared to diesel generators.

There are different kinds of hydrogen fuel cells, based on the type of electrolyte used. One kind is the solid oxide fuel cell (SOFC), which is a high-temperature device (operating between 600–1,000°C) having a fast ion conducting solid electrolyte (SE) made from electroceramics. SOFCs present opportunities for development of new SEs (oxides or ceramics) and electroceramic electrodes as well as their associated manufacturing processes, including advanced sintering techniques. In addition to solid electrolytes and SOFC electrodes, electroceramics are used in many different energy-relevant technologies such as various other kinds of electrodes (batteries, electrolyzer cell anodes and cathodes), capacitor and microwave dielectrics, and in piezoelectric devices. Their unique properties are tailored through defect engineering and are intricately tied to their precisely controlled non-stoichiometry (e.g.,

02/Nuclear%20Energy%20Supply%20Chain%20Fact%20Sheet.pdf

⁵⁷ Uria-Martinez R, White D, Oladosu G, DeSomber K, Johnson M. Hydropower: supply chain deep dive assessment. [Internet] Department of Energy; 2022 Feb 24 [cited 2024 Sep 13]; Available from: <u>https://www.osti.gov/biblio/1871571</u>

⁵⁸ Cooperman A. Large castings for wind turbines. [Internet] National Renewable Energy Laboratory; 2023 Aug [cited: 2024 Sep 13]. Available from: <u>https://www.nrel.gov/docs/fy23osti/84438.pdf</u>

⁵⁹ Dawnbreaker. Market research study domestic casting industry. [Internet] Department of Energy; 2022 Aug [cited: 2024 Sep 13]. Available from: <u>https://sc-dev.osti.gov/-/media/sbir/pdf/Market-Research/AMO---Metal-Casting-August-2022-Public.pdf</u>

⁶⁰ Department of Energy. Achieving American leadership in the wind supply chain. [Internet] Department of Energy; 2022 Feb 24 [cited: 2024 Sep 13]. Available from: <u>https://www.energy.gov/sites/default/files/2022-02/Wind%20Supply%20Chain%20Fact%20Sheet%20Final.pdf</u>

⁶¹ Department of Energy. Achieving American leadership in the hydropower supply chain. [Internet] Department of Energy; 2022 Feb 24 [cited: 2024 Sep 13]. Available from: <u>https://www.energy.gov/sites/default/files/2022-02/Hydropower%20Supply%20Chain%20Fact%20Sheet.pdf</u>

⁶² Department of Energy. Achieving American leadership in the nuclear energy supply chain. [Internet] Department of Energy; 2022 Feb 24 [cited: 2024 Sep 13]. Available from: <u>https://www.energy.gov/sites/default/files/2022-</u>

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vacancies and aliovalent ion impurities), which are highly dependent on the processing environment and operational parameters.

Hydrogen can also be used as a fuel in vehicle internal combustion engines (ICEs) and gas turbines, as previously discussed. Several manufacturers are already heavily investing in these two end-use applications, some independent of federal funding, with substantial progress being made in technology maturity. However, it is expected that equipment (engine/turbine) modifications will be needed to ensure a longer and safer service life. Public and private research is similarly underway to produce a 100% hydrogen-fueled turbine. The NETL anticipates that industry will achieve this technology by around 2030 based on current research progress and publicly announced forecasts.⁶³ The key technical challenges for hydrogen and related technologies are overall cost, materials durability, system reliability and performance, as well as the lack of hydrogen infrastructure. As an example, certain high entropy alloys (see discussion of HEAs in Section 2.3.1: high temperature industrial materials, below) are being investigated in bulk form and as coatings to protect critical components in hydrogen turbine systems from oxidation, spallation, and thermal shock. Material-related challenges associated with hydrogen technologies will be further discussed in the next section on advanced materials for efficient energy utilization in the industrial sector.

Key Takeaway

One kind of hydrogen fuel cell is the solid oxide fuel cell (SOFC), which is a high-temperature device (operating between 600-1,000°C) having a fast ion conducting solid electrolyte (SE) made from electroceramics. SOFCs present opportunities for development of new SEs (oxides or ceramics) and electroceramic electrodes as well as their associated manufacturing processes, including advanced sintering techniques. In addition to solid electrolytes (SEs) and SOFC electrodes. Electroceramics are used in many different energy-relevant technologies such as battery electrodes, electrolyzer anodes and cathodes, capacitor and microwave dielectrics, and in piezoelectric devices. Their unique properties are tailored through defect engineering and are intricately tied to their precisely controlled non-stoichiometry (e.g., vacancies and aliovalent ion impurities), which are highly dependent on the processing environment and operational parameters.

The broader hydrogen economy, or energy system, encompasses several aspects, from production, storage, delivery/transportation, conversion, to end-use applications, including integrated energy systems, where hydrogen can improve the economics and performance of existing and emerging electric power generators; these elements all face several material compatibility challenges.

Key Takeaway

Understanding the impact of hydrogen on infrastructure and materials is critical due to the wide range of service conditions, including temperatures from 253°C to 1,430°C, pressures from near vacuum to 1,000 bar, and pH ranges in aqueous solutions from highly acidic to highly basic. Hydrogen exposure can create chemically reducing environments, induce stress corrosion cracking, cause embrittlement, and lead to deformation (such as decompression and dislocation mobility enhancement).

To tackle these material challenges, two consortia have been established: the Hydrogen Materials Advanced Research Consortium (HyMARC), focusing on ceramics, sorbents, catalysis, and metal oxide frameworks for hydrogen storage systems, and the Hydrogen Materials Consortium (H-MAT), which focuses on polymers and metals for fuel cells, pressure vessels, and pipelines. The Hydrogen and Fuel Cell Technologies Office (HFTO)

⁶³ U.S. Department of Energy. NETL experts to discuss use of hydrogen-fueled turbines to drive clean energy economy [Internet]. Department of Energy; 2022 [cited 2024 Jul 23]. Available from: <u>https://netl.doe.gov/node/12058</u>

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recently published roadmap,⁶⁴ which outlines strategies for developing and adopting hydrogen as an effective energy source for maximum national benefit. The overarching goal is to reduce the cost of hydrogen production by 80%, reaching \$1 per kilogram by 2035. To be competitive in the long term, the total cost to the end-user, including infrastructure costs, needs to be around \$5/kg or even lower in some markets. Achieving this will require significantly lowering capital costs, reducing energy costs, increasing efficiencies, and improving durability and reliability to reduce maintenance costs.

2.3 Advanced Materials for Efficient Energy Utilization in the Industrial Sector

In the industrial sector, materials and components frequently endure harsh service environments requiring high temperature functionality and mechanical strength. Processing and refining industries, which produce chemicals, petrochemicals, textiles, food and beverages, paper and pulp, semiconductors, cement, metals, and mining typically face more severe conditions and are more energy and emissions-intensive than discrete product manufacturing assembly plants. Premature structural or functional component failures in these environments can be costly and time consuming to replace, leading to production losses from unplanned shutdowns and negatively impacting process and energy efficiency until repairs are made. For example, the 2002 NACE report estimated the annual cost of corrosion in the manufacturing/production and industrial sector to be at around \$17.6 billion.⁶⁵

2.3.1 High-temperature Industrial Materials

Starting with high-temperature applications, the field of alloys used at temperatures up to about 1,100°C is presently dominated by nickel-based superalloys, as described in the previous section on thermal power production technologies. Typical industrial applications for Ni-based superalloys at these temperatures include hearth rollers, radiant tubes, furnace muffles, burner nozzles, among many others. For higher temperatures, in the range of 1,400 to 2,000°C, refractory metals and alloys are used. There are ten refractory metallic elements (metals with melting points > 2,000°C), five of which—tungsten (W), niobium (Nb), tantalum (Ta), rhenium (Re), and molybdenum (Mo)— that are fundamental to several industrial sectors. The pure refractory metals and alloys containing these elements are used where materials are required to withstand extreme thermal, mechanical, and corrosive material stressors, which are present in many harsh industrial applications, including aerospace, chemical production, ceramic and glass manufacturing, petroleum processing, metallurgical tooling, and semiconductor fabrication. Although the refractory metals oxidize readily, this problem can be mitigated with alloying additions and/or barrier coatings. The pure refractory metals are hard, but W and Mo are brittle, as are most Ta-containing alloys making fabrication of high-performance parts difficult. Refractory metal parts are thus typically produced by power metallurgy techniques. However, when these elements are used as minor alloying additions, fabrication by casting and forging techniques can sometimes be used depending on the phase equilibria of the selected system.

Energy efficiency is affected by temperature such that higher temperature processes are more energy efficient. Because of the rapid innovation and development of modern industrial technologies, higher-temperature-resistant special alloys and coatings will be needed. One such foundational material family of interest for these service conditions are the high entropy alloys (HEAs), a subset of compositionally complex alloys (CCAs) or multi-principal element alloys (MPEAs), originally defined as those containing five or more elements in near-equal atomic concentrations (5 – 35 at. %) and, therefore, high configurational entropy (number of possible arrangements of the constituent particles) providing for greater thermodynamic phase stability (lower Gibbs free energy). Of particular interest are those containing refractory metals (RHEAs), some of which may be expected to have better high-temperature performance with respect to corrosion and oxidation resistance, and wear resistance, as well as fracture toughness and strength, balanced with ductility when the alloy is also a eutectic HEA (EHEA) containing

https://www.hydrogen.energy.gov/docs/hydrogenprogramlibraries/pdfs/us-national-clean-hydrogen-strategyroadmap.pdf?sfvrsn=c425b44f 5

⁶⁴ U.S. Department of Energy. U.S. national clean hydrogen strategy and roadmap [Internet]. Department of Energy; 2023 Jun [cited 2024 Jul 23]. Available from:

⁶⁵ Koch GH, Brongers MPH, Thompson NG, Virmani YP, Payer JH. Corrosion costs and preventative strategies in the United States [Internet]. NACE International; 2002 [cited: 2024 Sept 30]FHWA-RD-01-156. Available from: <u>http://impact.nace.org/documents/ccsupp.pdf</u>

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ductile face centered cubic (FCC) and strong body centered cubic (BCC) phases. Bulk RHEAs have been prepared by arc melting, induction melting, electron-beam melting, powder metallurgy, and additive manufacturing (all are low volume throughput) while coatings have been deposited by magnetron sputtering. RHEAs have been mentioned as potential replacements for nickel-based superalloys at temperatures at least as high as 1,200°C. This would correspond to a lower homologous temperature (fraction of the melting point), T_H , for the higher melting RHEAs compared to those of the nickel alloys that are often used in excess of $T_H = 0.7$. A lower T_H would result in lower diffusivities and less creep at the high service temperatures. However, more needs to be learned about all the HEA systems, which are ripe for physics-based approaches combining CALPHAD and First Principles, as well as datadriven design, as there are not many well-established phase diagrams for HEAs due to the vast compositional space available.

Combinatorics gives the number of possible alloy systems as $n! / [m! \cdot (n-m)!]$, where *n* is the number of different elements under consideration, and *m* is the order of the alloy system (i.e., m = 2 for binary, m = 3 for ternary, and so on). For example, there exist 252 possible quinary alloy systems (m = 5) comprised exclusively of five elements each from the ten refractory metals, and a much larger number of specific alloys when the different possible proportions between the constituents are considered. It is very time consuming and expensive to experimentally investigate the phase equilibria of many systems. Contrarily, CALPHAD is ideal for quickly extrapolating the phase diagram for a high-order system from its subsystems, particularly those high order systems that are less explored, so long as the subsystems have been thermodynamically assessed. Nevertheless, despite the early enthusiasm surrounding these alloys, it should be noted there are currently no significant industrial implementations of HEAs after two decades of research. The global market for all high entropy materials (alloys and ceramics) was only \$54.7 million in 2022^{66} Furthermore, some researchers are skeptical of the original premise that the high configurational entropy of equiatomic alloys can lower the single-phase solid solution free energy below that of potential precipitates and intermetallic phases, which if present would normally be detrimental to ductility⁶⁷ Clearly, many basic materials questions, as well as manufacturing scale-up challenges remain with HEAs.

The field of HEAs is also a materials class in which HPC could help with a direct design approach through the exploration of the local atomic structure or short-range chemical order (up to a few coordination spheres around a reference site) in a chosen refractory alloy (i.e., RHEA), to predict the alloy's solidification behavior by ab initio or quantum molecular dynamics. It is the local lattice distortions associated with different sized atoms occupying the same crystallographic site of a solid solution that seems to impart the mechanical properties to these alloys (i.e., solid solution strengthening). If the diffusivities of the different alloy constituents can be accurately predicted, the crystal nucleation from the melt, the formation of stable and metastable phases, grain formation and growth, phase transformations, nano- and micro- segregations, and defect formations, the properties of the alloys can be designed and controlled.

There are also intermetallic phases (mainly aluminides), carbides, metalloid-containing phases (e.g., silicides), and refractory metal-intermetallic composites that have either been used or studied for high-temperature applications like heating elements, furnace racks/fixtures, hot gas filters, high-speed cutting tools, etc. However, as expected, the general lack of room-temperature ductility and toughness of these materials hinder progress. If a viable approach for lowering the brittle-to-ductile transition temperature for some of these materials can be found, they could become more attractive for certain applications.

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https://www.mitsui.com/mgssi/en/report/detail/__icsFiles/afieldfile/2024/05/17/2404p_abe_e.pdf
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⁶⁶ Abe Y. Development and use of high-entropy materials – entering an era of new functional materials composed of multiple elements [Internet]. Mitsui & Co; 2024 Apr [cited: 2024 Sep 12]. Available from:

⁶⁷ Slobodyan M, Pesterev E, Markov A. Recent advances and outstanding challenges for implementation of high entropy alloys as structural materials. Mat today Comm [Internet]. 2023 Aug 1 [cited 2024 Sep 12];36:106422–2. Available from: https://doi.org/10.1016/j.mtcomm.2023.106422

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In addition to high-temperature alloys, monolithic ceramics and bricks are also used as refractories, for example, as thermal insulation linings in blast furnaces, electric arc furnaces, and transport vessels in the steel industry. Monolithic materials can be installed in continuous panels or rings using spray-on gunite or shotcrete techniques to reduce reliance on neighboring materials for lining integrity and eliminate joints between traditional bricks that offer paths for corrosion. Developing bricks or monolithic lining refractories with improved lifetimes would result in an increase in furnace thermal efficiencies as well as extend the time between maintenance and replacement schedules. As industrial process heating and energy production technologies become more thermally efficient, more components made from high-temperature superalloys, refractory metals and alloys, HEAs, RHEAs, EHEAs, and ceramics will be of increasing importance (e.g., as Joule/resistance heating elements, retort vessels, heat shielding/thermowells, refractory linings, radiant tubes, higher temperature H₂ combustion engine/turbine components, Gen-IV nuclear fission and fusion reactor components).

The Industrial Efficiency and Decarbonization Office (IEDO) recently published a roadmap that outlines transformative technology pathways to reduce fuel- and electricity-related emissions in the industrial sector.⁶⁸ These pathways include novel fuels, feedstocks, and energy sources (LCFFES); process heat electrification; energy efficiency measures, including waste heat recovery (WHR) technologies. Advanced materials are essential in each of these areas, such as phase-stable materials for WHR, functional surfaces, and hydrogen embrittlement-resistant materials that can withstand aging effects that are discussed below.

2.3.2 Hydrogen in Industry

High-performance materials are essential for ensuring affordable, safe, and reliable production, transport, storage, and use of hydrogen to enable large-scale adoption of hydrogen across sectors. These advanced materials, which include metals, ceramics, polymers, and composites, must be compatible for hydrogen service over a wide range of harsh conditions that could include cryogenic temperatures and high-pressures. Hydrogen can be produced from electrolyzer cells (reverse fuel cells ran in regenerative mode) powered by renewable or nuclear energy, such as proton exchange (or polymer electrolyte) membrane (PEM) electrolysis, anion exchange membrane (AEM), alkaline electrolysis, or high-temperature (500-1,000°C) solid oxide electrolyzer cells (SOECs). High-temperature electrolysis also requires integration and optimization with thermal sources, such as nuclear plants, to increase the efficiency of hydrogen production and electricity generation. When coupled or integrated with external sources that can provide high-grade process heat (300-500°C) for steam generation—such as from a steel, geothermal, or nuclear power plant-the heat can be reused in the SOEC to increase the overall electrical efficiency of hydrogen production. In this configuration, a SOEC system will require less energy than PEM or alkaline electrolyzers to produce the same quantity of hydrogen. Without such an external source of heat for steam generation, the potential efficiency advantage (up to 20%) of solid oxide systems over future competing electrolyzer architectures largely disappears. However, while advancements in high-temperature solid oxide electrolyzers are progressing, challenges to market adoption and commercialization include cost, durability (solid oxide stacks fail earlier than PEM and alkaline stacks due to higher thermal stresses), and difficulties with manufacturing scale-up to large systems in the hundreds of megawatts.⁶⁹

Hydrogen's versatility enables its use in numerous end-use applications. Government agencies are focusing on hydrogen to power industrial segments (e.g., chemicals, steelmaking, cement production) and heavy-duty transportation (e.g., trucks, buses, rail, maritime) that are difficult to electrify. In these applications, fossil fuels are currently used as a fuel, a chemical feedstock, or for generating high-temperature heat.

⁶⁸ Cresko J, Rightor E, Carpenter A, Peretti K, Elliott N, Nimbalkar S, et al. Industrial Decarbonization Roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 23] p. 1–241. Available from:

https://www.energy.gov/sites/default/files/2022-09/Industrial%20Decarbonization%20Roadmap.pdf ⁶⁹ Flis G, Wakim G. Solid oxide electrolysis: a technology status assessment [Internet]. Clean Air Task Force; 2023 Nov [cited 2024 Jul 23]. Available from: <u>https://cdn.catf.us/wp-content/uploads/2023/11/15092028/solidoxide-electrolysis-report.pdf</u>

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2.3.3 Carbon Capture Utilization and Storage (CCUS)

For CCUS and oxy-fuel combustion incorporating CO_2 capture, viable technologies are not anticipated to be materials-limited. For example, while there are some materials-related challenges (e.g., due to higher concentrations of CO_2 , SO_2 , H_2O , and high carbon activities), there are mixed results on the differences in the extent of corrosion and no significant difference observed in carburization of materials between air-fired and oxy-fuel fired combustion systems. Careful selection of materials for CCUS systems is required to ensure safe and economical operation, but it is believed that suitable plant infrastructure materials currently exist. Plant and facility CCUS infrastructure of pipes, pumps, ductwork, flues, and injection wells, etc. crosscut between the mission spaces of FECM, IEDO, and AMMTO. However, new CO_2 sorbent materials themselves fall within FECM's domain and are outside this landscape's scope.

2.3.4 Advanced Cement and Concrete

Many energy- and emissions-intensive industries produce products under harsh environments. For most of these sectors (e.g., iron/steel, glass, pulp/paper, chemicals), energy efficiency gains and CO₂ emissions reductions are expected to come from new or improved manufacturing processes to existing product formulations, with a notable exception being cement and concrete. Advanced, next-generation cement (binder) and concrete (hydrated binder plus aggregate for end-use) demonstrating comparable or even superior properties to those of ordinary Portland cement (OPC) formulations could drastically reduce process- and energy-related CO₂ emissions from industry.⁷⁰ However, the technical performance of such alternative materials is still not well characterized and proven/validated with regards to strength, durability, and long-term safety in environmentally demanding infrastructure applications. Thus, these cement formulations are currently limited in use for certain applications. Economic challenges also present significant barriers for adopting these materials. After water, concrete is the most widely used substance on Earth. As such, the cement industry is a mature, highly consolidated, highly competitive, and capital-intensive commodity business with relatively low profit margins compared to other industries. Cement manufacturers typically generate gross profit margins of around 5-10% of revenue.⁷¹ It is crucial that new formulations aimed at replacing OPC are not only proven to be technically performing, but also cost competitive and sustainable.

2.3.5 Waste Heat Recovery

Industrial waste heat recovery technologies include systems-level solutions that reuse waste heat streams for other thermal processing and waste heat-to-power (WHP) electric technologies. WHR system components include: regenerative and recuperative burners; economizers for low-to-medium temperature WHR (finned tube and coiled tube, condensing and non-condensing) typically fabricated from polytetrafluoroethylene, carbon, or stainless steel; waste heat boilers; air preheaters/heat exchangers, including metallic and ceramic recuperators (for medium-to-high temperatures), fixed and rotary regenerators (for high temperatures), and run around coils; plate heat exchangers; heat pipes (with screen mesh structure wicks) made from aluminum, copper, titanium, stainless steel, tungsten, or Inconel or Monel alloys; and heat recovery steam generators. (pressure systems). Additionally, devices for the direct conversion of recovered heat into electricity can be integrated into WHR systems.

Waste heat from industrial processes (often coupled with molten material, particulates, corrosive substances, or other material stressors), flue gases, cooling towers, or even wastewater are typically captured and transferred via a heat exchanger (HX), which must possess a high thermal conductivity for efficient heat transfer, in addition to corrosion resistance and high strength to prevent rupture. Typical HX materials include stainless steel, nickel alloys, copper-nickel alloys, carbon steel, and other metals, but also SiC, alumina, and other thermally conducing ceramics for high-temperature heat exchangers ($T > 900^{\circ}C$) that can tolerate more hostile environments involving corrosive

⁷⁰ Cresko J, Rightor E, Carpenter A, Peretti K, Elliott N, Nimbalkar S, et al. Industrial Decarbonization Roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 23] p. 1–241. Available from: <u>https://www.energy.gov/sites/default/files/2022-09/Industrial%20Decarbonization%20Roadmap.pdf</u>

⁷¹ Babu M. Cement industry in a slowdown, profitability shrinks further [Internet]. The Business Standard; 2022 [updated 2023 Feb 14, cited 2024 Jul 24]. Available from: <u>https://www.tbsnews.net/economy/stocks/cement-industry-slowdown-profitability-shrinks-further-413950</u>

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or abrasive fluid streams. There are many kinds of heat exchanger constructions found in industry, with the shell and tube type being the most common (~35%) in the process industries. In this type, a large pressure vessel (the shell) has a bundle of tubes inside it and heat is transferred between the fluid inside the tube and the fluid outside the tube through the tube walls. Joining the tubes and shell in this kind of heat exchanger is critical for safety because the system may be very hazardous if it carries fluids under high pressures.

Key Takeaway

More durable industrial heat exchangers obtained through advanced joining techniques (e.g., friction stir processing) represent a substantial innovation opportunity. Diffusion-bonded or brazed compact heat exchangers (CHX) have been developed to reduce the size of heat exchanger installations (e.g., aerospace, naval, automative applications). CHXs are designed to have a high area density, or area of heat-transfer surface to heat exchanger volume.

Most CHXs are formed of layers of plates or finned channels of fixed length and width, whose surface shape determines the performance via nondimensional heat-transfer coefficient and friction factor relationships (there is a significant resistance to flow with high-friction loss).

Key Takeaway

One type of CHX is the microchannel heat exchanger (MCHX), also known as a printed circuit heat exchanger (PCHX), in which thin, flat metal plates have fluid flow microchannels chemically etched in each layer to form a complex flow pattern. The layers are then diffusion-bonded together to create a dense solid core heat exchanger with superior airflow and heat-transfer properties without gaskets, interlayers, or brazing. Further advances in MCHXs are particularly advantageous for extreme environments as they could withstand very high pressures of tens of MPa's and extreme temperatures beyond 800°C.

Alternately, waste heat can be stored (a process discussed in the next section) within sensible, latent, or thermochemical storage, which allows for the waste heat to be utilized when heat generation does not directly match the timing or duty cycle. Waste heat from industrial processes can also be directly converted to electricity with arrays of advanced solid-state thermophotovoltaic (TPV) modules consisting of emitters (thermal radiators) and specialized PV materials tuned to convert infrared radiation photons directly to electricity, or by solid-state thermoelectric generator (TEG) modules, which are, essentially, assemblies of interconnected thermocouples known as thermopiles that generate a voltage in response to a temperature difference between the thermocouple ends via the Seebeck effect. TEGs are superior to TPVs due to their higher power density. Either type of solid-state device can be protected or shielded from harsh environments with barrier layers or sheaths. As of 2021, both TPVs and TEGs have laboratory observed maximum conversion efficiencies of around 325°C to 725°C. Between about 725°C and 1,725°C, future TPVs can benefit from higher efficiencies with a similar power density to TEGs. At temperatures above 1,725°C, TPVs suffer from cell heating.⁷³

2.4 Advanced Materials for Energy Storage

The global demand for energy storage solutions is expected to increase to more than 2,500 GWh by 2030, fourfold from a 2018 baseline. This creates enormous opportunity for American technology providers, manufacturers, and the broader U.S. economy. The DOE has set several storage goals for 2030 such as an aggressive 90%

⁷² LaPotin A, Schulte KL, Steiner MA, Buznitsky K, Kelsall CC, Friedman DJ, et al. Thermophotovoltaic efficiency of 40%. Nature [Internet]. 2022 Apr 13 [cited 2024 Jul 24];604(7905):287–91. Available from: https://doi.org/10.1038/s41586-022-04473-y

⁷³ Okanimba Tedah IA, Maculewicz F, Wolf DE, Schmechel R. Thermoelectrics versus thermophotovoltaics: two approaches to convert heat fluxes into electricity. Journal of Physics D: Applied Physics [Internet]. 2019 May 3 [cited 2024 Jul 24];52(27):275501. Available from: <u>https://doi.org/10.1088/1361-6463/ab1833</u>

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reduction in baseline 10+ hour stationary storage applications costs to \$0.05/kWh and a 44% reduction in 300-mile rated EV battery packs from \$143/kWh to \$80/kWh⁷⁴. Several DOE offices conduct energy storage activities, which include both electrical and thermal energy storage systems.

2.4.1 Thermal Energy Storage

Integrating TES within heat-to-electricity, heat-to-heat, and electricity-to-heat applications is being investigated as a path to achieve the desired \$0.05/kWh target. High-temperature thermal energy storage (HTTES) applications offer significant potential for improving the efficiency of energy-intensive industrial processes that require heat above 1,400°C, such as iron ore processing, metal fabrication, cement production, glass manufacturing, mineral processing, and chemical production. HTTES can reduce fuel consumption by preheating fuel, oxidizers, and process materials. Low temperature TES also provides benefits for heating, cooling, and some process heat applications in both electricity-to-heat and heat-to-heat configurations. TES for augmenting existing industrial process heat is attractive because it eliminates the energy penalty from thermal-to-electric conversion.

Characterization of TES systems include the storage media (e.g., water, molten salts), storage media containment vessels, and heat exchange/transfer (i.e., based on the ability of the TES system to support power generation or heat sources for efficient energy charging and discharging). Thermal energy storage media tanks/vessels are normally constructed of reinforced concrete (for water media) or stainless steel (for molten salt media) with exterior insulation. There are three main categories of thermal energy storage technologies: sensible heat, latent heat (associated with phase changes of the thermal storage material), and thermochemical (based on thermal energy released/absorbed during reversible chemical reactions). Sensible heat storage is the most common commercially deployed TES type and is applicable for both power generation and heating. It is the only kind discussed here. In sensible heat TES systems, energy is stored by raising the temperature of the thermal storage mediaum. The amount of energy stored is proportional to the physical properties of the storage material including density, volume, specific heat, and temperature change of the storage material.

Molten nitrate salts are commonly used as the thermal storage medium in commercial sensible TES systems that store energy between 290°C and 600°C, due to the phase stability of these salts at those high temperatures. The storage of thermal energy in solid media, such as particles, concrete, and graphite, has seen some deployment cases and can be utilized at very high temperatures (> 1,000°C). If a ceramic monolith is used as the storage media, it can be thermally cycled using a separate heat-transfer media. Solid storage media obtained from nature can be abundant, low cost, and environmentally compatible. Ceramic- or sand-type solid particles as thermal storage media overcome the corrosion issues as well as the low temperature freezing concerns of molten salt and are additionally attractive because of their high-temperature stability.⁷⁵ Material selection in all these thermal energy storage applications must consider the durability under high temperatures and the specific heat-transfer media chosen, such as molten salts or solid particles. Solid-state heat-transfer media for HTTES technologies appear promising for industrial process heat recovery due to their broader operating temperature range. While using solid-state heat-transfer media can mitigate some challenges associated with corrosive molten nitrate salts, new challenges arise, such as material erosion from moving abrasive granular particles and heat-transfer fluid issues.

2.4.2 Electrical Energy Storage

In addition to thermal energy storage devices, electrical energy storage technologies are emerging to ensure grid resilience during unusual grid events, like extreme weather, cyber-physical attacks, or sudden changes in

⁷⁴ U.S. Department of Energy. Energy storage grand challenge roadmap [Internet]. Department of Energy; 2020 Dec [cited 2024 Jul 24]. Available from:

https://www.energy.gov/sites/default/files/2020/12/f81/Energy%20Storage%20Grand%20Challenge%20Roadmap .pdf

⁷⁵ Balliet WH, McLaughlin L, Ma Z, Glusenkamp K. Technology strategy assessment findings from storage innovations 2030 thermal energy storage July 2023 [Internet]. Department of Energy; 2023 Jul [cited 2024 Jul 24]. Available from: <u>https://www.energy.gov/sites/default/files/2023-07/Technology%20Strategy%20Assessment%20-%20Thermal%20Energy%20Storage.pdf</u>

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renewable generation or loads. Such a network of energy storage units, if properly managed, can restore the grid by optimizing energy resource utilization and maintaining supply-demand balance. Similarly, the aerospace, automotive/electric vehicle, and industrial sectors are increasingly seeking reliable electrical energy storage systems based on electrochemical devices such as batteries and supercapacitors that can operate under extreme thermal conditions without experiencing thermal runaway (TR) failures. These electrochemical devices are comprised of cathodes, anodes, separators, and electrolytes, with solid electrolytes, or SEs (e.g., polymers, ceramics, composites), being an excellent choice to control TR in high temperature (> 85C°C) or harsh weather situations. SEs are safer under short circuit conditions (easing the risk of fire or explosions) and have greater ionic conductivity and electrochemical stability than conventional liquid electrolytes. Nevertheless, there are remaining challenges needing to be addressed with the design including defect engineering and computational modeling of thermally stable, eco-friendly and sustainable production of solid electrolytes, fundamental investigations of electrode-electrolyte interfaces, and scalability of SE fabrication techniques and their integration into energy storage devices⁷⁶.

There are also other kinds of electrochemical devices relevant to energy production and use, such as fuel cells and electrolyzer cells. These types of electrochemical devices were previously discussed under the Hydrogen section. Electrochemical devices present opportunities for development of new electroceramic materials together with their associated manufacturing processes, including advanced sintering techniques. In addition to fast ion conductor solid electrolytes, electroceramics are used in various kinds of electrodes (e.g., batteries, fuel cell anodes and cathodes), capacitor and microwave dielectrics, and in piezoelectric devices. Their unique properties are tailored through defect engineering and are intricately tied to their precisely controlled non-stoichiometry (e.g., vacancies and aliovalent ion impurities), which are highly dependent on the processing environment and operational parameters.

2.5 Materials Integration into Energy Systems

Materials integration presents significant opportunities in energy storage as well as energy production and utilization technologies, particularly with multi-material (composite) components and structures, and with the broadest inclusivity external claddings (free-standing materials mechanically placed over another material and often diffusion bonded), internal linings, and coatings (non-free-standing films chemically or physically deposited on a base material). These composite and multifunctional material systems combine the benefits of different materials to obtain optimal structural and functional properties like strength, stiffness, corrosion/oxidation/wear resistance, in addition to possible weight savings and reduced energy consumption. Their high strength and lightweight characteristics can make composites the preferred alternative to metals in certain structural components, including load-bearing structures. Decreasing the cost and weight of composites while improving their strength, resilience, and functional properties can boost their implementation and will increase the energy efficiency of U.S. energy sectors. Wide-ranging opportunities from heat exchangers to vehicle and aerostructure lightweighting provide quantifiable justification for pursuing R&D of composites with superior⁷⁷ Likewise, innovation in coatings with selfhealing properties and integrated sensors could be a promising solution for early detection problems, monitoring real-time conditions, and autonomous repairing, thereby helping to reduce operation and maintenance (O&M) costs. Functional surface technologies are covered exclusively in Focus Area 1 and will not be further discussed in this section, which is concerned primarily with joining and bonding techniques for the assembly or fabrication of composite structures and claddings.

⁷⁶ Kumaravel V, Bartlett J, Pillai SC. Solid electrolytes for high-temperature stable batteries and supercapacitors. Advanced Energy Materials [Internet]. 2020 Nov 26 [cited 2024 Jul 24];11(3):2002869. Available from: <u>https://doi.org/10.1002/aenm.202002869v</u>

⁷⁷ Hunt WH, Brindle R, James M, Justiniano M, Sabouni R, Seader M, et al. Linking transformational materials and processing for an energy-efficient and low-carbon economy, 2010 [Internet]. Department of Energy; 2010 [cited 2024 Jul 24]. Available from: <u>https://www.osti.gov/biblio/1219340/</u>

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Key Takeaway

Achieving suitable joints or bonds between materials is crucial in energy systems, especially when traditional fusion welding techniques are not effective for dissimilar metals. Weld defects during the manufacturing stage can be the cause of many failures in service. These include porosity, inclusions, lack of fusion, shrinkage cracks, and internal stress. Myriad aspects require consideration, such as base/weld material selection, welding process parameters, and post-weld heat treatments. Indeed, a branch of ICME has emerged, known as Integrated Computational Welding Engineering (ICWE), or ICME-W, to address the challenges associated with many highly coupled and nonlinear variables controlling the joint microstructure, properties, and performance.

There is a need for high-quality weld joints and improved methods for joining similar and dissimilar metals (e.g., aluminum and steel, or austenitic and ferritic steels) and other dissimilar materials, such as ceramic-ceramic and ceramic metal systems. While ceramics can theoretically be joined under some circumstances through fusion welding, this process is particularly challenging for metal-ceramic systems due to mismatches in composition, coefficients of thermal expansion (CTE), melting points, and thermal conductivities.

For SiC/SiC CMC composite-to-composite joining, several techniques such as diffusion bonding, hot press sinter bonding, electric current–assisted sintering (ECAS), transient liquid phase (TLP), among others, are promising routes for producing ceramic-ceramic joints in applications such as accident tolerant nuclear fuel cladding, which require hermetic seals in a variety of configurations with strength retention at high temperatures as well as high neutron flux. Ceramic composite cladding material is being considered as a replacement for the current zircaloy cladding to help improve the overall economics and performance of today's pressurized water reactors — and allow for longer response times at high temperatures in accident situations.⁷⁸

Key Takeaway

A more modern materials research approach for eliminating joints and interfaces is the concept of a functionally graded material (FGM) wherein a material's composition or microstructure and, hence, its properties change gradually with volume. FGMs could be designed for specific function and applications. Various techniques based on powder processing, preform processing, layer processing, and melt processing could potentially be used to fabricate FGMs.

When different metals must be joined, it is essential to avoid forming detrimental brittle intermetallic compounds or precipitates within the joint, as these can lead to failures under high-stress conditions, such as creep. The use of lightweight metals in automobiles and aerostructures is also constrained by challenges in joining and repairing metals, as well as issues with corrosion resistance and durability in high-friction environments. The most common class of welding technique is fusion welding. Within this class, concentrated focused energy sources such as lasers (LBW) and electron beams (EBW) can be used to produce high-precision narrow welds. While these are expensive techniques (particularly, EBW), they are much faster and more repeatable than conventional arc welding and they can be automated. EBW produces deeper penetrating welds and smaller heat affected zones (HAZ) than LBW, making it ideal for high-strength joints in critical applications. Moreover, a variant known as localized electron beam welding (LEBW) is not constrained to smaller workpiece sizes that fit within the vacuum chamber housing the electron gun.

Both EBW and LBW can be used for nickel- and cobalt-based super alloys with proper weld joint preparation and fit up. The welding of nickel- and cobalt-based-based superalloys, commonly used in turbine blades, waste incinerator boilers, seals, turbocharger rotors, and high temperature fasteners, is traditionally complicated by liquation cracking and microstructural segregation. However, there are some remaining technical barriers

⁷⁸ Office of Nuclear Energy. This new fuel cladding could transform nuclear fuels [Internet]. Department of Energy; 2024 [cited 2024 Jul 24]. Available from: <u>https://www.energy.gov/ne/articles/new-fuel-cladding-could-transform-nuclear-fuels</u>

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preventing EBW from reaching its full potential in other energy applications, such as welding in nuclear reactor pressure vessels (RPVs). Existing large RPVs in PWRs and BWRs are fabricated from stacked rings (single piece forgings or split bent sheet forgings) welded together. These hurdles include the need for preheating high carbon RPV steels (to reduce residual stress and distortion), the lack of EB weld repair methods, nondestructive evaluation methods, and proven surface techniques.

Key Takeaway

Diffusion bonding is a high temperate, low-to-moderate pressure solid-state joining technique that can provide favorable joints (i.e., exhibiting high strength and dimension control) to nickel- and cobalt-based superalloys— although voids, interfacial precipitates, and surface oxides present challenges. Techniques such as EFAS and hot isostatic pressing capable of simultaneously applying uniaxial pressure and heat can be used for diffusion bonding materials. In addition to superalloys, diffusion bonding finds many applications with a variety of other metals (e.g., refractories) as well as ceramics used in harsh environments, including steels, titanium, intermetallic phases, tungsten, MMCs, copper, aluminum, magnesium, oxide and carbide ceramics, silicon nitride, and zirconium diboride composites. Diffusion bonding carries the disadvantage of lower production volume throughput due to long diffusion times and stringent surface preparation (cleanliness and roughness) requirements.

Novel approaches have recently been used for diffusion bonding ceramics, which utilize EFAS in combination with hot isostatic pressing (HIP) in a two-step process to achieve high temperature and sufficient pressure in cases where poor surface quality (i.e., roughness) precludes the use of EFAS alone.⁷⁹

Similar to diffusion bonding, solid-state friction stir welding (FSW) also does not require any filler materials. Although FSW is conducted at a low ambient temperature, the frictional heat produced at the welding line by a rotating tool plunged into the materials allows for a solid-state joining method in which the severe plastic deformation experienced by the metals soften them without melting. While the tool is traversed along the joint line, it mechanically intermixes and joins the pieces of metal. Compared with fusion welding, friction stir welds have a more homogeneous grain structure and better mechanical properties such as tensile strength, hardness, and toughness. Additionally, the lower temperature melt-free nature of the solid-state process carries the advantage of avoiding the occurrence of unfavorable phase transformations in the weld and a reduction in the heat affected zone (HAZ). Thus, one potentially attractive harsh environment area of interest for FSW involves the joining of ODS steels in future Gen IV nuclear fission reactors, as well as nuclear fusion reactors. Traditional fusion-based welding would be expected to severely adversely impact the nano-oxide dispersion along the joint. Carried out at temperatures below the melting point, by comparison, FSW would be anticipated to largely, albeit not entirely, avoid this issue. Linear friction welding (LFW) offers the further advantage of near-net shaping (i.e., welding materials for special shaped components) without limitations on interface geometry, unlike the more established and widely used rotary friction welding (RFW). However, both friction welding methods still face challenges, particularly in joining thin-walled components.

FSW was originally adopted for lower melting metals like aluminum, magnesium, and copper alloys using highspeed steel FSW tools and is now quite widely used with aluminum in the aerospace, automotive, and railway industries. It has also been used with titanium. In recent years, significant progress has been made with friction stir welding of steels and nickel superalloys, but the joining cost is still high. Implementing FSW for high melting point alloys is quite challenging primarily due to the tool wear, which requires refractory metal (e.g., tungsten) or hard ceramic (e.g., cubic boron nitride) tools. One of the best methods to attain a prolonged FSW tool life is a hybrid approach, where preheating or in-situ heating techniques are used to soften the weld region before the tool is plunged into the material, reducing its wear rate.

⁷⁹ Cohen S, Barak Ratzker, Sergey Kalabukhov, Nachum Frage. Diffusion bonding of transparent ceramics by spark plasma sintering (SPS) complemented by hot isostatic pressing (HIP). Journal of the European Ceramic Society [Internet]. 2023 Nov 1 [cited 2024 Jul 24];43(14):6628–33. Available from: https://doi.org/10.1016/j.jeurceramsoc.2023.06.071

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Key Takeaway

The FSW concept has given rise to friction stir additive manufacturing (FSAM) and additive friction stir deposition (AFSD), which are subsets of solid-state metal additive manufacturing (SSMAM) that could be scaled to produce large area, multi-layered components in a plate addition fashion using FSW. Because of the solid-state nature of these SPD processes, the fabricated parts have ultra-fine grained (UFG) equiaxed microstructures, which lead to better mechanical properties (forged-like strength is possible) with less residual stresses and fewer solidification defects when compared to existing fusion-based additive manufacturing processes.

Another solid-state process, which was originally used as a coating deposition method (and still has applications in this space) that has now gained attention as a potential cost-effective fabrication route to nickel-based superalloys is cold spray additive manufacturing (CSAM). At this time, CSAM nickel alloys still suffer from inferior mechanical properties compared to other fusion-based AM nickel alloys, but this can be somewhat alleviated with post-processing heat treatments.

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3. Resource Allocation over the Five Landscape Focus Areas

In the past, AMMTO's predecessor office, the Advanced Manufacturing Office (AMO), categorized and considered harsh environment materials R&D funding based strictly on the types of environments experienced by components while in service (e.g., high temperatures, irradiation, corrosive media, etc.). However, as was discussed in the prior section, most energy applications involve coupled or multiple material stressors. Therefore, while consideration of the material stressors present in any given application is obviously critical to material selection and for the design of new components for use in the application, an environment-centric strategy is not fully adequate from an R&D investment perspective. Instead, a much more fruitful way to identify high-impact harsh environment materials related R&D opportunities begins with considering the crosscutting strategic goals outlined earlier in this landscape for advanced materials and manufacturing technologies. The overarching goal is to use advanced high-performance materials and manufacturing technologies to enable more energy efficient and cost-competitive forms of energy production/conversion, utilization, and storage, for which the material stressors are already known. It is then a straightforward matter of determining the objectives that will allow us to achieve these goals.

Identifying and investing in opportunities with the greatest potential for impact is extremely important to provide abundant and secure energy that the United States and the world will increasingly require. The prioritization methodology discussed in the Introduction section identified in a semi-quantitative manner the opportunities with the greatest impact and reach potential for each of the focus areas. The basis for selecting the five focus areas into which the opportunities are bucketed originated from a decade earlier multi-phased innovation impact study contracted to TMS through Oak Ridge National Laboratory in cooperation with ASM International and The Energy Materials Initiative. These focus areas were initially identified by the Energy Materials Blue Ribbon Panel in earlier phases of the work. The phased TMS studies focused on identifying the most significant opportunities for materials innovation that could deliver substantial energy savings, environmental gains, and economic advantage to the United States over 2–10 years from the time it was published. Focused research and development efforts in the topics outlined in that report were expected to deliver large energy, environmental, and economic impacts.

Now in 2024, we utilize this same strategy to elucidate updated R&D pathways for energy production/conversion, efficient utilization, and storage technologies within the same innovation impact focus areas as well as specific breakthrough opportunities within the R&D pathways. These breakthrough opportunities have significant potential to once again help address the nation's energy, environmental, and economic needs. While each material or processing breakthrough opportunity has the potential to individually benefit the United States, the true impact will occur when these innovations come together and are applied to energy sectors at scale.

The five focus areas, as originally described in the TMS study, are:

Focus Area 1: Functional Surface Technologies: Tomorrow's energy systems will require material surfaces that can effectively interact with service environments and withstand demanding operating conditions. Materials that can serve specific functions—such as speeding reaction times, capturing photons, and separating gases—can increase system efficiency.

Focus Area 2: Materials Integration into Energy Systems: Current and emerging energy systems are composed of different classes of materials that must work together to achieve desired system structure and functionality. Materials science and engineering advances have the potential to enable the integration of new materials and the effective interfacing of materials combinations as systems become more complex and service environments become more demanding.

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Focus Area 3: Higher-Performance Materials: For many energy systems, the path to realizing greater energy efficiency brings extreme conditions that today's materials cannot withstand, such as higher temperatures, more intense radiation, greater wear, or more corrosive environments. Higher-performance materials that can maintain their chemical, physical, and mechanical properties while increasing component and system life under extreme conditions can effectively enhance the efficiency of energy systems

Focus Area 4: New Paradigm Materials Manufacturing Processes: Materials manufacturing is fundamentally energy-intensive and often wasteful of resources. Process innovations and novel synthesis methods that minimize energy and material losses can improve manufacturing process efficiency and cost-effectiveness, ultimately enabling greater competitiveness in the U.S. manufacturing sector.

Focus Area 5: Materials and Process Development Acceleration Tools: Materials and process development tools, including computational modeling and data visualization, are critical to understanding the nature of materials, preventing detrimental defects and faults, and simulating system performance. Ultimately, developing and using these tools will help reduce the cost and time necessary to facilitate materials discovery and development.

For each focus area section below, specific technology opportunities are discussed. At the start of each section, an action plan is given that lays out the scope of technologies of interest, their current technoeconomic barriers as well as challenges that need to be addressed to overcome those barriers. Stakeholder roles and benefits are given. The action plans are followed by tables giving the current TRL of the specific identified technology challenges/opportunities (in order of deceasing impact factor) and the pace of TRL advancement needed (last column) to progress each technology's TRL to a state of completion through level 7 (i.e., entering TRL 8) by 2035. Thus, some challenges mut be addressed more aggressively than others, dependent on their current TRL. Most AMMTO projects seek to advance the TRL by a one-to-two step increase over a three-year period of performance. Thus, R&D should begin around 2025 for any high impact opportunity currently at TRL 3 or lower to attain completion of TRL 7 (i.e., enter TRL 8) by 2035. High impact opportunities currently at TRL 5 or higher could begin as late as 2030 to complete TRL 7 by 2035.

Most opportunities explicitly discussed in the following Focus Area sections are those that exist on the right side of the Opportunity potential vs. Effort plot (Figure 5), as denoted by the Location column in the tables. In this way, high-impact opportunities are easily identified in the tables for prioritization, although some may take more effort and resources than others, primarily based on the current TRL level as just described in the preceding paragraph.

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Figure 6. 2025-2030 timeline for covered challenges across the various focus areas with coding according to associated energy and application spaces.

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ROADMAP TO ADVANCE HIGH IMPACT MATERIALS RESEARCH FOR HARSH ENVIRONMENTS



Figure 7. 2030-2035 timeline for covered challenges across the various focus areas with coding according to associated energy and application spaces.

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3.1 Focus Area 1: Functional Surface Technology Recommendations

The action plan table below lists several details that should be used to inform funding strategies for next generation coatings and coating process research and development investments, as well as describing the roadblocks with the existing state of the art and challenges to be addressed for functional surface technologies. Specific opportunities with associated timelines follow the action plan.

Neglecting this R&D could have adverse implications across various energy technologies

More costly alternative solutions: Without the application of protective coatings, linings, claddings, and surface engineering (e.g., peening), where possible, the more extreme environments anticipated in future energy technologies will force our reliance on more expensive solutions—if they can be found—involving superior base materials that can survive unaltered and without thermal or environmental barrier coatings or anti-wear (tribological) coatings.

Action Plan for Focus Area 1

Table 3. Action Plan for Functional Surface Technologies.

Scope								
Surface technologies for improved component performance and/or durability in harsh service environments Coatings, cladding, films, self-healing surfaces, and engineered surface features that ser thermal or environmental barriers to protect the underlying base/substrate material form a by various agents encountered in the harsh environments of energy production/conve- utilization, and storage technologies.								
Technologies of Interest:	PVD, CVD, electrodeposition, cold spraying, laser cladding, friction surfacing, and multi-layer/multifunctional systems.							
Roadblo	ocks	Challenges to pursue						
 Oftentimes, incomplete knowled mechanism High cost associated with the la Coating/substrate incompatibilit Requirements for multiple differ Requirement for flawless (defection) 	lge of surface degradation Irge-scale deposition. y ent layers t-free), impermeable coatings.	 Modeling and simulation of surface degradation mechanisms Advanced deposition techniques Implementation of smart manufacturing methodologies to lower cost, and to monitor and optimize coating processes. 						
Stakeholders and Potential Roles								
Stakeholder	Role							
Product Manufacturers/Suppliers	 Synthesize and deposit high-quality protective coatings/cladding/films on base/substrate materials. Innovate in performance modeling and testing, manufacturing qualification. 							
End Users/Original Equipment Manufacturers (OEMs)	 End-use industries will benefit when technical roadblocks are overcome and field certification is completed. These end-use industries include the power generation and handling industries. Hydropower and geothermal industries are looking for hard coatings for wear, erosion, and cavitation resistance. The nuclear power industry is seeking molter salt and liquid sodium corrosion resistant materials as well as high-temperature, irradiation resistant materials. The hydrogen-based energy economy needs hydrogen- embrittlement resistant materials. 							

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ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C14	2565	Develop multi-material multifunctional claddings/coatings and FGMs for surface protection from attack by multiple mechanisms.	LR	e.g., Oxidation resistance at OT > 750°C	6	1	
C12	435	Extend the life of components and materials operation under harsh environments through improved coating/repair technologies.	LR	Repair depth > 10 mm	5	1.5	
C79	279	Improve structural materials exhibiting suitable molten salt and liquid metal corrosion resistance at high temperatures	UR	OT > 700-750°C	3	2.5	
C27	208	Develop coatings for material protection in molten salt applications.	UR	OT > 700°C	3	2.5	
C23	192	Develop complex multi-functional and stable coatings for variety of combined operating conditions/coupled materials stressors	LL	Properties exceeding WC coatings, Local OP > 7000 atm	6	1	
C126	94	Develop low cost SiC Fiber materials for use in Fission and Fusion reactor applications.	LL	> 75% reduction in \$ of SiC fiber	6	1	
C4	92	Develop materials and surface technologies with adequate contact and bending fatigue life for bearings, gears and shaft in wind turbine gearbox components.	LL	Enable 20-30-year lifetime	6	1	
C61	80	Develop sensor and protective coatings to mitigate hydrogen embrittlement of metallic structures and parts.	LR	Hydrogen permeability of < 10^-15 mol/s/m/Pa^0.5 at OT = 400-500°C	4	2	
C92	63	Develop component materials for highly corrosive and deposit forming geothermal brines.	LL	<u>QpH</u> = 2 or 12	4	2	(M)
C17	51	Develop energy efficient surface engineering process for component performance enhancement.	LR	Corrosion resistance better than AISI 300 series	4	2	
C39	50	Develop protective coatings to mitigate hydrogen embrittlement of metallic structures and parts.	UR	Hydrogen permeability of < 10^-15 mol/s/m/Pa^0.5 at OT = 400-500°C	4	2	
C11	42	Develop coatings and surface technologies for journal and thrust bearings in hydropower plant to enable frequent start and stop operating cycles for more flexible operations.	UL	Self-lubricating bearings	3	2.5	
C24	34	Develop abrasion resistant coatings for large wind turbine blades (critical for offshore blades).	LL	Erosion resistance at blade tip speeds > 300 KM/hr.	6	1	
C49	34	Develop advanced ceramic or composite coating to reduce hydrogen losses and improved fire safety in pipelines.	UL	Reduce losses by 50%	3	2.5	
C110	25	Develop surface modifications to improve high temperature performance (oxidation, corrosion, erosion, wear) of low-cost metallic materials.	LR	Oxidation resistance at OT > 425°C	5	1.5	
C25	17	Develop extreme environment coatings designed for recyclability with base part material.	UR	Recyclable with base material	3	2.5	
C60	15	Develop transportation of hydrogen enriched natural gas in the existing pipeline.	UL	Reduce losses by 50%	2	3	
C57	10	Develop surface technologies and coatings for high pressure compression of H2 and CO2 for pipeline transport.	LL	Reduce losses by 50%	5	1.5	

Table 4. Challenges identified for FA1 with potential impact and effort (pace of TRL advancement) needed.

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Manufacturing of Foundational Material Systems and High Temperature Fluid Transfer and Storage Coatings for Molten Salt and Liquid Metal Protection

Improve structural materials exhibiting suitable molten salt and liquid metal corrosion resistance at high temperatures (C79)

Molten salt and liquid metals are key for various energy production and storage applications due to their unique physical and thermal properties. Chloride and fluoride salts are under consideration for Gen-IV molten salt reactors,^{80,81,82} where they could serve as a coolant (in the temperature range of 500 to 900°C) for solid-fueled reactors or as a material that simultaneous acts as both a solvent and coolant for the nuclear fuel. Molten salts are attractive in these applications because they can operate at higher temperatures under ambient pressure for more efficiency, along with offering other safety and sustainability advantages. Liquid Na and Pb are being explored for Gen-IV sodium and lead-cooled fast reactors,⁸³ Li, PbLi, FLiBe (i.e., LiF-BeF₂), for fusion reactors,^{84,85} and nitrate and chloride salt for CSP applications.⁸⁶ In various experiments over the years, nickel alloys with lower chromium contents such as Hastelloy N, Haynes 230, Haynes 244, and Inconel 800 have been used as prototype structural materials due to their superior corrosion resistance in molten fluorides.

Other energy-relevant applications for molten salts include nuclear fuel reprocessing, metallurgical and materials processing (e.g., heat treating/annealing of steel, ceramic powder synthesis), batteries, and thermal energy collection, transport, and storage. In fact, due their importance to DOE, an Office of Science Energy Frontier Research Center (EFRC) for Molten Salts in Extreme Environments (MSEE) was established in 2018, led by Brookhaven National Laboratory (BNL) with partners ORNL, INL, Stony Brook University, the University of Iowa, and the University of Notre Dame. The EFRC was renewed for four years in 2022. One of its three fundamental research thrusts is the exploration of the dynamic properties of molten salts in bulk and at interfaces with other materials in order to develop an increased understanding of their physical and chemical properties for better prediction and control of materials corrosion in a variety of applications.

⁸⁰ International Atomic Energy Agency. Status of Molten Salt Reactor Technology. IAEA Technical Reports [Internet] International Atomic Energy Agency; 2023 [cited 2024 Jul 29]; Series No. 489. Available from: <u>https://www.iaea.org/publications/14998/status-of-molten-salt-reactor-technology</u>

⁸¹Serp J, Allibert M, Benes O, Delpech S, Feynberg O, Ghetta V, Heuer D, et al. The molten salt reactor (MSR) in generation IV: overview and perspectives. Progress in Nuclear Energy [Internet]. 2014 Nov [cited 2024 Jul 29]; 77: 308-319. Available from: https://doi.org/10.1016/j.pnucene.2014.02.014

 ⁸² Le Brun C. Molten salts and nuclear energy production. J. Nucl. Mater. [Internet] 2007 Jan [cited 2024 Jul 30];
 360: 1-5. Available from: <u>https://doi.org/10.1016/j.jnucmat.2006.08.017</u>

⁸³National Academies of Sciences, Engineering, and Medicine. Laying the foundation for new and advanced nuclear reactors in the United States. [Internet] The National Academies Press; 2023 [cited 2024 Jul 30]. Available from: https://nap.nationalacademies.org/catalog/26630/laying-the-foundation-for-new-and-advanced-nuclear-reactors-in-the-united-states

⁸⁴ Ihli T, Basu TK, Giancarli LM, Konishi S, Malang S, Najmabadi F, Nishio S, et al. Review of blanket designs for advanced fusion reactors. Fusion Engineering and Design [Internet] 2008 Dec [cited 2024 Jul 30]; 83 (7-9): 912-919. Available from: https://doi.org/10.1016/j.fusengdes.2008.07.039

⁸⁵Raffray AR, Akiba M, Chuyanov V, Giancarli L, Malang S. Breeding blanket concepts for fusion and materials requirements. J. Nucl. Mater. [Internet]. 2002 Dec [cited 2024 Jul 30]; 307-311(Part 1): 21-30. Available from: <u>https://doi.org/10.1016/S0022-3115(02)01174-1</u>

⁸⁶ Ding W, Bauer T. Progress in research and development of molten chloride salt technology for next generation concentrated solar power plants. Engineering [Internet]. 2021 Mar [cited 2024 Jul 30]; 7(3): 334–347. Available from: <u>https://doi.org/10.1016/j.eng.2020.06.027</u>

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A key technological challenge limiting operating temperature and system performance is the compatibility of structural materials with the molten salt or liquid metal fluids.^{87,88} In addition to developing new materials with intrinsic resistance to these fluids, coatings offer another promising opportunity to reduce the corrosion degradation in these media of high-strength, high-temperature alloys (for more information on this, see C27 immediately following). For example, various AI, Ni, and Cu coatings have been successfully tested at temperatures up to 700°C in molten salt (see Figure 8a).^{89,90} AI-based coatings can form an (AI,Li)-rich semi-protective oxide layer in Licontaining liquid metals such as PbLi.^{91,92}

The long-term compatibility of coatings with both the molten salt/liquid metal and substrate at temperatures greater than 700°C in realistic conditions remains a major challenge. Multi-layer coatings and functionally graded structures offer unique opportunities for the fabrication of stable multi-functional coatings compatible with molten salts and liquid metals.

Current roadblocks limiting the deployment of coatings for molten salt and liquid metal applications include:

- Complexity of the corrosion degradation mechanisms in flowing fluids with dissolution and redeposition depending on the hot and cool areas, with corrosion rate highly dependent on the salt chemistry and impurities present.
- Lack of understanding on the impact of irradiation on liquid metal and molten salt compatibility.
- Additional coating requirements such as irradiation or wear resistance.
- Cost associated with the large-scale deposition of coatings made of expensive elements such as Mo and Ni.
- Difficulty related to depositing multi-material functional coatings.
- Low state of technology development associated with moving from coating small coupons to coating structures needed for flowing experiments, such as tubing with inner diameter of ~1m.
- Low availability of molten salts of well-controlled chemistry.
- Safety concerns associated with molten salts and liquid metals production and handling.

A broad range of research opportunities exist to overcome these limitations:

⁸⁷ Kelleher BC, Gagnon SF, Mitchell IG. Thermal gradient mass transport corrosion in NaCl-MgCl₂ and MgCl₂-NaCl-KCl molten salts. Materials Today Communications [Internet]. 2022 Dec [cited 2024 Jul 30]; 33: 104358. Available from: <u>https://doi.org/10.1016/j.mtcomm.2022.104358</u>

⁸⁸ DeVan JH. Compatibility of structural materials with fusion reactor coolant and breeder fluids. J Nucl Mat [Internet]. 1979 Dec [cited 2024 Jul 30]; 85-86 (Part 1): 249-256. Available from: <u>https://doi.org/10.1016/0022-3115(79)90499-9</u>

⁸⁹ Fähsing D, Oskay C, Meißne TM, Galetz MC. Corrosion testing of diffusion-coated steel in molten salt for concentrated solar power tower systems, Surf Coat Tech. [Internet]. 2018 Nov [cited: 2024 Jul 30]; 354: 46–55. Available from: <u>https://doi.org/10.1016/j.surfcoat.2018.08.097</u>

⁹⁰ Weinstein M, Falconer C, Doniger W, Bailly-Salins L, David R, Sridharan K, et al. Environmental degradation of electroplated nickel and copper coated SS316H in molten FLiNaK salt. Corros. Sci. [Internet]. 2021 Oct [cited 2024 Jul 30]; 191;109735. Available from: <u>https://doi.org/10.1016/j.corsci.2021.109735</u>

⁹¹ Wulf SE, Krauss W, Konys J. Long-term corrosion behavior of Al-based coatings in flowing Pb–15.7Li, produced by electrochemical ECX process. Nuclear Materials and Energy [Internet]. 2018 Aug 1 [cited 2024 Aug 27]; 16:158–62. Available from: <u>https://doi.org/10.1016/j.nme.2018.06.019</u>

⁹² Romedenne M, Zhang Y, Su YF, Pint BA. Evaluation of the interaction between SiC, pre-oxidized FeCrAlMo with aluminized and pre-oxidized Fe-8Cr-2W in flowing PbLi. J. of Nuclear Materials [Internet]. 2023 Aug [cited 2024 Jul 30]; 581: 154465. Available from: <u>https://doi.org/10.1016/j.jnucmat.2023.154465</u>

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- Significant improvements have been made in understanding and modeling degradation in molten salt and liquid metals.⁹³ These improvements open new opportunities for the design of alloys compatible with these fluids using approaches described in Focus Areas 3, 4, and 5.
- New thermo-kinetics modeling tools have been developed to design stable multi-layer coatings or graded structures stable at high temperatures, which could be used for molten salt and liquid metal applications (see Figure 8b).
- Growing interest from industry is leading to the development of new molten salt and liquid metal facilities for production and testing.

Success will be measured through the development, testing, and validation of coatings stable at temperatures >700°C in flowing molten salts or liquid metals. The power generation and storage industries will benefit, as will the coating and feedstock companies that support these technologies. The sequence of research (R&D pathway) will start with the development and testing of new materials and coatings showing limited degradation in static and flowing molten salt/liquid metal for up to ~1,000 hours. This will be followed in the 2030–2035 timeframe by demonstration of the long-term performance of the coatings in realistic conditions (e.g., high flow rates, thermal cycling, irradiative environments).





Develop coatings for material protection in molten salt applications (C27)

As used in the energy, aerospace, automobile, manufacturing, and electronics industries, among others, high temperature materials can be polymers, ceramics, composites, cermets, metal matrix composites, metals, and alloys. What is considered a high temperature material varies depending on the material class and application. For instance, polymers used as seals in EGS high temperature wells need only be stable at temperatures as low as 200°C to 300°C,⁹⁴ while refractory materials like hafnium carbide can be used in environments with temperatures of

⁹⁴ Zeldin A, Kukacka LE, Carciello N. Polymer systems in geothermal applications. J of App Poly Sci [Internet] 1979 Jun [cited 2024 Jul 30]; 23(11): 3179-3191. Available from: <u>https://doi.org/10.1002/app.1979.070231104</u>

⁹³ Pillai R., Sulejmanovic D., Lowe T., Raiman, S.S., Establishing a Design Strategy for Corrosion Resistant Structural Materials in Molten Salt Technologies. JOM [Internet]. 2023 Jan;75, 994-1005. Available from: <u>https://doi.org/10.1007/s11837-022-05647-9</u>

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4,000°C.^{95,96,97,98} Some researchers have defined high temperature materials generally as those that can withstand temperatures above 540°C.^{99,100,101,102,103}

High-temperature materials are typically exposed to other stressors in addition to high temperature. For example, high temperature materials also commonly encounter some combination of high stress/loads, highly oxidizing species, corrosive fluids, and irradiation. Consequently, most, if not all, high temperature materials are engineered to resist several degradation mechanisms simultaneously. These materials are usually required to have a long service life, with appreciable safety margins, for safe plant and component operations and to recoup initial investment in the material within a reasonable amount of time. With higher service temperatures, materials' service lives tend to be shorter. However, the deployment of higher temperature materials facilitates higher thermal efficiencies in energy systems such as ultra-supercritical coal plant operations that use supercritical fluids at temperatures exceeding 700°C.^{104,105,106,107}

Known roadblocks for the development and manufacturing of high temperature materials include knowledge gaps in:

- The development of techniques and feedstocks optimized for cost-effective advanced manufacturing of materials that can function reliably at temperatures greater than 700°C. How to manufacture MAX phase feedstock and materials in a cost-effective way is one such knowledge gap.
- Knowledge gaps in Developing cost-effective high temperature materials, including refractory alloys, that can withstand highly oxidizing or corrosive molten salt environments for nuclear, solar (CSP), and other applications. These materials must also resist creep-fatigue and/or irradiation damage, depending on the application.
- Cost-effective industrial scale-up to manufacture high temperature materials.
- The development of materials that effectively resist the extreme plasma environments (first wall) in fusion reactors.
- The development of elastomeric materials required for seals in EGS high temperature wells, specifically, those that can function at temperatures between 200°C and 350°C.

⁹⁹ Simić M, Alil A, Martinović S, Vlahović M, Savić A, Husović TV. High temperature materials: properties, demands and applications. Hemijska industrija [Internet]. 2020 [cited 2024 Jul 30]; 74(4): 273-284. Available from: <u>https://doi.org/10.2298/HEMIND200421019S</u>

¹⁰⁰ Meetham GW, Van de Voorde MH. Materials for high temperature engineering applications. 1st edition. Berlin Heidlberg: SpringerVerlag; 2000.

- ¹⁰¹ Gupta OP. Elements of Fuels, Furnaces, and Refractories. 6th edition, New Delhi: Khanna Publishers; 2014. ¹⁰² Schacht CA. Refractories Handbook. 1st edition, New York, NY: Marcel Dekker, Inc.; 2004.
- ¹⁰³ Bengisu M. Engineering Ceramics. 1st edition, Berlin Heidelberg: Springer-Verlag; 2001.

¹⁰⁴ Huang EW, Liaw PK. High-temperature materials for structural applications: new perspectives on high-entropy alloys, bulk metallic glasses, and nanomaterials. MRS Bulletin [Internet] 2019 Nov [cited 2024 Jul 30]; 44: 894. Available from: <u>https://doi.org/10.1557/mrs.2019.257</u>

¹⁰⁵ Chu S, Majumdar A. Opportunities and challenges for a sustainable energy future. Nature [Internet]. 2012 Aug [cited 2024 Jul 30]; 488: 294. Available from: <u>https://doi.org/10.1038/nature11475</u>

¹⁰⁶ International PE. Critical thinking: Ultra and supercritical technology focus [Internet]. Power Engineering International. 2017 [cited 2024 Jul 30]. Available from: <u>https://www.powerengineeringint.com/coal-fired/critical-thinking/</u> thinking/https://www.powerengineeringint.com/coal-fired/critical-thinking/

¹⁰⁷ Myllyvirta L. How much do ultra-supercritical coal plants reduce air pollution? [Internet]. Energy Post. 2017 [cited 2024 Jul 30]. Available from: <u>https://energypost.eu/how-much-do-ultra-supercritical-coal-plants-really-reduce-air-pollution/</u>

⁹⁵ Pierson HO. Handbook of chemical vapor deposition (CVD): principles, technology, and applications. Noyes Publication; 1992.

⁹⁶ Husted R. Periodic table of elements: Los Alamos National Laboratory [Internet]. Lanl.gov. 1992. [updated: 2011, cited: 2024 Jul 30]. Available from: <u>https://periodic.lanl.gov/72.shtml</u>

⁹⁷ McGraw-Hill encyclopedia of science and technology: an international reference work in fifteen volumes including an index. Colume 6. New York: McGraw-Hill; 1977.

⁹⁸ Hafnium [Internet]. Encyclopedia Britannica [cited 2024 Jul 30]. Available from: https://www.britannica.com/science/hafnium

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- Knowledge gaps in the development of abrasion and corrosion-resistant coatings with optical properties. Such materials include those suitable for drill heads for very deep superhot geothermal rock to enable supercritical geothermal plant deployment. Knowledge gaps also exist for development of super-hard materials suitable for ball bearings, as well as abrasion resistance, when operating in extreme environments.
- Development of suitable ceramic and metal matrix composites for structural and primary pressure boundary applications.
- How to effectively deploy machine learning and artificial intelligence tools for efficient formulation and manufacturing of high temperature materials, especially when those materials must be exposed to other extreme conditions of pressure/stress and highly oxidizing/corrosive environments.

Crosscutting research opportunities include:

- The development of materials that resist high temperature and corrosion (oxidation) induced degradation in operating conditions of 700°C–1,000°C. The knowledge gained from the development of these materials can be further leveraged to develop irradiation-resistant materials.
- The development of feedstock optimized for advanced manufacturing of extreme temperature materials. The techniques for developing the temperature classes of materials highlighted above are expected to be similar to those for developing higher melting point feedstock materials.
- The development of high temperature materials will contribute to lowering energy generating costs, through lower OpEx and the ability to run the plants and system at higher temperatures and efficiencies.

The capabilities necessary to achieve applicable target metrics and DOE emissions/energy goals include:

- Science-based engineering approaches to help design application-appropriate, cost-effective high temperature materials.
- The deployment of machine learning (ML) to gather and leverage vast datasets that have been compiled in the past on alloys, materials chemistry, materials behaviors and characteristics, including those associated with manufacturing processes and pathways.
- Development of competitive industrial-scale manufacturing to support deployment of successfully developed alloys.
- In situ monitoring capabilities to support manufacturing processes.

The successful development and deployment of these HEMs will reduce the operating cost of plants and the manufacturing cost of components. More durable materials will allow for reduced inspection intervals as well as less frequent repair, replacement, and associated downtime. Success will be measured by the number of early industry adopters of the materials; by how many of those adopters are willing to help collect the necessary data to qualify and codify the materials or deployment; by the number of new technologies the materials make economically and technologically accessible; and by the extent to which the materials reduce the cost of currently deployed technologies. Industries likely to benefit include U.S. utilities, power generation equipment manufacturers, and energy storage equipment companies.

To achieve DOE goals, a deliberate R&D pathway must be established. Materials development activities come first, followed closely by or with concurrent development of the techniques to manufacture this class of materials and the accompanying feedstock. In the 2025–2030 timeframe, the R&D community must pursue creep- and irradiation-resistant materials for molten salt and liquid metal cooled reactors, SiC materials (fiber) for fusion applications, high temperature materials for hydrogen production, high temperature materials for geothermal and EGS, and sintering technologies for highly reactive high temperature materials. Between 2030–2035, high temperature materials for molten salt applications and high temperature abrasion resistant materials should be pursued. By 2035–2040, the R&D community should pursue high temperature plasma-facing materials for fusion energy applications and high temperature materials for fusion energy applications and high temperature materials for fusion energy applications.

This R&D pathway ensures that the product from one stage of research will be leveraged at a subsequent stage, as described above for nuclear power production. Gen-IV Molten salt and liquid sodium cooled reactors are potential game-changers that could enable safer, more cost-competitive and more sustainable nuclear power.
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Develop complex multi-functional and stable coatings for variety of combined operating conditions/coupled materials stressors (C23)

Key classes of high-temperature materials such as Ni-based superalloys, refractory alloys, SiC-based CMCs, ODS alloys (e.g., Ni-Cr based Inconel MA754 and Fe-Cr based Incoloy MA956), HEAs, etc., are of interest for a broad range of thermal power plant applications due to their superb high-temperature oxidation, corrosion, and creep resistance. Many of them will, however, require coatings specific to environmental conditions. SiC-based CMCs have demonstrated great potential at high temperatures with superior specific strength. In addition to high toughness, there is a need for protection against H₂O-rich environments in H₂-fired gas turbines,¹⁰⁸ supercritical water in nuclear plants,¹⁰⁹ or impurities in liquid metal systems for fusion and fission applications.¹¹⁰ Refractory multi-principal element alloys offer superior strength at very high temperature, but they suffer from poor oxidation resistance and developing EBC compatible with relevant environments (steam, CO₂, impure molten salt) is imperative.¹¹¹ Some classes of materials considered for structural applications also have a great potential as coatings. For wear and erosion resistance at various temperatures, multi-principal element carbide or nitride alloys have demonstrated excellent hardness properties up to 1300°C.¹¹²

In addition to traditional deposition techniques such as sputtering and CVD, new deposition methods such as laser cladding or friction surfacing are being explored.^{113,114} Research on multi-component rare earth oxides is also needed to develop the next generation of EBCs.¹¹⁵ While EBCs have been studied for decades for gas turbine applications, EBCs and TBCs could offer protection in other harsh environments such as molten salts, while potentially lowering the substrate in service temperature. Compatibility with conventional structural substrates such as steels and Ni-based superalloys is often challenging for multi-principal element coatings, but multi-material multi-layer coatings or graded structures are promising solutions.

Another class of advanced alloys very promising as coatings is oxide dispersion strengthened (ODS) alloys. The fine dispersion will harden the surface and ensure protection against erosion and wear at very high temperatures,

¹⁰⁸ Turcer LR, Padture NP. Towards multifunctional thermal environmental barrier coatings (TEBCs) based on rare-earth pyrosilicate solid-solution ceramics. Scr Mater [Internet]. 2018 Nov [cited 2024 Jul 30]; 154: 111–117. Available from: <u>https://doi.org/10.1016/j.scriptamat.2018.05.032</u>

¹⁰⁹ Park JY, Kim IH, Jung YI, Kim HG, Park DJ, Weon-Ju Kim WJ. Long-term corrosion behavior of CVD SiC in 360°C water and 400°C steam. J of Nucl Mat [Internet]. 2013 Nov [cited 2024 Jul 30]; 443: 603–607. Available from: <u>https://doi.org/10.1016/j.jnucmat.2013.07.058</u>

¹¹⁰ Yang X, Liu M, Gao Y, Zhang D, Feng S, Liu H, Yu G. Effect of oxygen on the corrosion of SiC in LiF–NaF–KF molten salt. Corrosion Sci [Internet]. 2016 Feb [cited 2024 Jul 30]; 103: 185-172. Available from: https://doi.org/10.1016/j.corsci.2015.11.014

¹¹¹ Yu Y-C, Poerschke DL. Design of thermal and environmental barrier coatings for Nb-based alloys for high temperature operation. Surf and Coatings Technology [Internet]. 2022 Feb [cited 2024 Jul 30]; 431: 128007. Available from: <u>https://doi.org/10.1016/j.surfcoat.2021.128007</u>

¹¹² Kirnbauer A, Kretschmer A, Koller CM, Wojcik T, Paneta V, Hans M, Schneider JM, et al. Mechanical properties and thermal stability of reactively sputtered multi-principal-metal Hf-Ta-Ti-V-Zr nitrides, Surf and Coatings Technology [Internet]. 2020 May [cited 2024 Jul 30]; 389: 25674. Available from: https://doi.org/10.1016/j.surfcoat.2020.125674

¹¹³ Yutao L, Hanguang F, Tiejun M, Kaiming W, Xiaojun Y, Lin Jian L. Microstructure and wear resistance of AlCoCrFeNi-WC/TiC composite coating by laser cladding. Materials Characterization [Internet]. 2022 May [cited 2024 Jul 30]; 194:112479. Available from: <u>https://doi.org/10.1016/j.surfcoat.2020.125674</u>

 ¹¹⁴ Zhu Q, Liu Y, Zhang C. Laser cladding of CoCrFeNi high-entropy alloy coatings: Compositional homogeneity towards improved corrosion resistance. Materials Letters [Internet]. 2022 Jul [cited 2024 Jul 30];
 318: 132133. Available from: <u>https://doi.org/10.1016/j.matlet.2022.132133</u>

¹¹⁵ Ridley MJ, Gaskins J, Hopkins P, Opila E. Tailoring thermal properties of multi-component rare earth monosilicates. Acta Mater [Internet]. 2020 Aug [cited 2024 Jul 30]; 195: 698–707. Available from: <u>https://doi.org/10.1016/j.actamat.2020.06.012</u>

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with Al-containing ODS alloys (e.g., Incoloy MA956) also offering improvement in oxidation/corrosion resistance via formation of a thin, highly adherent protective alumina surface layer.^{116,117} For thin components, the high creep strength of the coatings will enhance the composite structural integrity and improve its performance. If a very fine dispersion of nano oxide is achieved, the coating will be very compatible with high dose nuclear environments.¹¹⁸ A major advantage of ODS coating is their excellent compatibility with the substrate, since the coating chemistry can mimic the substrate chemistry, with a small addition of nano oxides.

Development of coatings for these foundational material systems or the use of these foundational material systems as coatings are hindered by:

- The rapid degradation of these materials in harsh environments requires flawless stable coatings
- Lack of material availability limiting coating fabrication and testing.
- Need for multi-layer coatings to ensure compatibility between coatings and substrates made of drastically different materials
- Cost of expensive coating elements such as refractory alloys, rare earth elements.
- Need for various industries to combine research efforts to reduce coating development cost.

Research opportunities to overcome the above limitations and accelerate the deployment of these foundational material systems include:

- New advanced deposition techniques allow the fabrication of multi-material coatings or graded structures for improved compatibility between substrates and coatings
- Improved understanding and modeling of the degradation mechanisms of these foundational material systems in various harsh environments
- In-situ reaction in O, C, or N-rich environments during the advanced deposition process allowing the formation of multi-principal element carbides or nitrides and ODS coatings¹¹⁹
- Government programs aiming at the development of these foundational material systems for multiple applications.

Success will be measured through the development of coatings allowing the use of these foundational alloy systems in multiple sectors and the deployment of foundational alloy coatings in several industries. Industries will benefit when technical roadblocks are overcome, including the power generation and handling industries. Hydropower and geothermal industries are looking for hard coatings for wear, erosion, and cavitation resistance. The R&D pathway will start with the development of advanced coatings for foundational alloy systems allowing their use in multiple industries (2025-2030). This will be followed by the fabrication of foundational alloy (2030-2035).

¹¹⁶ Bolelli G, Christoph Vorkotter C, Lusvarghi L, Stefania Morelli, Testa V, Vaßen R. Performance of wear resistant MCrAIY coatings with oxide dispersion strengthening. Wear [Internet]. 2020 May [cited 2024 Jul 30]; 444-445: 203116. Available from: <u>https://doi.org/10.1016/j.wear.2019.203116</u>

¹¹⁷ Dryepondt S, Unocic KA, Hoelzer DT, Massey CP, Pint BA. Development of low-Cr ODS FeCrAl alloys for accident-tolerant fuel cladding. J of Nucl Mat [Internet]. 2018 Apr [cited 2024 Jul 30]; 501: 59-71. Available from: <u>https://doi.org/10.1016/j.jnucmat.2017.12.035</u>

¹¹⁸ Ukai S, Fujiwara M. Perspective of ODS alloys application in nuclear environments. J of Nucl Mat [Internet]. 2002 Dec [2024 Jul 30]; 307–311: 749–757. Available from: <u>https://doi.org/10.1016/S0022-3115(02)01043-7</u>

¹¹⁹ Saptarshi S, Dejong M, Rock C, Anderson I, Napolitano R, Forrester J, Lapidus S, et al. Laser powder bed fusion of ODS 14YWT from gas atomization reaction synthesis precursor powders. JOM [Internet]. 2022 Aug [cited 2024 Jul 30]; 74: 3303-3315. Available from: <u>https://doi.org/10.1007/s11837-022-05418-6</u>

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Figure 9. Illustration of the experimental approach showing the dissolution of the Cr-rich oxide shell and stable Y-containing phases in the laser powder bed fusion (LPBF) melt pool and the in-situ reaction to form a homogeneous distribution of nano-scale Y–Ti rich oxides.¹²⁰

Hydrogen Embrittlement-Resistant Coatings

Develop protective coatings to mitigate hydrogen embrittlement of metallic structures and parts (C25)

Hydrogen has already been identified by industries and DOE as critical for the energy, industrial, and transportation sectors. The main challenges in realizing hydrogen's potential are infrastructure-related, namely, producing hydrogen in large volumes and ensuring its efficient transport and storage. The growing awareness of hydrogen's key role in the future of energy led to the H-Mat and HyBlend initiatives covering research and development on polymers and on low temperature metals (below 500°C) of interest for use in pressure vessels and pipelines.^{121,122,123}

Decades of research on the embrittlement of materials under pressurized hydrogen at room temperature have enabled the safety and reliability of hydrogen pipelines and storage infrastructure and has further led to the development of a *Technical Reference for Hydrogen Compatibility of Materials* from Sandia National

¹²⁰ Saptarshi S, Dejong M, Rock C, Anderson I, Napolitano R, Forrester J, Lapidus S, et al. Laser powder bed fusion of ODS 14YWT from gas atomization reaction synthesis precursor powders. JOM [Internet]. 2022 Aug [cited 2024 Jul 30]; 74: 3303-3315. Available from: <u>https://doi.org/10.1007/s11837-022-05418-6</u>

¹²¹ Department of Energy. Hydrogen from next-generation electrolyzers of water (H2NEW). [Internet] Department of Energy [cited: 2024 Jul 31]. Available from: <u>https://h2new.energy.gov/</u>

¹²² Abe, JO, Popoola API, Ajenifuja E, Popoola O.M. Hydrogen energy, economy and storage: Review and recommendation. International J of Hydrogen Energy [Internet]. 2019 Jun [cited 2024 Jul 30]; 44; 15072-15086. Available from: <u>https://doi.org/10.1016/j.ijhydene.2019.04.068</u>

¹²³ International Energy Agency. The future of hydrogen. [Internet] International Energy Agency; 2019 Jun [cited 2024 Mar 10]; Available from: https://www.iea.org/reports/the-future-of-hydrogen

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Laboratories.¹²⁴ Various mechanisms have been proposed for the low temperature hydrogen embrittlement of metallic alloys. For example, HEDE occurs through a stress concentration-driven migration of hydrogen to crack tips resulting in reduced fracture energy and cleavage-like failure. HELP is related to mobility of dislocations through an elastic shielding effect, resulting in enhanced localized plasticity.¹²⁵ Conventional metallic coatings are ineffective hydrogen permeation barriers due to rapid hydrogen diffusion, but a broad range of ceramic coatings have been evaluated as hydrogen isotope (deuterium and tritium) permeation barriers, mainly for use in nuclear fusion reactors.¹²⁶ (see Figure 10). The most promising permeation barrier candidates have so far been based on Al₂O₃, Er₂O₃ or Cr₂O₃,^{127,128} and while advanced coatings such as multi-component metal oxide glass, MAX phase, SiC and carbon-based (graphene) coatings are being developed,¹²⁹ additional evaluation is needed to consider these more advanced systems for long-term use as hydrogen permeation barriers. For lower temperature applications such as hydrogen storage and transport, polymers and polymer composites offer a cost-effective alternative that must be explored further.¹³⁰ All traditional coating application processes, including thermal spray, CVD, pack cementation, electro deposition, etc., have been utilized for permeation barrier deposition. Pre-oxidation of substrates or coatings allows for the formation of thermally grown oxides—i.e., alumina and chromia—with attractive hydrogen permeation properties.

Challenges related to the fabrication and use of hydrogen permeation barriers to hinder hydrogen embrittlement include:

- Complex degradation mechanisms in nuclear environments requiring layers resistant to irradiation, corrosion, etc., stable at 400°C–600°C.
- Cost associated with the deposition of coatings on large-scale components such as pipelines and storage vessels. Most promising materials have not been evaluated after long-term exposure in relevant environments.
- Lack of data correlating permeation barrier efficiency with substrate embrittlement.
- Limited work on the impact of low-cost polymer and polymer composite coatings on substrate embrittlement.

Great research opportunities exist to design, fabricate, and deploy hydrogen permeation barriers:

¹²⁴ San Marchi C, Somerday BPS. Technical Reference for Hydrogen Compatibility of Materials. [Internet] Sandia National Laboratories; 2012 [cited: 2024 Jul 30]; SAND2012-7321. Available from: <u>https://energy.sandia.gov/wp-content/uploads/2015/04/SAND2012_7321.pdf</u>

¹²⁵ Wetegrove M, Duarte MJ, Taube K, Rohloff M, Scheu C, Dehm G, Kruth A. Preventing hydrogen embrittlement: the role of barrier coatings for the hydrogen economy. Hydrogen [Internet]. 2023 May [cited 2024 Jul 30]; 4: 307-322. Available from: <u>https://doi.org/10.3390/hydrogen4020022</u>

¹²⁶ Rönnebro ECE, Oelrich RL, Gates RO. Recent advances and prospects in design of hydrogen permeation barrier materials for energy applications—a review. Molecules [Internet]. 2022 Oct [cited 2024 Jul 30]; 27: 6528. Available from: <u>https://doi.org/10.3390/molecules27196528</u>

¹²⁷ Field KG, Snead MA, Yamamoto Y, Terrani KA. Handbook on the Material Properties of FeCrAl Alloys for Nuclear Power Production Applications. Oak Ridge National Laboratory [Internet] 2017, [cited 2024 Jul 30]; ORNL/TM-2017/186. Available from: <u>https://info.ornl.gov/sites/publications/Files/Pub114121.pdf</u>

¹²⁸ Chikada T, Suzuki A, Adelhelm C, Terai T, Muroga T. Surface behaviour in deuterium permeation through erbium oxide coatings. Nuclear Fusion [Internet]. 2011 May 13 [cited 2022 Aug 23];51(6):063023. Available from: https://doi.org/10.1088/0029-5515/51/6/063023

¹²⁹ Hu L, Zhong F, Zhang J, Zhao S, Wang Y, Cai G, et al. High hydrogen isotopes permeation resistance in (TiVAlCrZr)O multi-component metal oxide glass coating. Acta Materialia [Internet]. 2022 Oct 1 [cited 2024 Aug 27];238:118204–4. Available from: <u>https://doi.org/10.1016/j.actamat.2022.118204</u>

¹³⁰ Li Y, Barzagli F, Lin Liu Q, Zhang X, Yang Z, Xiao M, et al. Mechanism and evaluation of hydrogen permeation barriers: a critical review. Ind & Eng Chem Research [Internet]. 2023 Aug 30 [cited 2024 Aug 27];62(39):15752–73. Available from: https://doi.org/10.1021/acs.iecr.3c02259

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- Further improvement of our understanding of hydrogen permeation mechanisms to enable development of more accurate physics-based models that will accelerate the design of advanced permeation barriers.
- Fabrication of multi-layer, multifunction permeation barriers with complex structures, enhanced stability, and improved compatibility with dissimilar substrates.
- Development of low-cost, large-scale deposition techniques for ceramics, metals, and polymers.
- In-situ formation of permeation barrier during coating deposition in reactive environments (O, C, or N-rich atmosphere).
- Integration of sensors into the coating fabrication process to monitor in-service hydrogen permeation.
- Development of new apparatus and methodologies to assess hydrogen permeation and embrittlement at various temperatures.

Success will be measured through the cost-effective development of hydrogen permeation barriers for low temperature applications such as hydrogen transport and storage and high temperature applications such as fusion reactors with a permeation reduction factor (PRF) at least 10 times greater than current permeation barriers. This will benefit power generation companies as well as pipeline and transportation industries.

The R&D pathway will start with the development and long-term performance evaluation of low-cost hydrogen permeation barriers for hydrogen storage and transport (2025-2030). This will be followed by the development of hydrogen permeation barriers for harsh environments such as fusion reactors and the integration of embedded/in situ sensors into the coating architecture for in-service/operando hydrogen detection and/or measurement (2030-2035).



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Figure 10. Hydrogen permeabilities for state-of-the-art barrier coatings containing various oxides, carbides and nitrides according to literature. Permeabilities for a selection of metals and alloys are shown for comparison. Values are given at 400-500°C.¹³¹

Develop sensor and protective coatings to mitigate hydrogen embrittlement of metallic structures and parts (C61)

The critical role that hydrogen will play in the energy, industrial and transport sectors, with hydrogen embrittlement being a major challenge both at low and high temperature.^{132,133,134,135} Developing efficient and reliable hydrogen energy storage industrial end uses that power generation systems such as H₂-fueled turbines, internal combustion engines and fuel cell technologies should be developed together for successful integration.^{136,137} A key difference is the common use of advanced austenitic steels and Ni-based alloys in gas turbines and engines, not acceptable in components subjected to high neutron irradiation such as fusion environment.^{138,139}

Limited understanding exists on the impact of high temperature combined with the presence of high temperature strengthening phases on the resistance to hydrogen embrittlement.^{140,141} Coatings might still be needed as hydrogen permeation barrier and coating material candidates have been discussed. Cost-effective solutions such as pre-oxidation to form a protective alumina or chromia scale or the deposition of low-cost chromia or alumina-forming coatings are particularly attractive.

¹³⁴ International Energy Agency. The future of hydrogen - analysis. [Internet] International Energy Agency; 2019 Jun [cited 2022 Mar 10]. Available from: <u>https://www.iea.org/reports/the-future-of-hydrogen</u>

https://www.sandia.gov/app/uploads/sites/158/2021/12/TechRef_Introduction.pdf

¹³¹ Wetegrove M, Duarte MJ, Taube K, Rohloff M, Scheu C, Dehm G, Kruth A. Preventing hydrogen embrittlement: the role of barrier coatings for the hydrogen economy. Hydrogen [Internet]. 2023 [cited 2024 Jul 31]; 4: 307-322. Available from: https://doi.org/10.3390/hydrogen4020022

¹³² US Department of Energy. Hydrogen from next-generation electrolyzers of water (H2NEW) [Internet]. [cited 2024 Jul 31]. Available from: https://h2new.energy.gov/

¹³³ Abe, JO, Popoola API, Ajenifuja E, Popoola OM. Hydrogen energy, economy and storage: review and recommendation. Int J of Hydrogen Energy [Internet]. 2019 [cited 2024 Jul 31]; 44: 15072-15086. Available from: https://doi.org/10.1016/j.ijhydene.2019.04.068

¹³⁵ Marchi CS, Somerday BP. Technical reference on hydrogen compatibility of materials. [Internet] Sandia National Laboratories; 2012 [cited 2024 Aug 8]. SAND2012-7321. Available from:

 ¹³⁶ Wetegrove M, Duarte MJ, Taube K, Rohloff M, Scheu C, Dehm G, Kruth A. Preventing hydrogen embrittlement: the role of barrier coatings for the hydrogen economy. Hydrogen [Internet]. 2023 [cited 2024 Jul 31]; 4: 307-322. Available from: https://doi.org/10.3390/hydrogen4020022

¹³⁷ Goldmeer J. Power to gas: hydrogen for power generation. [Internet] GE Power Technologies; 2019 Feb [cited 2024 Jul 31]. <u>https://www.gevernova.com/content/dam/gepower-new/global/en_US/downloads/gas-new-site/resources/GEA33861%20Power%20to%20Gas%20-%20Hydrogen%20for%20Power%20Generation.pdf</u>

¹³⁸ Siemens. Hydrogen power with Siemens gas turbines white paper. [Internet] Siemens; 2020 [cited 2024 Jul 31]. Available from: <u>https://www.siemens-energy.com/global/en/news/magazine/2019/hydrogen-capable-gas-turbine.html</u>

¹³⁹ Michler T, San Marchi C, Naumann J, Weber S, Martin M. Hydrogen environment embrittlement of stable austenitic steels. Int J of Hydrogen Energy [Internet]. 2012 Nov [cited 2024 Aug 2];37(21):16231–46. Available from: <u>https://doi.org/10.1016/j.ijhydene.2012.08.071</u>

¹⁴⁰ Michler T, Yukhimchuk AA, Naumann J. Hydrogen environment embrittlement testing at low temperatures and high pressures. Corrosion Sci [Internet]. 2008 [cited 2024 Jul 31]; 50: 3519-3526. Available from: https://doi.org/10.1016/j.corsci.2008.09.025

¹⁴¹ Gray HR. Embrittlement of nickel-, cobalt-, and iron-based superalloys by exposure to hydrogen. NASA [Internet]. National Aeronautics and Space Administration; 1975 [cited 2024 Aug 8]; 75N14884. Available from: <u>ntrs.nasa.gov/api/citations/19750006812/downloads/19750006812.pdf</u>

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Most challenges related to hydrogen passive coatings are similar for low and high temperature applications. Candidate materials have not been evaluated after long-term exposure in relevant environments and limited data has been generated to correlate permeation barrier efficiency with substrate embrittlement.

Additionally, specific challenges at high temperature need to be addressed:

- Lack of understanding of the hydrogen embrittlement mechanisms at high temperature
- Harsh thermo-mechanical conditions leading to accelerated coating degradation

Success will be measured through the development and establishment of multi-capability platform for testing and evaluating materials performance in high temperature and pressure hydrogen pre- and post-combustion environments. The platform is expected to be a cohesive unit integrating combinatorial materials design driven by additive fabrication techniques, physics-based coupled thermodynamic-kinetic modeling and in-situ atomic scale characterization methods. This is expected to benefit companies that focus on hydrogen power generation technologies, as well as hydrogen transportation, storage, and usage found within the automotive industry. Sequence of events will be the development of high temperature hydrogen testing capabilities and the selection/development of stable high temperature hydrogen passive coatings (2025-2030). This will be followed by the qualification, scale up and deployment of these hydrogen passive coatings (2030-2035).



Figure 11. Impact of 100h exposure in hydrogen at high temperature on the room temperature tensile elongation of alloy 718.

Develop protective coatings to mitigate hydrogen embrittlement of metallic structures and parts (C25)

Given its abundance in nature, hydrogen holds the potential for large-scale production, playing a pivotal role in meeting global energy demands.^{142,143} Serving as an energy carrier, hydrogen finds applications across transportation, power generation, and chemical industries. However, the primary hurdle for achieving industrial-scale hydrogen production lies in material-related challenges. Hydrogen embrittlement stands out as a significant

¹⁴² Ahad MT, Bhuiyan MMH, Sakib AN, Becerril Corral A, Siddique Z. An overview of challenges for the future of hydrogen. Materials [Internet] 2023 Oct [cited 2024 July 29]; 16: 6680. Available from: <u>https://doi.org/10.3390/ma16206680</u>

¹⁴³ Pivovar B, Rustagi N, Satyapal S. Hydrogen at scale (H2@ Scale): key to a clean, economic, and sustainable energy system. Electrochem. Soc. Interface [Internet] 2018 [cited 2024 July 29]; 27(1): 47. https://doi.org/10.1149/2.F04181if

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concern, alongside issues like permeation, high temperatures, and pressures in corrosive environments.^{144,145,146} Addressing these challenges necessitates the development of durable, cost-effective materials capable of withstanding extreme conditions, including temperatures up to 1430°C and pressures exceeding 900 bars, while resisting embrittlement and hydrogen permeation^{147,148} Consequently, the establishment of economically viable manufacturing techniques for materials and components, along with supporting feedstock production and joining technologies, is imperative to foster the growth of a sustainable hydrogen manufacturing industry.

Constraints in the current and emerging technical landscape for hydrogen production include the need for durable, low-cost materials that can withstand high temperatures up to 1430°C and pressures above 900 bars while resisting embrittlement and hydrogen permeation. Additionally, materials and surface technologies such as claddings and coatings are necessary for hydrogen storage and transportation. Advanced manufacturing techniques are required to produce these materials cost effectively, and joining technologies are essential for manufacturing components for hydrogen products.

The objectives being pursued, with crosscutting benefits to multiple application spaces, include the development of durable, low-cost, high temperature resistant materials that support operations at up to 1430°C and pressures above 900 bars, and that are resistant to embrittlement and hydrogen permeation. Achieving these goals requires specific capabilities, such as science-based engineering approaches to design application-appropriate, cost-effective materials and their feedstock development. Additionally, computational tools, ML, and AI are essential to gather and leverage extensive historical data on alloy or materials chemistry, material behaviors, and characteristics, including those associated with manufacturing processes and pathways. The development of industrial-scale manufacturing is also crucial to support the widespread deployment of successfully developed materials and components.

Pursuing crosscutting advanced materials and manufacturing R&D will benefit DOE priority areas such as energy production, storage and utilization. The production of durable, low-cost, high temperature resistant materials will increase and lower the cost of hydrogen production. Success will be measured by the increased operational performance and reduced costs in hydrogen production due to these advanced materials. U.S. industries likely to benefit from this R&D include gas and liquid pipeline manufacturers, hydrogen power generation, hydrogen storage vessel manufacturers, and fuel cell companies.

The sequence in which categorized challenges should be pursued to achieve future goals includes first developing suitable, durable, low-cost, high temperature resistant materials by 2025–2030. This effort will include producing

¹⁴⁴ Gray HR, Nelson HG, Johnson RE, McPherson WB, Howard FS, Swisher JH. Potential structural material problems in a hydrogen energy system. Int J of Hydrogen Energy [Internet], 1978 [cited 2024 Jul 29]; 3: 105-118. <u>https://doi.org/10.1016/0360-3199(78)90059-9</u>

 ¹⁴⁵ Alamiery A. Advancements in materials for hydrogen production: A review of cutting-edge technologies. Chem Phys Mater 3 [Internet] 2024 Jan [cited 2024 Jul 29]; 3(1): 64–73. <u>https://doi.org/10.1016/j.chphma.2023.09.002</u>
 ¹⁴⁶ Baum ZJ, Diaz LL, Konovalova T, Zhou QA. Materials research directions toward a green hydrogen economy: a review [Internet]. ACS Omega. 2022 Sep 20;7(37):32908–35 [cited 2024 Jul 31]. Available from: https://pubs.acs.org/doi/full/10.1021/acsomega.2c03996

¹⁴⁷ Sharma M, Pramanik A, Bhowmick GD, Tripathi A, Ghangrekar MM, Pandey C, Kim BS. Premier, progress and prospects in renewable hydrogen generation: A review. Fermentation. [Internet] 2023 May [cited 2024 Jul 29]; 9(6): 537. <u>https://doi.org/10.3390/fermentation9060537</u>

¹⁴⁸ Nguyen-Thi TX, Nguyen PQP, Tran VD, A ğbulut Ü, Nguyen LH, Balasub-ramanian D, Tarelko W, et al. Recent advances in hydrogen production from biomass waste with a focus on pyrolysis and gasification. Int J Hydrogen Energy [Internet] 2024 Feb [cited 2024 Jul 29]; 54: 124-160. https://doi.org/10.1016/j.ijhydene.2023.05.049

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coatings and claddings, ceramics, and other composite materials that resist hydrogen embrittlement and permeation, along with the necessary joining technologies for structural and functional materials. Ignoring this R&D sequence will lead to continued difficulties in producing cost-effective. The aim is to bring impactful technologies to market within a compressed schedule of 5 years, positively affecting hydrogen production and impacting other applications in solar and nuclear energy. The established timeframe and the order in which R&D is pursued are essential to meeting DOE energy goals

Functional Coatings

Develop extreme environment coatings designed for recyclability with base part material (C25)

Coatings in harsh environments typically serve as functional surfaces to protect structural substrate materials from surface degradation mechanisms such as corrosion, oxidation, wear, and erosion.¹⁴⁹ This protection can be achieved by depositing a degradation-resistant coating that prevents the diffusion of harmful species or by reducing/suppressing the degradation mechanisms, for example, with low friction coefficient coatings¹⁵⁰ or hydrophobic coatings.¹⁵¹ Additionally, functional coatings can be used to enhance component performance. Examples include high absorption coatings for CSP systems,¹⁵² coatings that improve interfacial stability in solid-state batteries,¹⁵³ and electrical insulation coatings. While these coatings can significantly enhance system performance, protective layers against harsh environments remain essential, leading to the development of multi-material, multi-functional coatings.

Excellent examples of multi-functional coatings are thermal barrier coatings (TBCs) and environmental barrier coatings (EBCs) used in gas turbine components. These coatings combine thermal and/or environmental ceramic top-coat layers with oxidation-resistant metallic bond coats^{154,155,156} (Figure 12). Recently, digital manufacturing has emphasized the need for operando data to monitor, control, and optimize manufacturing and energy production

¹⁴⁹ Fox R., Lalena JN, Snyder W. Materials for harsh environments: 2020 virtual workshop summary report [Internet]. Department of Energy; 2021 Mar 31 [cited: 2024 Jul 31]. Available from:

https://www.energy.gov/eere/ammto/articles/materials-harsh-environments-2020-virtual-workshop-summaryreport

 ¹⁵⁰ Hirvonen JP, Koskinen J, Jervis JR, Nastasi M. Present progress in the development of low friction coatings.
 Surf Coat Tech. [Internet]. 1996 [cited 2024 Jul 30]; 80: 139-150. Available from: https://doi.org/10.1016/0257-8972(95)02701-7

 ¹⁵¹ Bayer IS. Superhydrophobic coatings from ecofriendly materials and processes: a review.
 Adv. Mater. Interfaces [Internet]. 2020; [cited 2024 Jul 30] 7: 2000095. Available from: https://doi.org/10.1002/admi.202000095

¹⁵² Atkinson C, Sansom CL, Almond H J., Shaw C.P. Coatings for concentrating solar systems – a review, Renew Sustain Energy Rev. [Internet] 2015 May [cited 2024 Jul 30]; 45: 113-122. Available from: https://doi.org/10.1016/j.rser.2015.01.015

¹⁵³ Xiao Y, Wang Y, Bo SH, Kim JC, Lincoln J, Miara LJ. Understanding interface stability in solid- state batteries Nat. Rev. Mater. [Internet]. 2020 Feb [cited 2024 Jul 30]; 5:105-126. Available from: https://doi.org/10.1038/s41578-019-0157-5

¹⁵⁴ Turcer LR, Padture NP. Towards multifunctional thermal environmental barrier coatings (TEBCs) based on rare-earth pyrosilicate solid-solution ceramics. Scr Mater. [Internet]. 2018 May [cited 2024 Jul 30]; 154:111–117. Available from: https://doi.org/10.1016/j.scriptamat.2018.05.032

¹⁵⁵ Lee KN. Yb2Si2O7 environmental barrier coatings with reduced bond coat oxidation rates via chemical modifications for long life. J Am Ceram Soc. [Internet]. 2019 [cited 2024 Jul 30]; 102(3): 1507–1521. Available from: <u>https://doi.org/10.1111/jace.15978</u>

¹⁵⁶ Viswanathan V, Dwivedi G, Sampath S. Multilayer, multimaterial thermal barrier coating systems: design, synthesis and performance assessment. J Am Ceram Soc. [Internet]. 2015 Mar [cited 2024 Jul 30]; 98: 1769–1777. Available from: <u>https://doi.org/10.1111/jace.13563</u>

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processes.¹⁵⁷ Additive manufacturing has demonstrated the fabrication of unique embedded sensors.¹⁵⁸ Furthermore, materials recyclability is crucial for a sustainable circular economy. Protective coatings are vital in preventing degradation mechanisms that hinder substrate recycling. Reducing interdiffusion during operation between the substrate and the functional coatings is necessary to avoid substrate contamination. Another constraint pertains to cost and durability. Cost and durability of the functional coating are critical factors that limit the deployment of functional coatings. The technological, economic, and environmental benefits of these coatings need thorough evaluation to justify their additional costs. The coatings must remain stable and functional under various combined operating conditions.



Figure 12. Schematic of t multilayered TBC architecture comprised of YSZ and GDZ to simultaneously meet the requirements of cyclic durability, erosion, and environmental attack.

Opportunities related to the development and deployment of multi-material/multi-layered coatings have been discussed. The complexity of producing multi-layer coatings is also a cost and time burden. Thus, it would be beneficial to develop alternative materials, where possible, that could offer the same or better performance without the need for complex, multi-layer manufacturing. Additional opportunities for functional coatings are:

- Improving Coating Performance: Innovations in coating materials and application techniques to enhance performance and durability under extreme conditions.
- Cost Reduction Strategies: Developing cost-effective methods for producing and applying coatings without compromising quality.
- Recyclability Enhancements: Creating coatings that facilitate easier recycling of substrates by minimizing contamination.

¹⁵⁷ Huning A, Fair R, Coates A, Paquit V, Scime L, Russell M, Kane K, et al. Digital platform informed certification of components derived from advanced manufacturing technologies. [Internet] Oak Ridge National Laboratory (TN); 2021 Sept [cited 2024 Jul 30]; ORNL/TM-2021/2210. Available from: https://info.ornl.gov/sites/publications/Files/Pub166838.pdf

¹⁵⁸ Hyer HC, Sweeney DC, Petrie CM. Functional fiber-optic sensors embedded in stainless steel components using ultrasonic additive manufacturing for distributed temperature and strain measurements. Addit Manuf. [Internet]. 2022 Apr [cited 2024 Jul 30]; 52: 102681. Available from: <u>https://doi.org/10.1016/j.addma.2022.102681</u>

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• Integrated Sensor Technologies: Embedding sensors within coatings to provide real-time data on performance and degradation, aiding in predictive maintenance and optimization.

The following advancements will help in overcoming the current limitations and expanding the application of functional coatings in harsh environments:

- New computational tools accelerate the development of materials with unique functional properties.
 Processes allowing the cost-effective fabrication of coatings exhibiting unique functionality.
- New advanced fabrication process allowing the design and fabrication of complex geometries taking advantage of specific coating functionality (i.e., cooling system for thermal barrier coatings).
- Digital manufacturing approaches allow component lifetime and performance monitoring via sensing functional layers and embedded surface devices.
- New techno-economic analysis approaches combined with life cycle assessment tools to assess the benefit of functional coatings on component life cycle.

Success will be measured through the cost-effective development of stable multi-functional an/or multi-layered coatings. This will include the next generation of advanced topcoats combining thermal and environmental barrier layers with protection against CMAS and vibration. Similar architecture will develop for other energy systems such as MSR, SFR, CSP, hydropower where complex harsh environments require multi-function coatings. Integration of new sensing layers to monitor component performance and lifetime will also be of prime significance and would benefit primarily power generation equipment and powder manufacturers.

The R&D pathway will start with the development and validation of multi-functional coatings (2025-2030) for harsh environments. Integration of in situ surface sensing layers and devices for digital manufacturing integration/operando service will then follow (2030-2035).

Surface Engineering

Develop energy efficient surface engineering process for component performance enhancement (C17)

Machining a component to meet required/specified dimensions and tolerances is the most common surface engineering process. Surface finish will drastically impact properties such as fatigue, creep, corrosion,^{159,160} and will influence the performance of components such as heat exchangers and turbine blades.¹⁶¹ Surface engineering is also often used to modify the microstructure at the component surface and enhance properties. Various processes can result in surface hardness increase to enhance wear and fatigue resistance. Surface heat treatment aims at nucleating strengthening precipitates, for example martensite in carbon steels.¹⁶² When performed in environments with high carbon or nitrogen activities, formation of strengthening carbide or nitride can also be achieved.¹⁶³ Mechanical deformation to form a high density of dislocation at the surface, for example using shot peening, is

¹⁶² Lee J-H, Jang J-H, Joo B-D, Sonn Y-M, Moon Y-H. Laser surface hardening of AISI H13 tool steel. Trans. Nonferrous Met Soc China [Internet]. 2009 [cited 2024 Jul 30]; 19: 917 920. Available from: https://doi.org/10.1016/S1003-6326(08)60377-5

¹⁵⁹ Javidi A, Rieger U, Eichlseder W. The effect of machining on the surface integrity and fatigue life. International Journal of Fatigue [Internet]. 2008 [cited 2024 Jul 30]; 30: 2050–2055. Available from: https://doi.org/10.1016/j.ijfatigue.2008.01.005

¹⁶⁰ Lee SM, Lee WG, Kim YH, Jang H. Surface roughness and the corrosion resistance of 21Cr ferritic stainless steel. Corrosion Science [Internet]. 2012 [cited 2024 Jul 30]; 63: 404–409. Available from: https://doi.org/10.1016/j.corsci.2012.06.031

¹⁶¹ Webb RL, Eckert ERG. Applications of rough surfaces to heat exchanger design, Int J Heat Mass Transfer, [Internet] 1972 [cited: 2024 Jul 30]; 15:1647-1658. Available from: https://doi.org/10.1016/0017-9310(72)90095-6

¹⁶³ Schneider MJ, Chatterjee MS. Introduction to Surface Hardening of Steels, ASM Handbook Volume 4A, Steel Heat Treating Fundamentals and Processes, J. Dossett and G.E. Totten editors, 2013; 389-398.

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another efficient method to increase surface hardness.¹⁶⁴ Improving the corrosion and oxidation resistance can also be achieved by surface treatments .^{165,166,167} The goal is to grow a protective slow growing oxide scale at the surface, typically, AI, Cr or Si-rich. The surface treatment will either form the protective oxide scale before operating or the microstructure will be modified to favor the formation of a protective scale in service. The effectiveness of these surface treatments will decrease over time at high temperature due to microstructure evolution and/or spallation of the scale initially formed. Friction stir processing is an emerging solid-state technology allowing the production of surface composites.¹⁶⁸ The severe deformation taking place during friction stir allows the production of unique microstructure and properties. Additive manufacturing offers the opportunity to locally control the microstructure by changing printing parameters^{169,170} and could integrate surface engineering into the component fabrication process.

Hybrid manufacturing adds another surface engineering capability by locally tailoring the surface roughness, microstructure, and residual stress/hardness^{171,172} (Figure 13). The unique possibility with AM to generate complex near net shape components has also, however, led to the need for new surface engineering techniques specifically designed for AM components.¹⁷³ Finally, coating deposition was not considered/discussed here as surface engineering, but surface engineering is often needed in preparation of coating deposition, i.e. shot peening before thermal spray deposition.

While surface engineering is already used for most industrial components, limitations to further improve component properties via surface engineering are:

• Cost associated with the additional surface engineering step, for large-scale components.

¹⁶⁵ Zheng ZB, Zheng YG. Effects of surface treatments on the corrosion and erosion-corrosion of 304 stainless steel in 3.5% NaCl solution, Corr Sci. [Internet]. 2016 [cited 2024 Jul 30]; 112;657-668. Available from: https://doi.org/10.1016/j.corsci.2016.09.005

¹⁶⁶ Cooper L, Benhaddad S, Wood A, Ivey DG, The effect of surface treatment on the oxidation of ferritic stainless steels used for solid oxide fuel cell interconnects, J of Power Sources [Internet]. 2008 [cited 2024 Jul 30]; 184, 220–228. Available from: https://doi.org/10.1016/j.jpowsour.2008.06.010

¹⁶⁷ Pint BA, Jun J. Pre-Oxidation to Improve Liquid Metal Compatibility, Oxi Met. [Internet]. 2021 [cited 2024 Jul 30]; 96:231–240. Available from: <u>https://doi.org/10.1007/s11085-021-10057-4</u>

¹⁶⁸ Sharma V, Prakash U, Kumar BVM. Surface composites by friction stir processing: A review, Journal of Materials Processing Technology [Internet]. 2015 [cited 2024 Jul 30]; 224;117-134. Available from: https://doi.org/10.1016/j.jmatprotec.2015.04.019

¹⁶⁹ Fernandez-Zelaia P, Kirka MM, Dryepondt SN, Gussev. Crystallographic texture control in electron beam additive manufacturing via conductive manipulation, Materials and Design [Internet]. 2020 [cited 2024 Jul 30]; 195;109010. Available from: <u>https://doi.org/10.1016/j.matdes.2020.109010</u>

¹⁷⁰ Gu D, Shi X, Poprawe R, Bourell, DL, Setchi R, Zhu J. Material-structure-performance integrated laser-metal additive manufacturing, Science [Internet]. 2021 [cited 2024 Jul 30]; 372; 932-947. Available from: <u>https://doi.org/10.1126/science.abg1487</u>

¹⁷¹ Dilberoglu, UM, Gharehpapagh B, Yaman U, Dolen M. Current trends and research opportunities in hybrid additive manufacturing, The Int J of Adv Manufacturing Technology [Internet]. 2021 [cited 2024 Jul 30]; 113:623–648. Available from: https://doi.org/10.1007/s00170-021-06688-1

¹⁷² Feldhausen T, Paramanathan M, J. Heineman J, Hassen A, Heinrich L, Kurfess R, Fillingim K, et al. Hybrid manufacturing of conformal cooling channels for tooling, J. Manuf. Mater Process [Internet]. 2023 [cited 2024 Jul 30]; 7, 74. Available from: <u>https://doi.org/10.3390/jmmp7020074</u>

¹⁷³ Maleki E, Bagherifard S, Guagliano. Surface post-treatments for metal additive manufacturing: Progress, challenges, and opportunities, Addit Manuf [Internet]. 2021 [cited 2024 Jul 30]; 37;101619. Available from: https://doi.org/10.1016/j.addma.2020.101619

¹⁶⁴ Wu J, Liu H, Wei P, Zhu C,Lin Q. Effect of shot peening coverage on hardness, residual stress and surface morphology of carburized rollers, Surf Coat Tech [Internet]. 2020 [cited 2024 Jul 30]; 384;125273. Available from: <u>https://doi.org/10.1016/j.surfcoat.2019.125273</u>

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- Lack of techno-economic analysis tools to evaluate the long-term benefit of surface engineering.
- Limited experience in surface engineering using advanced (additive) manufacturing processes.
- Surface treatment needs to be compatible with other component manufacturing steps such as heat treatment.

Research opportunities to overcome the above limitations and develop new surface engineering approaches are discussed below:

- The fabrication of unique surface microstructure via friction stirs, additive, hybrid, and other advanced manufacturing processes, not achievable using traditional processes. Surface engineering can be integrated into the component fabrication strategy.
- Utilization of the same additive/hybrid platform for component production and surface engineering for cost reduction
- New modeling tools to predict and control microstructure and residual stress at the specimen surface.
- Improvement of life cycle analysis LCA tools to determine the impact of surface engineering on component cost and sustainability.
- Development of new surface engineering processes designed for advanced manufacturing.

Success will be measured through the development of new cost-effective engineering techniques to improve fatigue, wear and/or corrosion resistance in harsh environments and the integration of surface engineering in additive/hybrid processes. Most industries have surface engineering needs, such as power generation industries and aerospace and automotive manufacturers. The R&D pathway will start with the development of new cost-effective engineering techniques to improve fatigue, wear, and/or corrosion resistance in harsh environments (2025-2030). This will be followed by the integration of surface engineered features via advanced manufacturing (i.e., additive and hybrid processes) (2030-2035).





Figure 13. Mold fabrication by hybrid manufacturing, before and after surface finish, adapted from Feldhausen et al.¹⁷⁴

¹⁷⁴ Feldhausen T, Paramanathan M, J. Heineman J, Hassen A, Heinrich L, Kurfess R, Fillingim K, et al. Hybrid manufacturing of conformal cooling channels for tooling, J Manuf Mater Process [Internet]. 2023 [cited 2024 Jul 30];7,74. Available from: <u>https://doi.org/10.3390/jmmp7020074</u>

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Coating Repair Technologies

Extend the life of components and materials operation under harsh environments through improved coating/repair technologies (C12)

Coating repair is a key technology that can enable a sustainable and circular economy by extending the life of components and decreasing the need for new material extraction and transformation. For large expensive components repair is of critical economic importance as scraping is often driven by limited localized damage. Currently, the gas turbine industry has well established procedures for the inspection, maintenance and repair of components and coatings. For coating repairs multiple approaches can be considered but will typically include a removing step of the degraded coatings and underlaying substrate, deposition of a new protective coatings, and heat treatments.^{175,176} A broad range of traditional and advanced processing techniques such as thermal spray, brazing, welding, laser cladding or cold spraying are employed.^{177,178,179} Recently, use of large-scale wire arc additive manufacturing technologies for repair of metallic components has been deemed feasible and financially viable.¹⁸⁰ While wire arc additive manufacturing repair has been demonstrated to be viable for steels, while more exotic materials such as superalloy repair are less explored. There is an opportunity specifically in the powder bed space where technologies such as electron beam melting additive manufacturing have shown promise processing difficult to weld high temperature Ni-based superalloys. While repairs of these materials are currently done in industry, repairs are typically limited to surface-defects; powder bed AM potentially enabling repair of large volumes and heights (10+ mm).

Repair is not limited only to 'replacement' efforts (e.g., replication of the original geometry and material/coating system). Hybrid and additive manufacturing allow for modification of the original component geometry and material providing opportunity to improve overall component performance (Figure 14). Furthermore, more sophisticated designs conventionally not achievable can be realized, for example advanced cooling channels. As discussed previously, new complex multi-layer or graded structures can be deposited to improve compatibility between the coating/protective layer and the substrate. It is also worth noting that hybrid manufacturing allows us to efficiently remove and re-coat components using the same platform. While coating repair is a relatively mature technology for metallic components, repair of composite materials offers additional challenges. This is of particular importance in

¹⁷⁵ Pallos KJ. Gas turbine repair technology. [Internet] GE Power Systems (GA); 2001 [cited 2024 Jul 30]; . GER-3957B. Available from: <u>https://www.gevernova.com/content/dam/gepower-new/global/en_US/downloads/gas-</u> new-site/resources/reference/ger-3957b-gas-turbine-repair-technology.pdf

¹⁷⁶ Daleo JA, Ellison KA, Boone DH. Metallurgical considerations for life assessment and the safe refurbishment and requalification of gas turbine blades. J of Eng for Gas Turbines and Power [Internet]. 2002 Jun [cited 2024 Jul 30]; 124; 571-579. Available from: <u>https://doi.org/10.1115/1.1455638</u>

¹⁷⁷ Fiebig J, Bakan E, Kalfhaus T, Mauer G, Guillon O, Vaßen R. Thermal spray processes for the repair of gas turbine components. Adv Eng Mater [Internet]. 2020 Jan [cited 2024 Jul 30]; 22: 1901237. Available from: <u>https://doi.org/10.1002/adem.201901237</u>

¹⁷⁸ Brandt M, Sun S, Alam N, Bendeich P, Bish A. Laser cladding repair of turbine blades in power plants: from research to commercialisation. Int Heat Treatment and Surface Eng [Internet]. 2009 Sept [cited 2024 Jul 30]; 3: 5-114. Available from: <u>http://dx.doi.org/10.1179/174951409X12542264513843</u>

¹⁷⁹ Yin S, Cavaliere P, Aldwell B, Jenkins R, Liao H, Li W, Lupoi R. Cold spray additive manufacturing and repair: fundamentals and applications. Addit. Manuf [Internet]. 2018 May [cited 2024 Jul 30]; 21: 628–650. Available from: <u>https://doi.org/10.1016/j.addma.2018.04.017</u>

¹⁸⁰ Oak Ridge National Laboratory. Metal steam turbine blade shows cutting-edge potential for critical, large 3Dprinted parts. [Internet] Oak Ridge National Laboratory (TN); 12 Dec 2023 [cited 2024 Jul 30]. Available from: <u>https://www.ornl.gov/news/metal-steam-turbine-blade-shows-cutting-edge-potential-critical-large-3d-printed-parts</u>

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emerging energy sectors such as renewable wind energy,¹⁸¹ where degradation of leading-edge coatings due to erosion is a major concern for wind turbine blades.¹⁸²

As blade lengths continue to increase, so does the speed of the tip of the blade, which during their use life often experiences speeds more than 80 m/s, leading to significant erosion at the top of the blade. Blade coatings can be applied to extend their use life, and most coatings are often based on thermoset chemistries or tapes that are manually applied along the length of the blade. However, while these coatings increase resistance to leading-edge erosion during the use life, they are not easily repairable in the field and need to be regularly re-applied. The costs for this can be up to 12 times that of major structural damage throughout the blade lifetime.¹⁸³ There is very little drive for commonization in repair and maintenance of wind turbine blades, and very little understanding of where these materials are going once they are removed from the blade and replaced.

Limitations for coating repair technologies include:

- Cost associated with the repair of large-scale components requiring expensive facilities and/or on-site repair.
- Difficulty in fabricating stable multi-materials multilayer coatings (See Sub1)
- Limited options for coatings on large-scale composite coatings.

Research opportunities to overcome these limitations include:

- New advanced/hybrid fabrication techniques allowing the deposition of high temperature harsh environment advanced coatings (i.e., hard to weld Ni-based alloys).
- Development of new advanced materials tailored for specific repair processes.
- Hybrid fabrication techniques allow the efficient removal and deposition of coatings using the same platform.
- Possibility to upgrade components with modern design not achievable via traditional processing.

Success will be measured through the development of new coating repair technologies for metallic and composite substrates and the deposition of these advanced coatings on large-scale components utilized within power generation companies and maintenance/repair industries.

The R&D pathway will start with the development and qualification of new repair technologies using multi-layer functional coatings, graded structures, and new component designs (2025–2030). This will be followed by the successful demonstration of the repair of large-scale metallic and composite components after in-service operation (2030–2035).

¹⁸¹ Mishnaevsky L, Tempelis A, Kuthe N, Mahajan P. Recent developments in the protection of wind turbine blades against leading edge erosion: materials solutions and predictive modelling. Renewable Energy [Internet]. 2023 Oct [cited 2024 Jul 30]; 215: 118966. Available from: https://doi.org/10.1016/j.renene.2023.118966

¹⁸² Kuthe N, Mahajan P, Ahmad S, Mishnaevsky L. Engineered anti-erosion coating for wind turbine blade protection: computational analysis. Materials Today Communications [Internet] 2022 Jun [cited 2024 Jul 30]; 31: 103362. Available from: https://doi.org/10.1016/j.mtcomm.2022.103362

¹⁸³ Mishnaevsky L, Thomsen K. Costs of repair of wind turbine blades: influence of technology aspects. Wind Energy [Internet]. 2020 Jul [cited 2024 Jul 30]; 23: 2247–2255. Available from: <u>https://doi.org/10.1002/we.2552</u>

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Figure 14. Repair of cast irons cylinder heads on heavy-duty engines by AM DED using high Ni containing alloy

Multi-Material (layered) Claddings/Coatings and FGMs

Develop multi-material multifunctional claddings/coatings and FGMs for surface protection from attack by multiple mechanisms (C14)

Coatings and cladding are key to the successful development of HEMs as they allow optimization of the HEM substrate's bulk structural properties, protection from surface-based degradation mechanisms such as oxidation, corrosion, erosion, wear, etc. being ensured by the deposited protective layer. The critical need for coatings has been identified in previous reports on HEM and various reports and articles focused on sustainable energy systems.^{184,185,186} Multi-material coatings can take advantage of each layer's specific properties and often improve compatibility between the substrate and the coating,¹⁸⁷ as demonstrated for multi-layer thin films, for wear resistance or corrosion protection.^{188,189} Key challenges in harsh environments, for high temperature applications, are the chemical stability of the multi-material coatings and long-term compatibility with the substrate. Great examples of industrial multi-material coatings are thermal environmental barrier coatings (TBCs) deposited on gas turbine

¹⁸⁴ Fox R, Lalena JN, Snyder W. Materials for harsh environments: 2020 virtual workshop summary report [Internet]. Department of Energy; 2021 Mar 31 [cited: 2024 Jul 31]. Available from:

https://www.energy.gov/eere/ammto/articles/materials-harsh-environments-2020-virtual-workshop-summaryreport

¹⁸⁵ Li M, Anderson D, Dehoff R, Jokisaari A, Van Rooyen I, Cairns-Gallimore D. Advanced materials and manufacturing technologies (AMMT) 2022 roadmap. [Internet] Department of Energy; 2022 Sept [cited: 2024 Jul 31]; ANL-23/12. Available from: <u>https://publications.anl.gov/anlpubs/2023/02/180691.pdf</u>

¹⁸⁶ Bender R, Feron D, Mill D, Ritter S, Bassler R, Bettge D, De Graeve I. Corrosion challenges towards a sustainable society, Mater Corros [Internet]. 2022 Jul [cited 2024 Jul 31]; 73: 1730–1751. Available from: <u>https://doi.org/10.1002/maco.202213140</u>

¹⁸⁷ Bull SJ, Jones AM. Multilayer coatings for improved performance. Surf and Coat Tech [Internet]. 1996 Jan [cited 2024 Jul 31]; 78: 173-184. Available from: <u>https://doi.org/10.1016/0257-8972(94)02407-3</u>

¹⁸⁸ Carbonini P, Monetta T, Nicodemo L, Mastronardi P, Scatteia B, Bellucci F. Electrochemical characterization of multilayer organic coatings. Prog Org Coat [Internet]. 1996 Sept [cited 2024 Jul 31]; 29, 13-20. Available from: <u>https://doi.org/10.1016/S0300-9440(96)00628-5</u>

 ¹⁸⁹ Khaden M, Penkov OV, Yang HK, Kim DE. Tribology of multilayer coatings for wear reduction: a review.
 Friction [Internet]. 2017 Sept [cited 2024 Jul 31]; 5, 248–262. Available from: <u>https://doi.org/10.1007/s40544-017-0181-7</u>

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blades. The low thermal conductivity ceramic topcoat coupled with cooling channels drastically increases the allowable surface temperature, thus improving the turbine efficiency.

However, a bond coat (NiCrAlY-type) is also required to form a protective thermally grown oxide compatible with the ceramic topcoat.¹⁹⁰ A similar approach has led to the development of EBC on silicon carbide ceramic matrix composites as an alternative to Ni-base superalloy turbine components with increased stability at elevated temperatures. EBCs have a primary goal of reducing oxidation and volatilization of the thermally grown SiO₂ layer that will form at the surface of the Si bond coating. Coating modifications have resulted in improved properties, such as resistance to corrosion, oxidation, and thermal expansion matching between layers.^{191,192,193} As shown in Figure 15, compositionally complex coating designs^{194,195,196} and multi-layered architectures can result in a dual-purpose thermal/environmental barrier coating, further reducing component temperatures to improve coating lifetimes in service. The impact of multi-phase, functionally graded, layered, and compositionally complex solid solution coatings must be assessed in terms of effects on thermomechanical and thermochemical stability to further improve durability and performance. In the case of EBCs, durability is often limited to the SiO₂ thermally grown oxide, which undergoes a phase transformation during temperature cycling.^{197,198}

While the advantage of multi-material multi-function coatings is obvious, critical drawbacks that have limited the adoption of this technology for a broad range of technologies include:

- Heat treatments are often needed after material deposition and the selected heat treatment needs to be compatible with all the materials/layers.
- The design of durable multi-material claddings can be very challenging as long-term in-service compatibility between the layers and the substrate needs to be ensured.

¹⁹⁰ Clarke DR, Oechsner M, Padture NP. Thermal-barrier coatings for more efficient gas-turbine engines, MSR Bulletin [Internet]. 2012 Oct [cited 2024 Jul 331]; 37: 891-898. Available from: https://doi.org/10.1557/mrs.2012.232

¹⁹¹ Turcer LR, Padture NP. Towards multifunctional thermal environmental barrier coatings (TEBCs) based on rare-earth pyrosilicate solid-solution ceramics. Scr Mater [Internet]. 2018 Sept [cited 2024 Jul 31]; 154: 111–117. https://doi.org/10.1016/j.scriptamat.2018.05.032

¹⁹² Lee KN. Yb2Si2O7 Environmental barrier coatings with reduced bond coat oxidation rates via chemical modifications for long life. J Am Ceram Soc [Internet]. 2019 Mar [cited 2024 Jul 31]; 102(3): 1507–1521. Available from: https://doi.org/10.1111/jace.15978

¹⁹³ Ridley M, Kane K, Lance M, et al. Steam oxidation and microstructural evolution of rare earth silicate environmental barrier coatings. J Am Ceram Soc [Internet]. 2023 [cited 2024 Jul 31]; 106(1): 613–620. Available from: <u>https://doi.org/10.1111/jace.18769</u>

¹⁹⁴ Ridley MJ, Gaskins J, Hopkins P, Opila E. Tailoring thermal properties of multi-component rare earth monosilicates. Acta Mater [Internet]. 2020 Aug [cited 2024 Jul 31]; 195: 698–707. Available from: https://doi.org/10.1016/j.actamat.2020.06.012

¹⁹⁵ Ridley MJ, Tomko KQ, Tomko JA, et al. Tailoring thermal and chemical properties of a multi-component environmental barrier coating candidate (Sc0.2Nd0.2Er0.2Yb0.2Lu0.2)2Si2O7. Materialia [Internet]. 2022 [cited 2024 Jul 31]; 26: 101557. Available from: <u>https://doi.org/10.1016/j.mtla.2022.101557</u>

¹⁹⁶ Turcer LR, Sengupta A, Padture NP. Low thermal conductivity in high-entropy rare-earth pyrosilicate solidsolutions for thermal environmental barrier coatings. Scr Mater [Internet]. 2021 Jan [cited 2024 Jul 31]; 191: 40– 45. Available from: <u>https://doi.org/10.1016/j.scriptamat.2020.09.008</u>

¹⁹⁷ Lance MJ, Ridley MJ, Kane KA, Pint BA. Raman spectroscopic characterization of SiO₂ phase transformation and Si substrate stress relevant to EBC performance. J Am Ceram Soc [Internet]. 2023 [cited Jul 31]; 106(10): 6205–6210. Available from: <u>https://doi.org/10.1111/jace.19190</u>

¹⁹⁸ Aguirre TG, Lin L, Ridley MJ, Kane KA, Pint BA. Finite element modeling of the phase change in thermallygrown SiO2 in SiC Systems for Gas Turbines. JOM [Internet]. 2024 Apr [cited Jul 31]; Available from: <u>https://doi.org/10.1007/s11837-024-06507-4</u> National Landscape of High-Impact Crosscutting Opportunities for Next Generation Harsh Environment Materials and **90** Manufacturing Process Research, Development, and Demonstration / January 16, 2025

For a broad range of applications, thermal cycling will lead to significant thermal stresses due to differences in thermal expansion coefficients between layers. This remains a critical parameter for the lifetime of EBCs and TBCs and this will be of particular significance when layers of oxides or carbides are deposited at the surface of metals to take advantage of their specific resistance to corrosion, erosion, wear, etc. Cracking or spallation of protective layers can then result in rapid catastrophic failure of the components. Chemical interaction at high temperature between the layers will alter each layer chemistry and degrade the layer performance. Microstructure evolution will impact the layer of thermal properties and might result in unexpected failure after service exposure. Another key limitation of multi-material coatings is the cost associated with the deposition of these coatings, often requiring specific manufacturing platforms for each layer.



Figure 15. Cross-sectional SEM micrograph of a T/EBC on a CMC. Adapted from below.¹⁹⁹

Opportunities related to the development and deployment of multi-material coatings have been discussed in Opportunity 1. Below, additional opportunities for functional coatings are described. Fortunately, advanced manufacturing techniques, powerful modeling tools and innovative materials offer new opportunities for the development and deployment of cost-effective multi-material coatings.

New advanced manufacturing techniques such as directed energy deposition have demonstrated the fabrication of more complex multilayer components, in particular graded structures, allowing progressive microstructure changes and thus improving layer compatibility and suppressing potentially weak interfaces.^{200,201}

¹⁹⁹ Lee K, Fox DS, Eldridge JI, Zhu D, Robinson RS, Bansal NP, et al. Upper temperature limit of environmental barrier coatings based on mullite and BSAS. J of Am Ceram Soc [Internet]. 2003 Aug 1 [cited 2024 Aug 28];86(8):1299–306. Available from: <u>https://doi.org/10.1111/j.1151-2916.2003.tb03466.x</u>

²⁰⁰ Singh DD, Arjula S, Reddy AR. Functionally graded materials manufactured by direct energy deposition: a review, Materials Today: Proceedings [Internet]. 2021 [cited Jul 31]; 47: 2450-245. Available from: https://doi.org/10.1016/j.matpr.2021.04.536

²⁰¹ Pillai R, Ren Q, Su Y-F, Kurfess R, Feldhausen T, Nag S. Leveraging additive manufacturing to fabricate high temperature alloys with co-designed mechanical properties and environmental resistance. J of Eng for Gas Turbines and Power [internet]. 2024 [cited Jul 31]; GTP-23-1471, 146, 061018. Available from: <u>https://doi.org/10.1115/1.4063784</u>

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Hybrid platform combining additive and subtractive manufacturing allows for the precise fabrication of layers of controlled thickness.²⁰² Hybrid manufacturing also brings the opportunity to combine several deposition techniques into one cost-effective platform with improved processing control at each step, such as:

- The development of new advanced HEMs, as described in FA3 will lead to coating layers or graded structures of unique properties.
- Multi-material coatings and graded structures can reduce thermal expansion coefficient mismatches and limit in-service thermal stresses.
- Advanced manufacturing techniques can result in unique process-specific microstructure tailored to the multi-material coating function.

Controlling the coating fabrication process and microstructure might also suppress the need for heat treatments.

- New thermo-kinetics modeling tools have been developed to design stable graded structures at high temperatures.
- Analysis of in-situ process data using advanced modeling tools has led to new fabrication strategies to reduce residual stresses. Coating fabrication with low residual stress will likely result in reduced stresses during in-service thermal cycling.

Success will be measured through the cost-effective development and commercial deployment of multi-material graded structures. Demonstration that such multi-material coating could be stable at high temperature with superior corrosion, erosion or wear resistance could have a drastic impact on multiple energy sectors such as H2-fired gas turbines, Gen-IV nuclear reactors and CSP power plants. This benefits primarily the power generation industries along with associated powder and coating manufacturers. The R&D pathway will start with the development and qualification of processes allowing the fabrication of stable multi-material coatings and graded structures (2025-2030) for harsh environments. This will be followed by the demonstration of the in-service long-term performance of the multi-material coatings (2030-2035).

Antifouling Coatings

Develop surface modifications to improve high temperature performance (oxidation, corrosion, erosion, wear) of low-cost metallic materials (C110)

Fouling (scaling) is a major concern in various power generation systems as it will often accelerate corrosion degradation mechanisms. Hot corrosion in boilers or deposition of CMAS in gas turbines are examples of deposits from the flue gas leading to accelerated attack.^{203,204} This is a major challenge for biomass power plants where the deposit chemistry is highly dependent on the type of biomass fuels.²⁰⁵ Fouling in addition to corrosion and erosion

²⁰² Feldhausen T, Paramanathan M, Heineman J, Hassen, Heinrich L, Kurfess R, Fillingim K, et al. Hybrid manufacturing of conformal cooling channels for tooling. J Manuf Mater Process [Internet]. 2023 Apr [cited Jul 31];7:74. Available from: <u>https://doi.org/10.3390/jmmp7020074</u>

²⁰³ Mori S, Sanusi T, Simms N, Sumner J. Fireside corrosion and deposition on heat exchangers in biomass combustion systems. Mater High Temp [Internet]. 2023 Oct [cited 2024 Jul 31]; 40: 36–47. Available from: <u>https://doi.org/10.1080/09603409.2022.2138007</u>

²⁰⁴ Shifler DA, Choi SR. CMAS effects on ship gas-turbine components/materials. Proceedings of the ASME Turbo Expo 2018 [Internet]. 2018 Jun 11 [cited 2024 Aug 9];1. Available from: <u>https://doi.org/10.1115/GT2018-75865</u>

²⁰⁵ Lachman J, Balas M, Lisy M, Lisa H, Milcak P, Elbl P. An overview of slagging and fouling indicators and their applicability to biomass fuels. Fuel Processing Technology [Internet]. 2021 Jun [cited 2024 Jul 31]; 217: 106804. Available from: https://doi.org/10.1016/j.fuproc.2021.106804

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is also a major concern for geothermal power plants as geothermal brines can have complex and region-specific chemistries, leading to significant solid deposition and accelerated material degradations.^{206,207}

While corrosion-resistant coatings often focus on corrosion protection, anti-fouling coatings (or paints) aim at preventing/limiting the deposition of deleterious species at the component surface to reduce the driving force for corrosion. Anti-fouling coatings and paints have been developed for the marine industry to protect ships against organic deposits and microbially-induced corrosion (MIC). They mitigate fouling through various mechanisms such as changing the brine chemistry with coating catalyzed reactions, altering surface roughness, decreasing total surface energy, utilizing hydrophobic properties from highly aromatic organic molecules, as well as by other hierarchical nano- and micro-sized features. A broad range of materials (Polyurethane, aluminum, cermets, etc.) and deposition techniques (paints, thermal spray, HVOF, etc.) have been considered to fabricate antifouling coatings (Figure 16).

Limitations for the use of fouling coatings are described below:

- Variability in fluid chemistry (geothermal brine, biomass) leading to fouling requires coating specific to the local harsh environments.
- Combination of several degradation mechanisms (e.g., fouling, corrosion, erosion, or thermocycling). New deep geothermal systems with result in even harsher conditions
- Difficulty in fabricating multi-materials multilayer coatings (See sub1)
- Environmental concerns related to coating fabrication processes (i.e., Cr[VI]).

Opportunities for research to overcome these limitations are described below:

- New advanced/hybrid fabrication techniques leading to local coating geometry and roughness designed for fouling suppression.
- New coating materials or graded structure with unique properties to prevent fouling, i.e., superhydrophobic and low surface energy coatings.
- Improved understanding and modeling of complex degradation mechanisms in flowing fluids
- Initial lab-scale performance validation of new coatings and following evaluation in selected field exposure of the coated materials.

Success will be measured through the development and validation of anti-fouling metallic and organic coatings deposited on low-cost materials used in biomass and geothermal plants. This will benefit a variety of industries such as power generation (biomass, hydro, nuclear, geothermal), sea water treatment, and wastewater treatment. Research sequence will start with the fabrication and testing of (multi-material) anti-fouling coatings (2025-2030) using advanced deposition techniques. This will be followed by the fabrication of multi-function coatings for protection against multi-degradation modes (e.g., fouling, corrosion, and erosion) (2030-2035).

²⁰⁶ Fanicchia F, Karlsdottir S.N. Research and development on coatings and paints for geothermal environments: a review. Adv Mater Technol [Internet]. 2023 Aug [cited 2024 Jul 31]; 8: 2202031. Available from: <u>https://doi.org/10.1002/admt.202202031</u>

²⁰⁷ Haklidir FS, Balaban TO. A review of mineral precipitation and effective scale inhibition methods at geothermal power plants in West Anatolia (Turkey). Geothermics [Internet]. 2019 Jul [cited 2024 Jul 31]; 80: 103-118. Available from: https://doi.org/10.1016/j.geothermics.2019.02.013

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Figure 16. Cross-sectional SEM micrograph of HVOF WC-Co-Cr cermet coating deposited onto carbon steel, showing vertical cracks and voids at the interface after in-situ exposure test at the Hellishei geothermal power plant. Adapted with permission from Ragnarsdottir, et al.²⁰⁸

Cavitation Resistant Coatings

Develop complex multi-functional and stable coatings for variety of combined operating conditions/coupled materials stressors (C23)

Cavitation and cavitation-erosion are known to be two key synergistical degradation mechanisms for hydropower turbines (Figure 17).^{209,210} In its glossary of hydropower terms, the waterpower technologies office defined cavitation as a "phenomenon that affects hydropower turbines when vapor bubbles form and implode due to rapid pressure changes, generating shock waves that create cavities on the metal surface.".²¹¹ In many practical applications, cavitation is assisted by the presence of particles enhancing erosion. A variety of hard coatings have been used for

²⁰⁸ Ragnarsdottir KR, Karlsdottir SN, Leosson K, Arnbjornsson A, Guolaugsson S, Haraldsdottir HO, Buzaianu A, et al. Corrosion testing of coating materials for geothermal turbine application. In: NACE Corrosion, [Internet] 2017 Mar 26-30. [cited: 2024 Jul 30] New Orleans, Louisiana. Access from:

https://onepetro.org/NACECORR/proceedings-abstract/CORR17/All-CORR17/NACE-2017-9185/125469 ²⁰⁹ Kumar P, Saini RP. Study of cavitation in hydro turbines—A review. Renewable and Sustainable Energy

Reviews [Internet]. 2010 [cited 2024 Jul 31]; 14: 374–383. Available from: https://doi.org/10.1016/j.rser.2009.07.024

²¹⁰ Kumar P, Saini RP. A review on operation and maintenance of hydropower plants. Sustainable Energy Technologies and Assessments [Internet]. 2022 [cited 2024 Jul 31]; 49: 101704. Available from: https://doi.org/10.1016/j.seta.2021.101704

²¹¹ Water Power Technologies Office. Glossary of hydropower terms. [Internet] Department of Energy. n.d. [cited 2024 Jul 31]. Available from: <u>https://www.energy.gov/eere/water/glossary-hydropower-terms</u>

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protection against cavitation-erosion, including carbides, nitrides, borides, etc. as well as cermets with carbides embedded in Ni, Cr or Mo-based alloys and epoxy-based coatings.²¹² A broad range of coating deposition techniques have been utilized, including plasma nitriding, CVD, thermal spray, pack cementation, laser cladding, etc..²¹³ More recently, new advanced techniques such as deep cryogenically treated thermal spray,²¹⁴ nanostructured and multi-modal or multi-layer coatings,^{215,216} and solid-state processing techniques such as cold spray and friction stir.^{217,218}

The complexity of cavitation-erosion degradation renders coating optimization challenging. While the overall phenomenon has been analyzed in detail, microstructural features impacting cavitation-erosion resistance are not well understood.²¹⁹ Coating hardness, while a valuable parameter, is not sufficient for the selection of coatings resistant to cavitation-erosion, and specific testing apparatus and standards have been developed for cavitation-erosion evaluation.²²⁰

The development and deployment of cavitation resistant coatings is limited due to:

- Lack of understanding and modeling tools for cavitation-erosion material degradation mechanisms
- Additional degradation mechanisms to be considered such as corrosion, wear, etc.
- Lack of techno-economic tools to assess the benefit of coating deposition.

Research opportunities to develop and deploy coatings for cavitation-erosion are listed below:

• New advanced techniques to deposit stable multilayer multifunction components (see sub1)

²¹² Singh R, Tiwari SK, Mishra SK. Cavitation erosion in hydraulic turbine components and mitigation by coatings: current status and future needs. JMEPEG [Internet]. 2012 [cited 2024 Jul 31]; 21: 1539–1551. Available from: https://doi.org/10.1007/s11665-011-0051-9

²¹³ Prashara G, Vasudev H, Thakur L. Performance of different coating materials against slurry erosion failure in hydrodynamic turbines: A review. Eng Failure Analysis [Internet]. 2020 [cited 2024 Jul 31]; 115: 104622. Available from: <u>https://doi.org/10.1016/j.engfailanal.2020.104622</u>

 ²¹⁴ Babu A, Perumal G, Arora HS, Grewal HS. Enhanced slurry and cavitation erosion resistance of deep cryogenically treated thermal spray coatings for hydroturbine applications. Renewable Energy [cited 2024 Jul 31];
 2021 [cited 2024 Jul 31]; 180: 1044-1055. Available from: https://doi.org/10.1016/j.renene.2021.09.006

²¹⁵ Krella AK , Czyzniewski A, Gilewicz A, Gajowiec G., Experimental study of the influence of deposition of multilayer crn/crcn pvd coating on austenitic steel on resistance to cavitation erosion. Coatings [Internet]. 2020 [cited 2024 Jul 31]; 10: 87. Available from: <u>https://doi.org/10.3390/coatings10050487</u>

 ²¹⁶ Xiang D, Ke D, Chengqing Yuan C, Ding Z, Cheng X. Microstructure and cavitation erosion resistance of HVOF deposited WC-Co coatings with different sized WC. Coatings [Internet]. 2018 [cited 2024 Jul 31]; 8: 307. Available from: https://doi.org/10.3390/coatings8090307

²¹⁷ Jiang X, Overman N, Smith C, Ross K. Microstructure, hardness and cavitation erosion resistance of different cold spray coatings on stainless steel 316 for hydropower applications. Materials Today Communications [Internet]. 2020 [2024 Jul 31]; 25: 101305. Available from: <u>https://doi.org/10.1016/j.mtcomm.2020.101305</u>

 ²¹⁸ Jiang X, Overman N, Smith C, Ross K. Friction stir processing of dual certified 304/304L austenitic stainless steel for improved cavitation erosion resistance. Applied Surface Science [Internet]. 2019 [cited 2024 Jul 31]; 471: 387–393. Available from: <u>https://doi.org/10.1016/j.apsusc.2018.11.177</u>

²¹⁹ Bregliozzia G, Di Schino A, Ahmed SI, Kenny JM, Haefke H. Cavitation wear behaviour of austenitic stainless steels with different grain sizes. Wear [Internet]. 2005 [cited 2024 Jul 31]; 258: 503-510. Available from: <u>https://doi.org/10.1016/j.wear.2004.03.024</u>

²²⁰ American Society for Testing and Materials. Standard test method for erosion of solid materials by cavitating liquid jet. [Internet] American Society for Testing and Materials; 2023 [cited 2024 Jul 31]; ASTM G134-17(2023). Available from: https://www.astm.org/standards/g134

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- Hybrid platform combining additive and subtractive manufacturing allows the control of microstructure and residual stress.
- Opportunity to produce coatings of more complex geometries for local reinforcement against localized erosion.
- Advanced characterization and modeling tools to drastically improve our understanding of microstructural degradation mechanisms.
- New advanced HEMs offer unique properties to be deposited as (multi-layer) coatings or graded structures.
- Advanced sensors and data analytics tools allowing operando monitoring of cavitation-erosion degradation.
- LCA tools to demonstrate the economic benefit of coating deposits.

Success will be measured through the development, and validation of cavitation-erosion coatings with an improvement by a factor of 5 to 10 in mass loss and lifetime compared to the base materials. A reduction of cost by 2–5x compared to repair approaches is also a key target goal. Industries to benefit from this include predominantly those in hydropower generation and associated coating manufacturers. The R&D pathway will start with the development and qualification of cavitation-erosion coatings deposited using cost-effective advanced manufacturing techniques (2025-2030). This will be followed by the demonstration of in-service long-term performance of cavitation-erosion of complex multi-material and/or multi-function coatings (2030-2035).



Figure 17. Examples of runner blades showing cavitation erosive failure.²²¹

²²¹ Singh R, Tiwari SK, Mishra SK. Cavitation erosion in hydraulic turbine components and mitigation by coatings: current status and future needs. J Mat Eng and Perf [Internet]. 2011 Oct 15 [cited 2024 Jul 31]; 21: 1539–1551. Available from: https://doi.org/10.1007/s11665-011-0051-9

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3.2 Focus Area 2: Materials Integration into Energy Systems Recommendations

The action plan table below lists several details that should be used to inform funding strategies for next generation process research and development investments for materials integration into energy systems, as well as describing the roadblocks with the existing state of the art and challenges to be addressed for material integration technologies. Specific opportunities with associated timelines follow the action plan.

Neglecting this R&D could have adverse implications across various energy technologies

Critical need not addressed: Similar to FA1, without the availability of adequate joining and bonding methods, it could be impossible to construct or assemble reliable systems at the lowest cost for some of the high-impact, high-performance energy technologies that will require advanced materials of the future.

Action Plan for Focus Area 2

Table 5. Action Plan for Materials Integration into Energy Systems.

Scope				
Advanced joining technologies for integrating materials/components into energy systems with harsh service environments	Achieving suitable joints or bonds between materials is crucial in energy systems. Weld defects during the manufacturing stage can be the cause of many failures in service. There is a need for high-quality weld joints and improved methods for joining similar and dissimilar metals (e.g., aluminum and steel, or austenitic and ferritic steels) and other dissimilar materials, such as ceramic-ceramic and ceramic-metal systems. A more aggressive materials research goal is to altogether eliminate joints and interfaces with functionally graded materials (FGMs), in which a material's composition or microstructure and, hence, its properties change gradually with volume. FGMs can be designed for specific functions and applications.			
Technologies of Interest:	FSW, Diffusion bonding (HIP, EFAS), FGMs, ICWE			
Roadblocks		Challenges to pursue		
 Bonding dissimilar materials often difficult and widely variable (material system dependent), e.g., in metal-ceramic systems due to mismatches in composition, coefficients of thermal expansion, melting points, and thermal conductivities. Welding nickel-based superalloys, commonly used in turbine blades, waste incinerator boilers, seals, turbocharger rotors, and high-temperature fasteners, complicated by cracking and microstructural segregation. Friction welding challenges, particularly in joining thin-walled components. 		 Integrated Computational Welding Engineering (ICWE), or ICME-W, to address the challenges associated with many highly coupled and nonlinear variables controlling the joint microstructure, properties, and performance. More advanced joining materials such as multi-principal element alloys (MPEA) that could be fit for joining some ceramics to metals. Composite interlayer designs to tune the coefficient of thermal expansion (CTE) mismatch (e.g., an MPEA with ceramic particles scattered inside it to control the CTE). 		
Stakeholders and Potential Roles				
Stakeholder	Role			
End Users/Original Equipment Manufacturers (OEMs)	 Advances in joining would reduce failure rates, thus lowering maintenance costs and increasing the longevity of systems and components. Capital costs would also be reduced. For example, innovations in this area would allow advanced materials to be used with lower cost parts, using the expensive components only where strictly necessary. With better coating or claddings, expensive exotic materials could be used to prevent corrosion, but strength could be derived from less expensive materials. Advances in joining would benefit companies in a diverse array of sectors, including concentrating solar power/thermal (CSP/T). nuclear power, geothermal power, metal refining, and more. 			

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ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C1	2328	Develop multi-material integration through joining and other fabrication techniques	LR	Diffusion bonding times < 30 min	4	2	
C45	542	Develop solid state joining of solid materials using EFAS (similar, dissimilar, titanium, ferrous, non-ferrous, refractory, ceramic, composite, etc.)	UR	Diffusion bonding times < 30 min	3	2.5	
C35	206	Develop Joining and integration methods for HEMs	UR	Diffusion bonding times < 30 min	3	2.5	(R)
C118	132	Develop joining/welding approaches for ceramic and composite materials to enable more complex component manufacturing	UR	Diffusion bonding times < 30 min	2	3	
C108	64	Develop joining Technology Innovations of solid materials using EFAS (similar, dissimilar, titanium, ferrous, non-ferrous, refractory, ceramic, composite, etc.)	UR	Diffusion bonding times < 30 min	3	2.5	

Advanced Manufacturing Integration/Joining Techniques

Develop multi-material integration through joining and other fabrication techniques (C1)

Improving materials joining techniques is of vital importance for the continued development of processes that must endure harsh environments, including energy production and industrial processes. Failures often occur at joining points, such as welds, as they can be the weakest part of structural material frames and systems. Some aspects of this field, e.g., metal-to-metal joining and mortar-joined ceramics, have been used for thousands of years. Gas metal arc welding (GMAW) and gas tungsten arc welding (GTAW) are relatively mature and commonly used fusion joining technologies. However, more specialized joining techniques for harsh environments are under development.

In fusion joining technologies, residual stresses and resulting failures are a commonly occurring issue. Methods to evaluate and control microstructural changes are needed to mitigate stress evolution effects. Reduction in residual stress and distortion through novel welding procedures (e.g., segment welding) and post-weld treatments (e.g., induction and ultrasonic treatment) are being pursued but are still in earlier stages. Potential mitigation methods to lower the likelihood of stress relaxation cracking (a.k.a. reheat cracking) include using welding filler materials and welding groove geometries to produce more homogenous microstructures and reduce residual stress, respectively. In large industrial applications such as molten salt tanks, cracking problems are compounded by size, as joining techniques and post-weld treatment strategies are more limited. Solutions must be suitable and easy to implement in the field over large areas. Cladding and coating methods have been used to address stress and corrosion concerns using methods like explosion welding and centrifugal rotation, but issues with these techniques remain due to delamination and strain induced by differences in chemistry and coefficients of thermal expansion.

A significant barrier is that joining techniques for different combinations of materials vary widely. Metal-to-metal joining, involving welding, brazing, soldering, and bonding, fundamentally changes material microstructure and properties of the heat affected zone and, if the joined materials are dissimilar, can also cause galvanic corrosion. Metal-to-ceramic joining is even more complex, due to mismatches in composition, coefficients of thermal expansion (CTE), melting points, and thermal conductivities. Ceramic-to-ceramic joining is also challenging, especially at high temperatures, since joining temperatures for brazing or diffusion bonding must exceed the ultimate use temperature of the joined assembly.^{222,223}

 ²²² Yang L, Miyanaji H, Janaki Ram D, Zandinejad A, Zhang S. Functionally graded ceramic based materials using additive manufacturing: review and progress. Ceramic transactions [Internet]. 2016 May 31 [cited 2024 Aug 29];258(CCLVIII):43–55. Available from: <u>https://doi.org/10.1002/9781119236016.ch5</u>
 ²²³ M.R. Locatelli, B.J. Dalgleish, K Nakashima, A.P. Tomsia, A.M. Glaeser. New approaches to joining ceramics

²²³ M.R. Locatelli, B.J. Dalgleish, K Nakashima, A.P. Tomsia, A.M. Glaeser. New approaches to joining ceramics for high-temperature applications. Ceramics International [Internet]. 1997 [cited 2024 Jul 30];23(4):313-22. Available from: <u>https://doi.org/10.1016/S0272-8842(96)00024-7</u>

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In researching joining solutions, it is therefore necessary to focus on specific material systems. While it is not reasonable to compile an exhaustive list of material systems necessary to achieve applicable metric targets and DOE emissions/energy goals, there are a few standout systems in which advances in joining capabilities could have key impacts. For example, as discussed more with C35 next, innovation with silicon carbide (SiC)-to-metal joining, would allow advanced ceramic materials to be used with lower cost parts.²²⁴

Three major advances are required in this area:

- Functionally graded materials (e.g., a metal-ceramic composite with changing composition along a certain direction) and processing techniques (e.g., 3D printing or extrusion with varying feed composition) which may reduce the joining problem to a metal-to-metal joint and a ceramic-to-ceramic joint.
- More advanced joining materials such as multi-principal element alloys (MPEA) that could be fit for joining some ceramic to metal
- Composite interlayer design to tune the mismatch of coefficient of thermal expansion (CTE) (e.g., an MPEA with ceramic particles scattered inside it to control the CTE).

Alternate tactics to reduce the constraints brought on by stresses and dissimilar material properties could include advances in welding techniques that enable reductions of heat input and residual stress or development of novel filler materials that demand less heat input.

Advances in joining would reduce failure rates, thus lowering maintenance costs and increasing the longevity of systems and components. Capital costs would also be reduced since more expensive components would only be used where strictly necessary. With better coating or claddings, expensive exotic materials could be used to prevent corrosion, but strength would be derived from less expensive base materials. Success must be evaluated by mechanical testing at operating temperature with microstructure characterization to reveal failure mechanisms as necessary. The strengths of joints produced by new techniques should be compared to base metals and assessed for corrosion resistance and mechanical properties. Other metrics may be more technology-specific (i.e., thermal conductivity, specific heat, and solar radiation absorptivity in the case of concentrating solar power applications). Advances in joining would benefit companies in a diverse array of sectors, including concentrating solar power/thermal (CSP/T), nuclear power, geothermal power, metal refining, and more.

This high impact R&D field will result in decreases for capital and operational costs of systems and increase viability of emerging technologies. Therefore, it is a top priority for Materials Integration into Energy Systems. It is essential that experimental research guided by computational materials/welding engineering be pursued. In particular, CSP/T requires a significant reduction in materials joining costs for cost competitiveness with other technologies such as solar PV, wind, and electrified heating.

Failure and limitations in joining methods are key hurdles holding back materials performance across many sectors and, in some cases, preventing the viability of new technologies. However, new joining methods require code approval prior to field implementation, which should be factored into overall development timescales. It is thus crucial to address these challenges within the next decade.

Develop Joining and integration methods for HEMs (C35)

Sensitivity to heat input can erase the hard-won performance attributes derived from their unique chemistries and microstructures of advanced materials. Development of new techniques for joining dissimilar materials, such as metals to non-metals, is also needed.

²²⁴ Uday MB, Ahmad-Fauzi MN, Alias Mohd N, Srithar R. Current issues and problems in the joining of ceramic to metal. Joining Technologies [Internet]. 2016 [cited 2024 Jul 30];Ch 8. Available from: <u>https://doi.org/10.5772/64524</u>

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Welding and joining techniques are usually designed and optimized to serve particular purposes or for joining particular classes of materials. For example, while not originally designed for this, methods like tungsten inert gas (TIG), plasma transferred arc (PTA), and metal inert gas (MIG) welding are used to make weld overlays to add materials to surfaces as part of degradation management to extend service life of components. Other methods are now being optimized for 3D printing operations. Welding and joining techniques must be studied and optimized to join HEMs of the future at a reduced cost.

For example, weldments are a challenge for molten salt tanks due to their large size, long welding beads, need for multiple passes, and the use of backing plates. As a result of welding, high residual stress and distortion are often generated. Due to the size of the tanks, heat treatment to relieve residual stress is extremely difficult. Reduction in residual stresses and distortions through welding procedures (segment welding) and post-weld treatments (induction, ultrasonic treatment) are being pursued for optimizing weldment design and fabricability. Reduction in stress relaxation cracking (reheating cracking) susceptibility by using welding filler materials that produce microstructures with a more homogeneous composition and fewer precipitates is also being pursued. Similarly, studies are being performed to optimize weld groove geometries that reduce residual stress and are easy to implement in the field.

In molten salt tanks, claddings and coatings are increasingly being used, which increases joining difficulty and necessitates development new joining techniques. Cladding methods include explosion welding and centrifugal rotation, but these techniques do not eliminate the differences in chemistry and coefficient of thermal expansion (CTE) that creates strain during thermal cycling and may lead to cracking. Coating methods include thermal spray, air plasma spray, and electron beam-physical vapor deposition (EB-PVD).

Additional challenges encountered in welding and joining include chemical segregation; loss of ductility; porosity; slag formation; lack of fusion; limited or nonexistent solid-state diffusion; cracking, including ductility dip cracking; and significant generation of strain through material shrinkage. Each materials system comes with its own challenges that must be resolved for joining to be successful. Metal-to-ceramic joining is even more complex, due to mismatches in composition, coefficients of thermal expansion (CTE), melting points, and thermal conductivities and continuous functionally graded metal-to-ceramic materials do not yet exist.^{225,226} In ceramic-to-ceramic joining, especially for use in high temperature environments, the joining temperatures for brazing or diffusion bonding must exceed the ultimate use temperature of the joined assembly.²²⁷

It is therefore necessary to focus on specific material systems in researching joining solutions. While an exhaustive list of material systems necessary to achieve applicable target metrics and DOE emissions/energy goals is not reasonable to compile, there are some critical areas worth highlighting. Innovations in capabilities in joining in these systems could have key impacts. One is silicon carbide (SiC) to metal joining.²²⁸ Advances in this area would reduce the cost of advanced ceramic materials.

Advances required in this area are:

²²⁵ Yang L, Miyanaji H, Janaki Ram D, Zandinejad A, Zhang S. Functionally graded ceramic based materials using additive manufacturing: review and progress. Ceramic transactions /Ceramic transactions [Internet]. 2016 May 31 [cited 2024 Aug 28];43–55. Available from: <u>https://doi.org/10.1002/9781119236016.ch5</u>

²²⁶ Locatelli MR, Dalgleish BJ, Nakashima K, Tomsia AP, Glaeser AM. New approaches to joining ceramics for high-temperature applications. Ceramics International [Internet]. 1997 Jan [cited 2024 Aug 28];23(4):313–22. Available from: <u>https://doi.org/10.1016/S0272-8842(96)00024-7</u>

²²⁷ Locatelli MR, Dalgleish BJ, Nakashima K, Tomsia AP, Glaeser AM. New approaches to joining ceramics for high-temperature applications. Ceramics International [Internet]. 1997 Jan [cited 2024 Aug 28];23(4):313–22. Available from: https://doi.org/10.1016/S0272-8842(96)00024-7

²²⁸ Uday MB, Ahmad-Fauzi MN, Noor AM, Rajoo S. Current issues and problems in the joining of ceramic to metal. Joining Technologies [Internet]. 2016 Sep 21 [cited 2024 Aug 28]; Available from: <u>https://doi.org/10.5772/64524</u>

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- Functionally graded materials (e.g., a metal-ceramic composite with varying composition along a particular direction) and processing techniques (e.g., 3D printing with varying feed composition) which may reduce the joining problems for a metal-to-metal joint or a ceramic-to-ceramic joint.
- More advanced joining materials such as muti-principal element alloys (MPEA) for joining ceramics to metals
- Composite interlayer designs to reduce the abrupt mismatch of CTE (e.g., a MPEA with ceramic particles dispersed within the MPEA to control the CTE).

It is also necessary to explore novel techniques such as electric field assisted sintering (EFAS), which has been shown to facilitate diffusion bonds/welds with excellent solid-state diffusion of material across interfaces/joints (Figure 1818). It is expected that new joining techniques or the optimization of old ones will be needed for HEMs currently being developed or planned.



Figure 18. Example of INL carbon-carbon EFAS die heating during processing.

Advances in joining would have many benefits and market impacts. First, failure rates would be reduced, increasing longevity of systems and components and decreasing maintenance/operational cost. A reduction in capital costs may also be achieved in some cases. New joining techniques or optimized current ones seem to provide additional speed to complete the joining process, as well as make currently impossible or difficult to join materials accessible and will be one of the focus areas of technology development. It is expected that many powerful modeling and simulation tools (e.g., ICWE) will be used to optimize joining techniques to mitigate traditional and new challenges encountered. Progress in welding and joining will allow advanced materials to be used at a lower cost per part, using the expensive materials only where necessary. More corrosion resistant coatings or claddings derived from expensive exotic materials can be applied to cheaper materials to prevent corrosion, without compromising strength. Success shall be evaluated at operating conditions through mechanical and electrochemical testing in combination with microstructural characterization to reveal failure mechanisms. This will benefit many industries in a diverse array of energy and manufacturing sectors, including concentrating solar power/thermal (CSP/T), nuclear power, geothermal power, metal refining, specialty metals manufacturers, fabricators, feedstock and materials processing organizations

3.3 Focus Area 3: High-Performance Materials Recommendations

The action plan table below lists several details that should be used to inform funding strategies for next generation harsh environment materials research and development investments, as well as describing the roadblocks with the existing state of the art and challenges to be addressed for advanced harsh environment material technologies. Specific opportunities with associated timelines follow the action plan.

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Neglecting this R&D could have adverse implications across various energy technologies

Innovation pipeline choked off: It takes years for new materials to be manufacturing qualified, field certified, and utilized in commercial products. Though it may not be felt until later, if we do not begin to develop durable harsh environment materials with superior properties now, component property/performance requirements of advanced energy systems of the future will be difficult to meet.

Action Plan for Focus Area 3

Table 7. Action Plan for High-performance materials.

Scope					
Technologies for foundational harsh environment material stems	Accelerate the exploration, design, development, and demonstration of advanced high- performance structural and functional materials/components engineered for harsh service conditions in energy production/conversion, utilization, and storage applications, with consideration given to materials circularity and sustainability.				
Technologies of Interest:	With the broad energy application space in focus for this landscape, a plethora of material families are of interest. These include high entropy or multi-principal element materials, superalloys (Ni-, Co-, and Fe-based), refractory alloys, oxide dispersion strengthened (ODS) alloys, advanced high-strength steels, ductile intermetallic phases, bulk metallic glasses, monolithic technical ceramics (e.g., oxides, carbides, borides, nitrides, silicides, various electroceramics, and ceramics with room temperature plasticity), fiber-reinforced composites (e.g., ceramic matrix composites and metal matrix composites), cermets (ceramic/metal composites), MAX phases, functionally/compositionally graded materials, and ultra-wide bandgap semiconductors that can be used to fabricate in situ sensors (e.g., for operando measurement of strain, pressure, gas, temperature) as well as power electronic and control devices for service in extreme environments beyond the capability of more established semiconductor materials. Materials for various forms of energy production/conversion, energy utilization, and energy storage are of prime focus.				

Roadblocks	Challenges to pursue
 High-temperature service limitations of materials. Coupled harsh service environments (multiple simultaneous material stressors) usually present Ceramics often possess advantageous functional properties that cannot be obtained in other materials, but also low fracture toughness and plasticity Excessive material processing cost Incomplete knowledge of materials degradation mechanisms Material properties intricately tied to their processing history 	• Facilitation through tools such as multi-scale physics- based deterministic methods (e.g., integrated computational materials engineering) and data-driven stochastic methods (e.g., artificial intelligence, machine learning).

Stakeholders and Potential Roles				
Stakeholder	Role			
Product Manufacturers/Suppliers	 Synthesize and fabricate advanced materials with enhanced properties and improved performance in demanding service applications. Innovate in material properties, performance modeling and testing, and manufacturing qualification. 			
End Users/Original Equipment Manufacturers (OEMs)	• Selected material R&D pathways will deliver more efficient waste heat recovery systems, energy production/conversion, and energy storage systems, leading to increased energy savings and a higher likelihood of achieving energy goals.			

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ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C5	163	Develop corrosion resistant materials for hydropower (e.g. AI-Ce-Mg alloys)	UL	Greater corrosion resistance than Al6160	3	2.5	
C121	132	Develop bulk components made from ultra- high temperature ceramic materials (e.g., borides, carbides, oxides, nitrides) with improved ability to withstand oxidative/corrosive atmospheres and mechanical stresses	LL	OT > 1,500°C	6	1	
C112	118	Develop materials for handling high- temperature HTFs in nuclear reactor and CSP	UL	OT >700-750°C	3	2.5	
C133	81	Develop plasma facing materials for magnetic fusion reactors that are resistant to particle sputtering, neutron damage and high heat fluxes	UL	OT > 1,000°C	2	3	
C100	72	Develop durable materials for EGS wells (low pH environments)	UL	OT = 200-350°C	2	3	
C102	64	Develop casing, cement, drilling fluids, proppants, elastomers. Either new materials or ways of using existing materials	LL	OT > 250°C	6	1	(M)
C109	60	Develop ultra-high temperature CMCs with suitable oxidation/corrosion and thermal shock resistance, as well as optical properties like spectral selectivity for CSP/T applications	LL	OT > 1500°C	2	3	
C69	56	Develop materials for more efficient process heating (e.g. WHR and electrification)	UR	OT > 400°C	2	3	
C9	41	Develop new materials for offshore wind turbine leading edges	UL	Erosion resistance at blade tip speeds > 300 KM/br	3	2.5	
C96	31	Develop materials for supercritical wells	LL	OT > 375°C	4	2	
C101	21	Develop high-temperature, hard materials for deep geothermal well drilling	LL	OT > 300°C, penetrate rock at 100 ft/ <u>hr</u>	4	2	
C91	12	Leverage feedstock preparation for reactive sintering of high temperature ceramic systems.	UL	OT>1300°C (Achieve high degree of filament homogeneity, low viscosity, high elongation at break, and/or powder surface purity (e.g., native oxide reduction))	3	2.5	

Table 8. Challenges identified for FA	3 with potential impact and effort (p	pace of TRL advancement) needed.
U		

Materials for High Temperature Waste Heat Recovery

Develop materials and components for more efficient process heating (e.g. WHR and electrification) (C69)

Waste heat recovery involves capturing and redirecting waste heat generated by industrial processes to serve as an additional energy source elsewhere.²²⁹ IEDO notes that in the industrial sector, process heating consumes more energy than any other operation does and that this energy is predominantly sourced from fossil fuels. Therefore, maximizing efficiency and resource utilization, particularly in the thermal energy cascade (e.g., waste heat recovery, heat upgrading/reuse), is crucial for transitioning to electricity and other energy sources. IEDO focuses on waste

²²⁹ Cresko J, Rightor E, Carpenter A, Peretti K, Elliott N, Nimbalkar S, et al. Industrial Decarbonization Roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 23] p. 1–241. Available from: <u>https://www.energy.gov/sites/default/files/2022-09/Industrial%20Decarbonization%20Roadmap.pdf</u>

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heat recovery across five key sectors: iron and steel, chemical production, food and beverage, petroleum refining, and cement manufacturing.

Approximately 20%–50% of industrial energy input is lost as waste heat, including hot exhaust gases, cooling water, and heat dissipated from equipment surfaces and heated products, amounting to an estimated 5–13 quadrillion Btu/year.²³⁰ Recovering these waste heat losses presents an appealing opportunity for emissions-free and cost-effective energy resources, significantly benefiting the industrial sector.

Waste heat recovery technologies encompass systems-level solutions enabling the reuse of waste heat streams for other thermal processes and WHP electric technologies.²³¹ Additionally, waste heat can be stored using various thermal storage methods such as sensible, latent, or thermochemical storage, allowing for productive utilization when the generation of waste heat does not align directly with potential uses in terms of timing or heat demand.²³²

Various challenges hinder the design of more efficient heat recovery systems, necessitating research and development efforts in several areas. Current and emerging technical constraints involve producing cheaper materials suitable for high temperature streams, those with high chemical activity, and exhaust streams cooled below condensation temperatures. These materials are crucial for waste heat recovery systems utilized in industries such as nickel and steel production, iron and steel manufacturing, cement production, and hydrogen production, each of which presents unique temperature and chemical challenges. Additionally, there are knowledge gaps in developing materials resistant to corrosion, scaling, and fouling, which will be essential for reducing maintenance costs and increasing productivity. Furthermore, cost-effective materials that retain mechanical and chemical properties at high temperatures are needed to prevent dilution of waste heat so that energy quality is maintained for recovery. Other needed innovations include materials capable of withstanding thermal cycling and novel heat exchangers with improved heat-transfer coefficients. Moreover, developing low-cost manufacturing techniques for these technologies is essential. The overarching objective is to develop low-cost, novel WHR system materials and components resistant to corrosive contaminants and elevated temperatures, categorized into three temperature ranges: high temperatures (>400°C), medium temperatures (>200-400°C), and low temperatures (<100°C).

Success will be measured by the extent to which novel, low-cost corrosion and high temperature resistant materials for waste heat recovery systems are developed and deployed. Because most industries produce waste heat, the emergence of such materials is likely to benefit a wide range of operations. Examples include metal foundries, food and beverage companies, and chemical feedstock and processing organizations.

The sequence of research (R&D pathway) is to first develop cost-effective high-temperature, corrosion-resistant materials for WHR, then developing the manufacturing methods for WHR components fabricated from these materials, and then integration of these components into WHR systems, including components for the direct conversion of waste heat into electricity. WHR system components include: regenerative and recuperative burners; economizers for low-to-medium temperature WHR (finned tube and coiled tube, condensing and non-condensing) typically fabricated from Teflon, carbon, or stainless steel; waste heat boilers; air preheaters/heat exchangers, including metallic and ceramic recuperators (for medium-to-high temperatures), fixed and rotary regenerators (for high temperatures), and run around coils; plate heat exchangers; heat pipes (with screen mesh structure wicks) made from aluminum, copper, titanium, stainless steel, tungsten, or Inconel or Monel alloys; and heat recovery

https://www.energy.gov/sites/prod/files/2016/06/f32/QTR2015-6I-Process-Heating.pdf.

²³⁰ Johnson I, Choate W, Davidson A. Waste Heat Recovery: Technology and Opportunities in U.S. Industry. [Internet]. 2008 Mar [cited 2024 Jul 29] Available from: <u>https://doi.org/10.2172/1218716</u>

²³¹ U.S. Department of Energy, Quadrennial Technology Review 2015, Chapter 6: Innovating Clean Energy Technologies in Advanced Manufacturing: Technology Assessment for Process Heating [Internet]. Department of Energy; 2015 Sept [cited 2024 Jul 29]. Available from:

²³² Harvey AL, The latest in thermal energy storage. Power Magazine [Internet]. 30 June 2017 [cited 2024 Jul 29]. Available from: <u>https://www.powermag.com/thelatest-in-thermal-energy-storage</u>

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steam generators. (pressure systems). Additionally, devices for the direct conversion of recovered heat into electricity can be integrated into WHR systems. These direct conversion devices include not only thermoelectric and thermophotovoltaic generators, as discussed in the introduction section of the landscape, but also thermionic and piezoelectric generators.

This R&D pathway promises more efficient waste heat recovery systems, leading to increased energy savings and a higher likelihood of achieving energy goals. The established timeframe for advanced WHR materials and component development and deployment, between 2025 to 2030, aligns with that of IEDO's roadmap.

New Materials for Hydropower

Develop corrosion resistant materials for hydropower (e.g., AI-Ce-Mg alloys) (C5)

Hydropower has provided reliable, low-cost electricity for more than a century as the nation's first renewable source of electricity.²³³ New technologies and practices are emerging, and power systems are evolving to make hydropower more flexible and sustainable. This creates new opportunities for hydropower to be even more relevant and impactful in the nation's energy economy.²³⁴ In 2020, hydropower provided 7.3% of the electricity on the grid and accounted for 37% of U.S. renewable electricity generation.²³⁵ Global installed hydropower capacity in 2020 was 1,308 GW; it is expected to grow by approximately 60% by 2050 to help satisfy growing global energy demand and limit the rise of global temperature²³⁶ New and advanced high-performance materials, manufacturing techniques, and capabilities will play a role in achieving this goal. According to the WPTO multi-year program plan (MYPP), one of the office's foundational research activities is advanced materials and manufacturing for marine power applications, focusing on basic and applied science to increase longevity, reduce operations and maintenance costs, reduce capital costs, and improve energy capture performance. Innovation is required in four main areas: 1) new manufacturing and materials to lower component costs; 2) corrosion, biofouling, fatigue, and abrasion resistant materials; 3) new materials for fish screens; and 4) new materials for energy converter systems and subsystems such as converter hulls and tidal energy converter blades. Materials being investigated include lightweight alloys, including carbon fiber composites. The overarching goal is to bring these new materials and manufacturing methods to market cost effectively.

This landscape is one of the tools that can strengthen the current collaboration between AMMTO and WPTO to better understand the opportunities for advanced manufacturing and materials for marine energy.

Known constraints include knowledge gaps in:

• Developing cost-effective at-scale manufacturing capabilities for hydropower energy applications, resulting in long lead times and high costs for materials and components, including those targeted at the development of new, small, low-impact hydropower projects.

²³³ Waterpower Technologies Office. U.S. Department of Energy Waterpower Technologies Office Multiyear Program Plan. [Internet] Department of Energy. 2022 [cited 2024 Jul 31]. Available from: https://www.energy.gov/eere/water/multi-year-program-plan

²³⁴ Quaranta E,Davies P. Emerging and Innovative Materials for Hydropower Engineering Applications: Turbines, Bearings, Sealing, Dams and Waterways, and Ocean Power. Engineering [Internet]. 2022 [cited 2024 Jul 31];8:148–158. Available from: <u>https://doi.org/10.1016/j.eng.2021.06.025</u>

²³⁵ Energy Information Administration. Electricity in the U.S. [Internet]. Energy Information Administration; 2024 Feb [cited 2024 Jul 31]. Available from: <u>https://www.eia.gov/energyexplained/electricity/electricity-in-the-us.php#:~:text=Hydropower%20plants%20produced%20about%207.3,from%20renewable%20energy%20in%202 020</u>

²³⁶ International Hydropower Association. 2020 hydropower status report sector trends and insights. [Internet]. London: International Hydropower Association Central Office; 2020 [cited: 2024 Jul 31]. Available from: https://www.hydropower.org/publications/2020-hydropower-status-report

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- Developing advanced manufacturing techniques targeted at repair and replacement of older/legacy components, as well as those that can handle new designs that include embedded sensors for condition monitoring.
- Incorporating durable lightweight materials (e.g., carbon fiber and thermoplastic composites) that can resist corrosion, fatigue, erosion, and cavitation in a cost-effective way, as well as in advanced manufacturing techniques in marine power components.
- Developing cost-effective metal matrix composite ceramics components for structural and pressure boundary applications.

Specific objectives to be pursued with crosscutting benefits include the development of cost-effective lightweight materials and manufacturing techniques for hydropower components with enhanced fatigue, erosion, corrosion, and cavitation resistance.

Achieving applicable target metrics and DOE emissions/energy goals requires science-based engineering approaches for designing application-specific, cost-effective materials and developing the feedstocks for those materials. Utilizing computational tools, machine learning, and AI to analyze extensive historical data on alloy chemistry, material behaviors, and manufacturing processes is essential for producing suitable feedstocks. Furthermore, developing industrial-scale manufacturing capabilities is necessary for the widespread deployment of successfully developed materials and components.

Success will be measured by improved operational performance, removal of bottlenecks, and applicability across multiple fields. Specific measures include the successful development of cost-effective lightweight materials and manufacturing techniques for fatigue, erosion, corrosion, and cavitation resistance, as well as cost-effective metal matrix composite components for structural and pressure boundary applications. U.S. industries likely to benefit from this crosscutting R&D include power generation companies that are hydropower oriented as well as those that service and maintain the hydropower sector.

The sequence of addressing challenges involves developing cost-effective metal matrix composite components for structural and pressure boundary applications between 2025 and 2030, followed by developing ultra-lightweight materials for fatigue, erosion, corrosion, and cavitation resistance between 2030 and 2040.

This R&D pathway could help increase hydropower's market share and reduce its LCOE. It is aligned with WPTO market share growth goals for supplying reliable hydropower energy.

Materials for Nuclear Applications

Develop plasma facing materials for magnetic fusion reactors that are resistant to particle sputtering, neutron damage and high heat fluxes (C133)

Through its Advanced Materials Manufacturing Technology (AMMT) program, the DOE Nuclear Energy office seeks to impact the nuclear industry by developing high-performance radiation-, corrosion-, and high temperature-resistant materials for advanced manufacturing and by accelerating the deployment of AMMTs to enable reliable and economical nuclear energy.²³⁷ Often, nuclear plants and components therein must withstand these harsh environment conditions for periods exceeding 40 years. The irradiation challenges experienced by materials in nuclear power reactors are usually compounded by high temperature, high stress, and highly oxidizing or corrosive environments. Whereas traditional light or heavy water reactors operate at temperatures below 350°C, some reactors in the new generation of advanced gas cooled as well as molten salt and metal (coolant) reactors operate at over 1,000°C. The advent of nuclear fusion reactors will push materials under irradiation to even more extreme operating conditions, with the first-wall plasma-facing materials expected to face temperatures up to 1,000°C.

 ²³⁷ Li M, Andersson D, Dehoff R, Jokisaari A, Van Rooyen I, Cairns-Gallimore D. Advanced materials and manufacturing technologies (AMMT) 2022 roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 24]. Available from: <u>https://www.energy.gov/sites/default/files/2023-03/ne-ammt-roadmap-030823.pdf</u>

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coupled with continuous bombardment by highly energetic 14 MeV neutrons.^{238,239,240} The Office of Nuclear Energy's AMMT program has a goal to develop cost-effective manufacturing techniques for robust radiation-resistant materials and their accompanying feedstocks to support these and other technologies in nuclear energy. AMMTO is in a position to be able to provide valuable support to these efforts. Known technical roadblocks in the field include significant knowledge gaps in producing suitable high-performance, irradiation-resistant structural and first-wall (plasma-facing) materials for fusion reactors that can resist creep and high heat fluxes. Gaps also exist in the development of low-cost SiC fiber and other high-performance materials for fusion reactors to support license applications for nuclear power plant life extensions. Additionally, there are challenges in creating low-cost, high-performing advanced radiation-resistant materials that can withstand radiation and corrosion at operating temperatures above 1,000°C for molten and advanced reactors. The long lead times for materials and manufacturing technique qualification further compound these issues.

Crosscutting research opportunities exist for developing nuclear fusion materials. For instance, some DOE offices, like ARPA-E, have been pursuing these opportunities with initiatives such as the Creating Hardened And Durable fusion first Wall Incorporating Centralized Knowledge (CHADWICK) program. AMMTO will collaborate with other stakeholders by developing manufacturing methods for viable materials identified in efforts like CHADWICK. Moreover, collaborative research is essential for developing materials that resist irradiation at operating temperatures above 1,000°C in corrosive environments, which is critical for nuclear fission applications such as molten salt and metal reactors.

The capabilities needed to achieve these advanced materials for nuclear fusion goals include science-based engineering approaches to design application-appropriate, cost-effective high temperature irradiation and corrosion-resistant materials. The deployment of computational tools, as well as ML and AI, is necessary to gather and leverage the extensive data collected on alloy or materials chemistry, material behaviors, and characteristics, including those associated with manufacturing processes and pathways of irradiation-resistant materials. Developing industrial-scale manufacturing capabilities is crucial to support the widespread deployment of successfully developed alloys and their feedstock. Additionally, *in-situ* monitoring capabilities are needed to support manufacturing processes.

The knowledge gained from developing materials that resist temperature, irradiation, and corrosion (oxidation)induced degradation at operating conditions above 1,000°C can be leveraged across several areas, including high temperature materials and feedstock development. These advancements will contribute to lowering energy generation costs by reducing operational expenses (OpEx) and enabling plants and systems to operate at higher temperatures, higher neutron fluxes, and greater efficiencies. Success will be measured by the cost-effective production and deployment of high temperature irradiation- and corrosion-resistant materials for their identified applications, as well as the development of feedstock and advanced manufacturing methodologies to produce these materials economically and shorten their supply chains. U.S. industries likely to benefit include power generation and electronic component manufacturers.

Critical to success is the sequence in which research is pursued. The first priority is developing high-performance materials for molten salt and sodium-cooled fast reactors with superior creep, corrosion, and radiation resistance

²³⁹ Abdou M, Morley NB, Smolentsev S, Ying A, Malang S, Rowcliffe A, Ulrickson M. Blanket/first wall challenges and required R&D on the pathway to DEMO. Fusion Engineering and Design [Internet]. 2015 [cited 2024 Jul 31]; 100: 2–43. Available from: http://dx.doi.org/10.1016/j.fusengdes.2015.07.021

²³⁸ Kumar D, Hargreaves J, Bharj A, Scorror A, Hardinga LM, Dominguez-Andradea H, Holmes R, Burrows R, et al. The effects of fusion reactor thermal transients on the microstructure of Eurofer-97 steel. J of Nucl Mat [Internet]. 2021 [cited 2024 Jul 31];554:153084. Available from: <u>https://doi.org/10.1016/j.jnucmat.2021.153084</u>

²⁴⁰ Nagasaka T,Muroga T. 6.01 - Vanadium for nuclear systems. Comprehensive Nuclear Materials, 2nd edition [Internet]. 2020 [cited 2024 Jul 31];6. Available from: <u>https://doi.org/10.1016/B978-0-12-803581-8.00730-X</u>

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at operating temperatures above 1,000°C, including refractory alloys or coatings for component protection, in the 2030 to 2035 timeframe. The next priority, in the 2040 to 2050 timeframe, is developing high-performance materials for fusion reactors with superior creep, corrosion, and radiation resistance at operating temperatures above 500°C, including refractory alloys or coatings for component protection. Currently, this effort is still in the exploratory phase.

High Temperature, Oxidation/Corrosion-Resistant Materials

Develop ultra-high temperature CMCs with suitable oxidation/corrosion and thermal shock resistance, as well as optical properties like spectral selectivity for CSP/T applications (C109)

Develop bulk components made from ultra-high temperature ceramic materials (e.g., borides, carbides, oxides, nitrides) with improved ability to withstand oxidative/corrosive atmospheres and mechanical stresses (C121)

High-temperature oxidation/corrosion-resistant materials are essential in many industries. They can be found in numerous applications, including molten salt and liquid metal cooled nuclear reactors;²⁴¹ CSP;²⁴² geothermal technologies;²⁴³ various types of turbomachinery (gas, steam, and hydraulic turbines, jet and rocket engines, and heat recovery systems), especially those that handle supercritical fluids;^{244,245} and hydrogen production;²⁴⁶ among others. As such, the temperature conditions under which corrosion resistance must be maintained vary by application and system. This landscape addresses corrosion resistance materials for applications with widely varying temperatures, between 150°C to higher than 1,400°C.

Compact, high energy density generating plants and machinery are required to meet rising energy demand. To produce large quantities of energy efficiently, these systems must operate in corrosive environments at very high temperatures. Many high-temperature oxidation/corrosion-resistant materials exist on the market today, but many of them are cost-prohibitive for targeted applications. In other cases, the required materials for sustained, exceedingly high temperature operations in corrosive environments are still under development.^{247,248} The overarching goal is to produce high temperature corrosion-resistant materials cost effectively.

https://www.energy.gov/sites/default/files/2021-

 ²⁴¹ Li M, Andersson D, Dehoff R, Jokisaari A, Van Rooyen I, Cairns-Gallimore D. Advanced materials and manufacturing technologies (AMMT) 2022 roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 24]. Available from: <u>https://www.energy.gov/sites/default/files/2023-03/ne-ammt-roadmap-030823.pdf</u>
 ²⁴² Silverman TJ, Huang H. Solar Energy Technology Office Multiyear program Plan. [Internet] Department of Energy; 2021 May [cited: 2024 Jul 31];DOE/EE-2346. Available from:

^{06/}Solar%20Energy%20Technologies%20Office%202021%20Multi-Year%20Program%20Plan%2006-21.pdf ²⁴³ Porse S. Geothermal technologies office fiscal years 2022-2026 multi-year program plan. [Internet] Department of Energy; 2022 Feb [cited: 2024 Jul 31];DOE/EE-2557. Available from:

https://www.energy.gov/sites/default/files/2022-02/GTO%20Multi-Year%20Program%20Plan%20FY%202022-2026.pdf

²⁴⁴ Allison TC, Moore J, Pelton R, Wilkes J, Ertas B. Turbomachinery. Elsevier eBooks [Internet]. 2017 Jan 1 [cited 2024 Aug 28];147–215. Available from: <u>https://doi.org/10.1016/B978-0-08-100804-1.00007-4</u>

 ²⁴⁵ Guinzburg A. Pumping machinery. ASME Fluids Engineering Division Annual Summer Meeting. [Internet] 2001
 May 29 [cited: 2024 Jul 31]. Available from: https://files.asme.org/divisions/fed/16300.pdf

²⁴⁶ Ahad MT, Bhuiyan MMH, Sakib AN, Becerril Corral A, Siddique Z. An overview of challenges for the future of hydrogen. Materials [Internet]. 2023 Jan 1 [cited 2024 Aug 28];16(20):6680. Available from: https://doi.org/10.3390/ma16206680

²⁴⁷ Pillai R, Chyrkin A, Quadakkers WJ. Modeling in high temperature corrosion: a review and outlook. Oxidation of Metals [Internet]. 2021 May 21 [cited 2024 Aug 28];96(5-6):385–436. Available from: https://doi.org/10.1007/s11085-021-10033-y

²⁴⁸ Li K, Zhu Z, Xiao B, Luo JL, Zhang N. State of the art overview material degradation in high-temperature supercritical CO2 environments. Progress in Mat Sci [Internet]. 2023 Jul 1 [cited 2024 Aug 28];136:101107. Available from: https://doi.org/10.1016/j.pmatsci.2023.101107

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Technical roadblocks include knowledge gaps in producing:

- Suitable materials for molten salt-based concentrating solar-thermal power towers, heat exchangers, and thermal energy storage systems (2025–2030 timeframe).
- Structural materials that exhibit suitable molten salt corrosion resistance above 700°C (2030–2035 timeframe).
- Performance materials for molten salt reactors with superior creep, corrosion, and radiation resistance (2030–2035 timeframe).
- Refractory alloys or coatings for component protection in molten salt reactors (2030-2035 timeframe).
- High-performance structural materials for sodium-cooled fast reactors with superior creep, corrosion, and radiation resistance (2030–2035 timeframe).
- Ultra-high-temperature monolithic ceramics (e.g., MAX phases) and CMCs with suitable thermal shock and oxidation resistance and optical properties such as spectral selectivity for use in CSP/T applications (2035–2040 timeframe).

Crosscutting research opportunities focus on developing materials with excellent corrosion resistance at service temperatures above 700°C in molten salt systems, molten sodium metal systems, and other high temperature environments. This includes materials that can withstand service temperatures above 1,400°C in non-molten salt and non-sodium liquid metal high temperature other environments, as well as materials that maintain corrosion resistance at moderately high temperatures (up to 430°C) in other applications, such as geothermal systems.

To achieve this material developments, several capabilities are needed. Science-based engineering approaches are essential for designing cost-effective, high-temperature oxidation/corrosion-resistant materials. The deployment of computational tools, along with machine learning and AI, is crucial for analyzing extensive data on alloy chemistry, material behaviors, and manufacturing processes. Developing industrial-scale manufacturing capabilities will support the widespread deployment of these materials, and *in situ* monitoring will enhance manufacturing processes.

Achieving these advanced materials developments will result in materials that resist high temperatures and oxidation/corrosion-induced degradation at operating conditions between 700 and 1,000°C. The knowledge gained from developing these materials can be leveraged to create irradiation-resistant materials and those that can withstand even higher temperatures of 1,400-1,500°C. Additionally, developing optimized feedstock for advanced manufacturing of these materials will help lower energy generation costs by reducing operational expenses (OpEx) and enabling higher temperatures and therefore higher efficiencies in plants and systems. Success will be marked by the cost-effective production and deployment of high temperature corrosion-resistant materials, the development of feedstock and advanced manufacturing methodologies, and the shortening of supply chains. Success will also be measured by the number of new technologies these materials enable and by their impact on cost reductions for existing technologies. U.S. industries likely to benefit include those in the power generation space, as well as well as heavy industries such as smelters, casters, and forgers.

This research opportunity requires a rigorous and sequential approach. From 2025 to 2030, the focus will be on developing structural and functional materials for molten salt-based concentrating solar-thermal power towers, heat exchangers, and thermal energy storage systems. From 2030 to 2035, the goal is to develop high-performance materials for molten salt and sodium-cooled fast reactors with superior creep, corrosion, and radiation resistance, including refractory alloys or coatings for component protection. From 2035 to 2040, the focus could be on development of advanced ultra-high temperature monolithic ceramics (e.g. MAX phases) and CMCs (e.g., carbon fiber reinforced borides) with oxidation/corrosion and thermal shock resistance and suitable optical properties (i.e., spectral selectivity) for possible application as high-temperature solar absorbers in CSP systems and in concentrated solar thermal (CST) systems for driving endothermic reactions at high temperatures such as the production of hydrogen and sustainable aviation fuels.
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Well Materials for Geothermal Energy

Develop casing, cement, drilling fluids, proppants, elastomers, new materials or ways of using existing materials (C102)

Naturally occurring geothermal systems, known as hydrothermal systems, are characterized by three essential elements: heat, fluid, and permeability at depth.²⁴⁹ Enhanced geothermal systems (EGS) are artificially created reservoirs in areas with hot rock but limited natural permeability or fluid saturation. The Geothermal Technologies Office (GTO) envisions a robust domestic geothermal sector contributing to a diverse energy sector.²⁵⁰ Accessing the subsurface through drilled and completed wells is essential for all forms of geothermal energy exploration, characterization, and development. The costs associated with accessing the reservoir are critical factors determining the economic viability of geothermal energy projects, making cost reduction imperative.²⁵¹ Geothermal wells and wellbores endure extreme temperature, pressure, and chemical conditions that strain well construction materials and often lead to failure, resulting in significant repair costs for operators.

Common materials used in geothermal well construction include elastomers for seals, packers, and motors; metals for casing and drilling tools; organic and inorganic components in cements, solders; bearing materials and lubricants. Casing materials and cement constitute up to 50% of the cost of a geothermal well, underscoring the importance of cost reduction efforts.^{252,253} IEDO is exploring improved cement technologies to reduce manufacturing costs, while AMMTO focuses on enabling technologies from electronics to elastomers that can withstand harsh drilling conditions.²⁵⁴ GTO's MYPP prioritizes efforts to address these challenges, focusing on three key areas: elastomers, lower cost and high-performance casing, and lower cost and high-performance cement. These efforts aim to enhance materials that currently underperform and to reduce costs without compromising performance.

Current and emerging technical constraints on the application landscape include the need for specialized materials and tool designs for high temperature environments. There are significant knowledge gaps in producing better casing materials and fabrication methods to reduce the cost of drilling geothermal wells. The cost of casing materials and cement accounts for about 50% of the total cost of a geothermal well, with steel being the predominant material. Research aims to use alternative materials and leaner casing designs for safe, long-term well operations, as well as to develop cost-effective cement production technologies, though this latter area is primarily handled by IEDO. The temperature requirement for casing and cementitious materials is 225°C and above.

Another constraint is the need for durable high temperature elastomers for seals and electric power components used in bottom hole assembly components. These components, which include motors, steering systems, logging-while-drilling/measurement-while-drilling tools, shock subs, and other tools, must be durable at temperatures above

https://www.energy.gov/eere/geothermal/articles/geovision-full-report-0

²⁴⁹ Department of Energy. Clean domestic power. [Internet] Department of Energy; 2012 Feb [cited: 2024 Jul 31]; DOE/GO-102012-3542. Available from: <u>https://www.energy.gov/eere/geothermal/articles/geothermal-technologies-program-fact-sheet</u>

 ²⁵⁰ Department of Energy. Geothermal Technology Office Fiscal Years 2022-2026 Multi-Year Program Plan.
 [Internet]. Department of Energy; 2022 Feb [cited 2024 Jul 31]; DOE/EE-2557. Available from: https://www.energy.gov/eere/geothermal/articles/geothermal-technologies-office-multi-year-program-plan-fy-2022-2026

²⁵¹ Department of Energy. GEO Vision: Harnessing the Heat Beneath our Feet. [Internet] Department of Energy; 2019 May [cited 2024 Jul 31]; DOE/EE–1306, MAY 2019.

²⁵² Lowry T, Finger J, Carrigan C, Foris A, Kennedy M, Corbet T, Doughty C, et al. GeoVision analysis: Reservoir Maintenance and Development Task Force Report. [Internet] Sandia National Laboratory (NM); 2017 [cited 2024 Jul 31];SAND2017-9977. Available from: <u>https://doi.org/10.2172/1394062</u>

²⁵³ Cresko J, Rightor E, Carpenter A, Peretti K, Elliott N, Nimbalkar S, et al. Industrial Decarbonization Roadmap [Internet]. Department of Energy; 2022 Sep [cited 2024 Jul 23];p.1–241. Available from: <u>https://www.energy.gov/sites/default/files/2022-09/Industrial%20Decarbonization%20Roadmap.pdf</u>

²⁵⁴

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175°C. Knowledge gaps exist in improving elastomers or finding alternatives to the organic elastomers currently used, which is crucial for developing high temperature drilling tools, casing, and test packers.

Significant knowledge gaps also exist in developing high-performance, low-cost materials and approaches for well construction and reservoir development, including casing, cement, drilling fluids, proppants, and elastomers. Materials for electronic components that can log data long-term at temperatures above 225°C are also needed. Advanced manufacturing innovations and tools that could reduce costs for all geothermal resource technologies are needed, including manufacturing with high-grade materials, specialized geometries, novel coatings for downhole equipment, and new well construction materials. Additionally, materials must be durable under the conditions of EGS HT wells at 200°C-350°C in acidic environments.

Future goals that have crosscutting benefits include reducing in-ground materials costs (casing and cement) by developing manufacturing methods to address the outlined issues. Since casing and cement costs account for up to 50% of geothermal well construction costs, reducing these costs is crucial. Achieving these advanced materials goals requires science-based engineering approaches to design cost-effective materials and their feedstock development. The deployment of computational tools, as well as ML and AI, is essential to leverage extensive historical data on alloy or materials chemistry, behaviors, and manufacturing processes. Development of industrial-scale manufacturing and in situ monitoring capabilities to support these processes is also necessary.

Pursuing crosscutting advanced materials and manufacturing R&D can benefit DOE priority areas such as energy production, storage, and utilization. Reducing the time to complete a well to depth can substantially impact the cost of drilling a geothermal well; for example, doubling the average daily drilling rate could reduce the drilling cost by 10–15%. Success will be measured by the development of high temperature, corrosion-resistant, durable materials that can prolong the life cycles of geothermal wells and bottom hole components, reducing costs and improving geothermal project economics. U.S. industries likely to benefit from this crosscutting R&D include piping, well lining, and energy generation companies.

Selected high-impact R&D pathways can lead to cost reductions in drilling and maintaining geothermal wells and can contribute to achieving a diversified energy sector.

3.4 Focus Area 4: New Paradigm Materials Manufacturing Processes Recommendations

The action plan table below lists several details that should be used to inform funding strategies for next generation manufacturing research and process development investments for harsh environment materials, as well as describing the roadblocks with the existing state of the art and challenges to be addressed for advanced manufacturing technologies. Specific opportunities with associated timelines follow the action plan.

Neglecting this R&D could have adverse implications across various energy technologies

Increased failure rates: Incomplete R&D efforts often lead to inadequate understanding of material/component performance and behavior, manufacturing nuances, and design limitations.

Quality and reliability issues: Without thorough R&D, the quality and reliability of manufactured components may suffer due to unforeseen material defects, suboptimal manufacturing processes, or inadequate design considerations.

Cost overruns and delays: R&D serves as a critical phase for identifying and mitigating potential issues early in the development cycle. It is necessary to avoid costly design flaws, production inefficiencies, and post-production remediation efforts.

Missed innovation opportunities: Inadequate R&D stifles innovation potential, limiting opportunities for market differentiation, competitive advantage, and long-term business success.

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Action Plan for Focus Area 4

Table 9. Action Plan for New Paradigm Materials Manufacturing Processes.

Scope						
Technologies for platform manufacturing systems for harsh environment materialsDrive improvements to existing manufacturing technologies as well as develop and de competitive novel AMTs with the highest possible degree of process repeatability, reproducil and sustainability to produce HEM components at industrially relevant scales with consist high quality in conformance to design specifications. Success for FA4 will improve capabilities, efficiencies, and cost competitiveness of traditional HEM bulk component fabric and coating/cladding methods as well as advance the technology readiness levels (TRL AMTs, advanced characterization techniques, and feedstock materials production ro Manufacturing routes are sought that are capable of competitively producing fully dense porosity), high strength, high dimensional precision and shape fidelity; high-performance or parts/coatings with lower residual stress; or UFG high strength HEMs from secondary (so feedstock with lower environmental impacts.						
Technologies of Interest:Harsh environment components can be fabricated by a variety of traditional manufacturin technologies and AMTs, including additive manufacturing (e.g., various kinds of 3D printing subtractive manufacturing (e.g., machining and drilling), and formative/deformation processir (e.g., casting, forging, rolling, and extrusion). The latter also includes powder metallurg processing techniques (e.g., HIP, EFAS, and high-energy ball milling and compaction) and SP for the production of bulk, sheet, and tubular UFG components. Some of the main challenges AMTs and SPD processing are the limited throughput and small sample size, including the lengi and cross-sectional area. Convergent/hybrid manufacturing routes also exist. Components f service in harsh environments are high-performance parts engineered for demandir applications. As such, the highest quality is required.						
Roadblocks Challenges to pursue						
 Excessive material processing of Inadequate supply of process for precursors Incomplete knowledge of how preaterial properties Scalability of process to fabricat components Most fabrication processes indu- manufactured components, whi and be detrimental to the perfor Quantifying residual stress thro- difficult Complex part geometries not ex- produced components 	cost; low throughput eedstock materials or processing parameters impact tion of large-scale NNS uce residual stress in tich can lead to part distortion mance of the component ugh modeling and simulation asily fabricated erial performance with AMT-	 Facilitation through tools such as multi-scale physics- based deterministic methods (e.g., integrated computational materials engineering) and data-driven stochastic methods (e.g., artificial intelligence and machine learning). A suite of smart manufacturing digital tools (e.g., sensors and digital twins) to monitor, optimize, and adjust operational parameters in real time, particularly with self-learning or autonomous closed-loop control systems, in order to more efficiently achieve production of components with the desired properties. A key challenge with FA4 is the re-establishment of not only large-scale production capabilities (tonnage quantities) but also recapturing expertise on AMTs through education and workforce development efforts. 				
	Stakeholders and F	Potential Roles				
Stakeholder		Role				
Product Manufacturers/Suppliers	 Synthesize and fabricate a performance in demanding Innovate in material proper qualification. 	advanced materials with enhanced properties and improved g service applications. arties, performance modeling and testing, and manufacturing				
End Users/Original Equipment Manufacturers (OEMs)	Selected material R&D pail energy production/conversions savings and a higher likelih	thways will deliver more efficient waste heat recovery systems, sion, and energy storage systems, leading to increased energy nood of achieving energy goals.				

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ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C16	1079	Lower the cost of AMTs for high temperature alloys	LR	Cost parity with traditional processes	4	2	
C7	1022	Develop materials and components operating in harsh environment with circularity in terms of recycling.	LR	Recyclable materials	4	2	
C18	749	Develop AMTs to make complex structures using HEMs	LR	High surface area to volume ratio	5	1.5	
C28	654	Deploy feedstock preparation for extreme environment materials	LR	Industrial scale homogenous, narrow PSD powders	5	1.5	
C2	609	Employ nondestructive evaluation (NDE) methods for large part analysis (porosity, internal cracks, grain structure/size)	UR	NDE for 10+ ton parts	2	3	
C3	514	Scale-up of large component manufacturing including forging of pressure vessel via methods such as DED-AM, PM-HIP	UR	10+ ton parts	3	2.5	
C77	270	Domestic fabrication of high-temperature ceramic and CMC components must scale, and their costs must be reduced, to meet growing demand	UR	Densification infrastructure for processing temperatures above 1700°C including sintering and faster infiltration and Advanced Mfg Techniques to create complex geometry parts with tailored properties and lower residual porosity (< 5%) not achievable using traditional methods	3	2.5	
C81	195	Lower the cost and energy input for manufacturing of high-temperature ceramics and composites	LL	50% reduction in cost and energy input	5	1.5	
C13	180	Develop 3D printed continuous fiber composite design for custom anisotropic thermal transport, electrical and mechanical properties. Immediate use as carbon-carbon EFAS tooling.	UR	50% energy savings	2	3	
C71	136	Enable near net shaping of hard, brittle, high temperature ceramics using unique die design or 3D printed preforms and pressure transfer media in EFAS	LR	50% energy savings	4	2	
C42	132	Develop manufacturing and densification processes for ceramic and CMC materials for hydrogen turbine hot gas path components.	LL	OT > 1600°C	4	2	
C82	129	Securing a domestic Supply of Critical HEM Precursor Materials	UR	50% reduction in \$ and lead times	3	2.5	
C129	87	Develop manufacturing of high-performance (creep resistant, radiation resistant) structural materials for fusion reactors	UL	OT > 1000°C	2	3	
C8	86	Scale up continuous/high-throughput EFAS system	UR	Processing times < 30 min	2	3	
C21	78	Develop advanced manufacturing of ceramics (Si3N4, ZrO2) for full-ceramic rotating shaft applications	UR	50% \$ reduction	3	2.5	

Table 10. Challenges identified for FA4 with potential impact and effort (pace of TRL advancement) needed.

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ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C50	61	Develop functionally graded and interpenetrating phase CMCs and the processes to fabricate them, to create very high temperature capable materials	UR	OT > 1600°C	3	2.5	
C46	60	Develop advanced preforming and densification processes need to be developed for ceramic and CMC structures for TPMS high heat transfer efficiency, high temperature heat exchangers for industrial decarbonization.	UR	heat transfer coefficient > 8 W/m^3*K	3	2.5	
C43	57	Develop fabrication processes for high efficiency, high-temperature heat exchangers	UR	OT > 1400°C	3	2.5	
C111	53	Produce SiC/SiC composite as structural material for housing molten salt heat storage applications. Cost of SiC fiber must be reduced for SiC/SiC composites cost to be competitive.	LL	> 75% reduction in \$ of SiC fiber	4	2	
C122	51	Develop Hybrid Manufacturing Methods for large NNS parts	UR	10+ ton parts	3	2.5	(R)
C85	36	Develop power conversion and associated HEM heat exchangers in High temperature systems has not yet been demonstrated over durations relevant to industry (e.g., CSP and high temperature reactor)	UR	OT > 400°C for 30 years	2	3	
C95	19	Develop novel cementitious materials for applications in geothermal wells.	UL	Non-OPC formulations	2	3	

Abrasion and Wear-Resistant Materials

Develop advanced manufacturing of ceramics (Si₃N₄, ZrO₂) for full-ceramic rotating shaft applications (C21)

Mechanical energy transmission via shafts from turbines to generators or vice versa is needed in a broad range of industries. Large gearboxes are needed for diffuse renewable energy such as wind and hydroelectric power, and wind turbine gearboxes have been identified as critical components due to harsh service conditions.^{255,256} In addition to contact and bending fatigue, degradation mechanisms include wear, scuffing, fretting, and corrosion pitting. Severe tribological conditions (friction, wear) are also encountered in gearboxes of hydropower plants where flexible operation requires frequent starting and stopping. In addition to carburization (absorption of carbon) and nitriding (formation of nitrides) treatments to harden gear and bearing surfaces, hard and low friction coatings have the potential to significantly increase surface fatigue life and gear efficiency.

 ²⁵⁵ Bhardwaj U, Teixeira A, Guedes Soares C. Reliability prediction of an offshore wind turbine gearbox.
 Renewable Energy [Internet]. 2019 Oct [cited 2024 Aug 29];141:693–706. Available from: https://doi.org/10.1016/j.renene.2019.03.136

²⁵⁶ Salameh JP, Cauet S, Etien E, Sakout A, Rambault L. Gearbox condition monitoring in wind turbines: A review, Mechanical Systems and Signal Processing [Internet]. 2018 Oct [cited 2024 Jul 31];111:251–264. Available from: <u>https://doi.org/10.1016/j.ymssp.2018.03.052</u>

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Diamond-like carbon (DLC) coatings have demonstrated the potential for improvement in gear lifetime (see Figure 19b).^{257,258,259} Other types of hard coatings include carbide-based coatings as well as MoS₂-containing coatings.²⁶⁰ Advanced deposition techniques such as laser cladding have also been explored to achieve multi-layer coatings.²⁶¹

Limitations for the development of coatings for severe tribological applications include:

- Complex and diverse degradation mechanisms requiring multi-functional coatings.
- Difficult deposition of multi-layer multi-functional coatings.
- Specific tools for coating deposition required for large gearbox components.
- High cost of coating deposition compared with carburizing or nitriding treatments.

Some research opportunities to overcome these limitations are:

- New cost-effective fabrication and deposition techniques (directed energy deposition [DED], chemical/physical vapor deposition [CVD/PVD], cold spray, laser cladding, etc.).
- Local control of microstructure and composition via advanced manufacturing resulting in coatings with graded structures possessing unique mechanical and tribological properties (friction behavior, hardness, shear strength, fracture toughness, wear resistance, and rolling contact fatigue life), reliable bonding with the substrate, and compatibility with the lubricant.
- Development of coatings based on Si₃N₄ and other high-performance materials that are too expensive to be used for large bulk gearbox components.

Industries likely to benefit from research include wind turbine manufacturers and end-users, the hydropower industry, and bearing manufacturers. The research sequence starts in the 2025 to 2030 timeframe with the development of coatings with superior tribological performance using advanced deposition techniques. Demonstration of in-service long-term performance of coatings exposed to complex and diverse degradation mechanisms follows in the 2030 to 2035 timeframe.

²⁵⁷ Krantz T, Cooper C, Townsend D, Hansen B. Increased surface fatigue lives of spur gears by application of a coating. J of Mech Design [Internet]. 2004 Nov [cited 2024 Jul 31]; 126: 1047-1054. Available from: https://doi.org/10.1115/1.1799651

²⁵⁸ Wu J, Wei P, Liu G, Chen D, Zhang X, Chen T, Liu H. A comprehensive evaluation of DLC coating on gear bending fatigue, contact fatigue, and scuffing performance. Wear [Internet]. 2024 Jan 15 [cited 2024 Jul 31]; 536-537: 205177. Available from: <u>https://doi.org/10.1016/j.wear.2023.205177</u>

²⁵⁹ Jiang JC, Meng WJ, Evans AG, Cooper CV. Structure and mechanics of W-DLC coated spur gears, Surface and Coatings Technology [Internet] 2003 Nov-Dec [cited 2024 Jul 31];176:50–56. Available from: https://doi.org/10.1016/S0257-8972(03)00445-6

²⁶⁰ Martins RR, Amaro R, Seabra J. Influence of low friction coatings on the scuffing load capacity and efficiency of gears. Tribology International [Internet]. 2008 Apr [cited 2024 Jul 31];41:234–243. Available from: https://doi.org/10.1016/j.triboint.2007.05.008

²⁶¹ Wang X, Zhang Z, Men Y, Li X, Liang Y, Ren L. Fabrication of nano-TiC functional gradient wear-resistant composite coating on 40Cr gear steel using laser cladding under starved lubrication conditions. Optics and Laser Technology [Internet] 2020 [cited 2024 Jul 31]; 126: 106136. Available from: https://doi.org/10.1016/j.optlastec.2020.106136

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Figure 19. TEM cross-sectional micrographs (a) of an As-deposited W-DLC coated steel spur gear showing the W-C:H layer/transition layer(T)/Cr adhesion layer/steel structure (b). Reproduced from Wang et al., 2020.²⁶²

Secure and Sustainable HEM Precursors

Develop manufacturing of high-performance (creep resistant, radiation resistant) structural materials for fusion reactors (C129)

Irradiation challenges experienced with materials in nuclear power reactors are coupled with high temperatures, high stress, and highly oxidizing or corrosive environments. Advanced Materials Manufacturing Technology (AMMT) program run by DOE's Nuclear Energy office seeks advancements to benefit the nuclear industry through development of high-performance radiation-, corrosion- and high temperature-resistant materials for use in advanced manufacturing techniques, and by accelerating the deployment of advanced materials and manufacturing technologies to enable reliable and economical nuclear energy.²⁶³ Often, the plants and their components are required to last for more than gas cooled as well as molten salt and liquid metal cooled, some of which operate at over 1,000°C, exacerbate the irradiation issue because of the increase to even more extreme operating temperatures compared with traditional light or heavy water reactors that operate at temperatures below 350°C

https://doi.org/10.1016/j.optlastec.2020.106136

²⁶² Wang X, Zhang Z, Men Y, Li X, Liang Y, Ren L. Fabrication of nano-TiC functional gradient wear-resistant composite coating on 40Cr gear steel using laser cladding under starved lubrication conditions. Optics and Laser Technology [Internet] 2020 [cited 2024 Jul 31];126:106136. Available from:

²⁶³ Li M, Andersson D, Dehoff R, Jokisaari A, Van Rooyen I, Cairns-Gallimore D. Advanced Materials Manufacturing Technologies (AMMT) 2022 Roadmap [Internet]. Department of Energy; 2022 [cited 2024 Jul 29]; ANL-23/12. Available from: <u>https://www.energy.gov/ne/articles/advanced-materials-and-manufacturing-technologies-2022-roadmap</u>

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developed, further push materials under irradiation to even more extreme operating conditions, with the first plasmafacing materials expected to face up to 550°C coupled with 14 MeV neutrons.^{264,265,266}

Known technical roadblocks in the field include significant knowledge gaps in producing suitable high-performance irradiation-resistant structural and first-wall (plasma-facing) materials for fusion reactors that can resist creep and high heat fluxes. There are also gaps in developing low-cost SiC fiber materials for fusion reactors and high-performance materials to support license applications for nuclear power plant life extensions. Additionally, there are challenges in creating low-cost, high-performing advanced radiation-resistant materials that can withstand radiation and corrosion at operating temperatures above 1,000°C for molten and advanced reactors. The long lead times for materials and manufacturing technique qualification further compound these issues. In many instances, either the ability to manufacture the feedstocks does not exist or the ability to scale their manufacture is not economical due to currently low market demand for these materials. Additionally, from feedstocks to components, a robust domestic supply chain does not exist for advanced manufacturing.

Crosscutting research opportunities exist for developing nuclear fusion materials. For instance, some DOE offices, like ARPA-E, have been addressing this issue with initiatives such as CHADWICK (Creating Hardened and Durable Fusion First Wall Incorporating Centralized Knowledge). AMMTO will collaborate with other stakeholders by developing manufacturing methods for viable materials identified in efforts like CHADWICK. Moreover, collaborative research is essential for developing materials that resist irradiation at operating temperatures above 1,000°C in corrosive environments, which is critical for nuclear fission applications such as molten salt and metal reactors.

Science-based computational approaches are needed to design application-appropriate, cost-effective high temperature irradiation and corrosion-resistant materials. The deployment of such computational tools, as well as ML and AI, is necessary to gather and leverage the extensive data collected on alloy or materials chemistry, material behaviors, and characteristics, including those associated with manufacturing processes and pathways of irradiation-resistant materials. Developing industrial-scale manufacturing capabilities is crucial to support the widespread deployment of successfully developed alloys and their feedstocks. Additionally, *in situ* monitoring capabilities are needed to support manufacturing processes.

The knowledge gained from developing materials that resist temperature, irradiation, and corrosion (oxidation)induced degradation at operating conditions above 1,000°C can be leveraged across several areas, including high temperature materials and feedstock development. These advancements will contribute to lowering energy generation costs by reducing operational expenses (OpEx) and enabling plants and systems to operate at higher temperatures, higher neutron fluxes, and greater efficiencies.

Success will be measured by the cost-effective production and deployment of high temperature irradiation and corrosion-resistant materials for their identified applications, as well as the successful development of feedstock and advanced manufacturing methodologies to produce these materials economically and shorten supply chains.

 ²⁶⁴ Kumar D, Hargreaves J, Bharj A, Scorror A, Hardinga LM, Dominguez-Andradea H, Holmes R, Burrows R, et al. The effects of fusion reactor thermal transients on the microstructure of Eurofer-97 steel. J of Nucl Mat [Internet] 2021 Oct [cited 2024 Jul 29];554:153084. Available from: https://doi.org/10.1016/j.jnucmat.2021.153084
 ²⁶⁵ Abdou M, Morley NB, Smolentsev S, Ying A, Malang S, Rowcliffe A, Ulrickson M. Blanket/first wall challenges and required R&D on the pathway to DEMO. Fusion Eng and Des [Internet]. 2015 Nov [cited 2024 Jul 29]; 100: 2–43. Available from: http://dx.doi.org/10.1016/j.jnucmat.2021.153084

²⁶⁶ Nagasaka T, Muroga T. 6.01 - Vanadium for nuclear systems. Comprehensive Nucl Mat 2nd edition [Internet]. 2020 [cited 2024 Jul 29]; 6. Available from <u>https://doi.org/10.1016/B978-0-12-803581-8.00730-X</u>

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U.S. industries likely to benefit include power generation, power management, power storage, and supporting manufacturers.

Critical to success is the sequence in which research is pursued. The first priority is developing high-performance materials for molten salt and sodium-cooled fast reactors with superior creep, corrosion, and radiation resistance at operating temperatures above 1,000°C, including refractory alloys or coatings for component protection (2030–2035). The next priority is developing high-performance materials for fusion reactors with superior creep, corrosion, and radiation resistance at operating temperatures above 500°C, including refractory alloys or coatings for component protection (2040–2050). Currently, this materials effort is still in the exploratory phase.

Deploy feedstock preparation for extreme environment materials (C28)

Developing suitable feedstock for AM is crucial for ensuring the production of high-quality parts. AM feedstock comes in various form factors and compositions.²⁶⁷ The two most common form factors are powder and wires. Powders are extensively used in techniques like laser powder bed fusion (L-PBF), direct laser deposition (DLD), laser engineered net shaping (LENS), digital laser printing (DLP), and EFAS. Depending on the technique, these powders can be used with or without a binder to aid printing. For instance, binders are typically required with DLP and the newly developed Continuous Electric-Field Assisted Sintering (CEFAS) system at Idaho National Laboratory (Figure 20). Wires are used in techniques like wire arc additive manufacturing (WAAM), the multi-wire variant (mWAAM), and wire laser additive manufacturing (WLA). Powders, whether they consist of pure metals, alloys, oxides, nitrides, borides, or carbides, must have specific chemical and physical properties for optimized processing through the required machine and for good product outcomes.²⁶⁸ Important characteristics include particle morphology, size distribution, and the ability of the powder particles to flow.^{269,270,271,272,273}

²⁶⁷ Mathias LET, Pinotto VE, Batisto BF, Rojas-Arias N, Figueira G, Adreoli AF, Gargarella P. Metal powder as feedstock for laser-based additive manufacturing: From production to powder modification. J of Mat Research [Internet] 2024 Jan [cited 2024 Jul 29];39:19-47. <u>https://doi.org/10.1557/s43578-023-01271-8</u>

²⁶⁸ Khairallah SA, Anderson AT, Rubenchik A, King WE. Laser powder-bed fusion additive manufacturing: physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones. Acta Mater. 2016 [cited 2024 Jul 29];108:36–45. <u>https://doi.org/10.1016/j.actamat.2016.02.014</u>

²⁶⁹ Sutton AT, Kriewall CS, Leu MC, Newkirk JW. Powder characterisation techniques and effects of powder characteristics on part properties in powder-bed fusion processes. Virtual Phys. Prototyp. [Internet]. 2017 [cited 2024 Jul 29];12:3–29. <u>https://doi.org/10.1080/17452759.2016.125060</u>

²⁷⁰ Vock S, Klöden B, Kirchner A, Weißgärber T, Kieback B, Powders for powder bed fusion: a review. Progr Addit Manuf [Internet] 2019 Feb [cited 2024 Jul 29];4,383–397. <u>https://doi.org/10.1007/s40964-019-00078-6</u>

²⁷¹ Chu F, Zhang K, Shen H, Liu M, Huang W, Zhang X, Liang E, et al. Influence of satellite and agglomeration of powder on the processability of AlSi10Mg powder in laser powder bed fusion. J Market Res. [Internet] 2021 Apr [cited 2024 Jul 29];11:2059–2073. <u>https://doi.org/10.1016/j.jmrt.2021.02.015</u>

²⁷² Pasebani S, Ghayoor M, Badwe S, Irrinki H, Atre SV. Effects of atomizing media and post processing on mechanical properties of 17-4 PH stainless steel manufactured via selective laser melting. Addit Manuf. [Internet] 2018 Aug [cited 2024 Jul 29];22:127–137. <u>https://doi.org/10.1016/j.addma.2018.05.011</u>

²⁷³ Shanthar R, Chen K, Abeykoon C. Powder-Based Additive Manufacturing: A Critical Review of Materials, Methods, Opportunities, and Challenges. Adv Eng Mater. [Internet] 2023 Jun [cited 2024 Jul 29];25(19):2300375, <u>https://doi.org/10.1002/adem.202300375</u>

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Figure 20. CEFAS system at INL.

The challenges involved in feedstock development and manufacturing encompass both technical and economic aspects. For powders, common production methods include atomization, electrolytic methods, mechanical processing (such as ball milling and vortex milling), and chemical processing (involving reduction and decomposition of compounds). Atomization is the predominant method, despite its relatively high cost.^{274,275,276} While drawing materials into wires is a well-established technology, the challenge lies in manufacturing materials with the appropriate composition and characteristics for feedstock.

Technical obstacles include knowledge gaps in:

- Developing techniques that can produce a cost-effective homogeneous distribution of powder particle sizes and shapes. This would eliminate the costly post-processing currently required to remove undesirable particles and achieve size categorization.
- Reducing high-energy consumption and high consumption rate of materials, especially for atomizationbased processes, which are considered less environmentally friendly and lack long-term sustainability.
- Optimizing powder characteristics to specific AM techniques.
- Preparing cost-effective feedstock for HEMs. Technical constraints prevent feedstock manufacturing on a large enough scale to support ubiquity of some promising materials, such as MAX phase materials.²⁷⁷
- Preparing feedstock for reactive sintering of high temperature ceramics.
- Bridging the transition gap between the development of new materials and the production of suitable feedstock to produce the material through AM.

Researchers must pursue crosscutting research opportunities to resolve the technical challenges with feedstock production for materials in operating environments above 1,300°C and with a high degree of filament homogeneity, low viscosity, high elongation at break, and/or powder surface purity (e.g., native oxide reduction).

²⁷⁴ Popovich A, Sufiarov V. in Metal Powder Additive Manufacturing, ed. by I. V. Shishkovsky. New Trends in 3D Printing [Internet] 2016 Jul 13 [cited: 2024 Jul 31]);p.227. <u>https://doi.org/10.5772/63337</u>

²⁷⁵ Spierings AB, Voegtlin M, Bauer T, Wegener K. Powder flowability characterisation methodology for powderbed-based metal additive manufacturing. Progr Addit. Manuf. [Internet]. 2015 Jul 23 [cited 2024 Jul 29];1,9–20. <u>https://doi.org/10.1007/s40964-015-0001-4</u>

²⁷⁶ Neikov OD, Naboychenko SS, Dowson G. editors. Handbook of non-ferrous metal powders technologies and applications, 1st edn. Elsevier: Amsterdam; 2009.

²⁷⁷ Gonzalez-Julian J. Processing of MAX phases: from synthesis to applications. J of Am Cer Soc [Internet]. 2020 Oct 29 [cited: 2024 Aug 29];104(2),659-692. Available from: <u>https://doi.org/10.1111/jace.17544</u>

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Needed research capabilities include:

- Science-based engineering approaches to help design application-appropriate, cost-effective feedstock materials.
- The deployment of computational as well as ML and AI tools to help gather and leverage the vast amount of data from past work on alloy or materials chemistry as well as on material behaviors and characteristics, including those associated with manufacturing processes and pathways to produce appropriate feedstocks.
- Development of industrial-scale manufacturing to support deployment of successfully developed feedstocks.

The availability of appropriate feedstock is central to the continued growth and wider application of AM techniques to produce HEMs. Success will be measured by the length of the HEM feedstock supply chain (how long it takes to acquire appropriate feedstock) and by the cost of acquiring application-specific materials. The industries likely to benefit the most from suitable HEM feedstock development include aerospace, automotive, lower tiered component manufacturers, and power generation.

To realize DOE goals, the R&D pathway below should be pursued:

- Prioritize capability development for versatile cost-effective technologies, followed by scale-up to produce HEM feedstock. For 2025 to 2030, the priority should be to develop a cost-effective way to derive carbon-based feedstock, and feedstock for materials operating above 1,300°C.
- Develop techniques and pathways to accelerate the feedstock production of new and exotic materials from 2030 to 2035.

Space Enabling Component Manufacturing

Develop Hybrid Manufacturing Methods for large NNS parts (C122)

Convergent manufacturing platforms combine multiple manufacturing processes into a single platform to yield unprecedented flexibility, portability, and modularity to enable new complex devices or systems and transformative approaches in the modern industrial landscape. Convergent manufacturing approaches are directly applicable to enabling new materials and components for harsh environments.^{278,279} This is a strategic shift from traditional batch manufacturing to adaptive *in situ* manufacturing processes, alongside the demonstration of prototypes that withstand extreme conditions. Convergent methodologies significantly reduce production times, enhance material properties, and streamline the transition from prototype to deployment.^{280,281,282,283} In the rapidly evolving

²⁷⁸ Lalena JN, Fox RV, Snyder SW. Material for harsh environments: 2020 virtual workshop summary report. [Internet] Department of Energy; 2021 [cited 2024 Jul 29]. Available from:

https://www.energy.gov/eere/ammto/articles/materials-harsh-environments-2020-virtual-workshop-summaryreport

²⁷⁹ Pillai R, Ren Q, Su YF, Kurfess R, Feldhausen T, Nag S. Leveraging additive manufacturing to fabricate high temperature alloys with co-designed mechanical properties and environmental resistance. J of Eng for Gas Turbines and Power [Internet]. 2024 Jun [cited 2024 Jul 29];146(6):061018. Available from: <u>https://doi.org/10.1115/1.4063784</u>

²⁸⁰ Feldhausen T, Raghavan N, Saleeby K, Love L, Kurfess T. Mechanical properties and microstructure of 316L stainless steel produced by hybrid manufacturing. J of Mat Process Technology [Internet]. 2021 Apr [cited 2024 Jul 29];290:116970. Available from: <u>https://doi.org/10.1016/j.jmatprotec.2020.116970</u>

²⁸¹ Saleeby K, Feldhausen T, Love L, Kurfess T. Rapid retooling for emergency response with hybrid manufacturing. Smart and Sustainable Manufacturing Systems [Internet]. 2020 Nov [cited 2024 Jul 29];4(3):245-249. Available from: <u>https://doi.org/i0.1520/SSMS20200050</u>.

²⁸² Lorenz K, Jones J, Wimpenny D, Jackson M. A review of hybrid manufacturing. In: Solid Freeform Fabrication Conference Proceedings [Internet], 2015 [cited 2024 Aug 8]; 53: 96-108.Available from: <u>https://utw10945.utweb.utexas.edu/sites/default/files/2015/2015-8-Lorenz.pdf</u>

²⁸³ Feldhausen T, Heinrich L, Saleeby K, Burl A, Post B, MacDonald E, Saldana C, et al. Review of computeraided manufacturing (CAM) strategies for hybrid directed energy deposition. Additive Manufacturing [Internet]. 2022 May [cited 2024 Jul 29];102900. Available from: <u>https://doi.org/10.1016/j.addma.2022.102900</u>.

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manufacturing sector, the demand for flexible and efficient production systems is increasingly critical.²⁸⁴ Convergent manufacturing methodologies, which integrate diverse technological processes into seamless operations, offer substantial advantages over traditional methods,²⁸⁵ including the ability to create novel materials to enable in situ process adjustments in harsh environments.



Figure 21. a) Section of an injection molding screw with a heating fluid passage fabricated via directed energy deposition and machining on bar stock. b) Robotic system and press setup for convergent manufacturing (additive manufacturing and compression molding) where multiple materials can be consolidated into final component. c) Example of using additive manufacturing with powder metallurgy for a valve body; internal material can be different than exterior skin.

Despite its potential, the adoption of convergent manufacturing faces several challenges, including high initial costs and the complexity of integrating new technologies into existing workflows. However, the opportunities for innovation, particularly in the automation of optimizing manufacturing processes, are vast. Addressing the challenges through continued research and collaborative efforts could significantly enhance the scalability and applicability of convergent manufacturing technologies for HEM.

Critical roadblocks that have limited the adoption of these technologies for HEM applications include:

- Materials compatibility and integration: Different materials have distinct properties, such as melting points, thermal expansion coefficients, and mechanical strength, which can complicate their integration in a single build process.
- Process stability and control: Convergent manufacturing processes involve complex thermal management control to achieve the desired microstructure of materials. Maintaining consistent temperature gradients and cooling rates across processes, which is critical for achieving desired material properties, can be difficult.
- Surface finish and integrity: Production of final geometries is challenging and, if it is not achieved during the manufacturing process, can lead to non-usable components. Integration of subtractive processes is needed to achieve finer finishes for fatigue, wear, and corrosion, but integrating these processes seamlessly can be complex.
- Equipment and technological complexity: Hybrid manufacturing systems are highly sophisticated and require integration of different technologies, including software for design and control systems for process management, leading to higher capital costs and maintenance requirements.
- Quality assurance and certification: The unique nature of each part, coupled with variations in material properties and the lack of extensive historical data, complicates certification processes. Standardized

²⁸⁴ Crean RC. Benchmarking DoD use of additive manufacturing and quantifying costs. [thesis on the internet]. Air Force Institute of Technology; 2017 [cited 2024 Jul 29]. Available from: <u>https://scholar.afit.edu/cgi/viewcontent.cgi?article=1790&context=etd</u>

²⁸⁵ Dilberoglu UM, Gharehpapagh B, Yaman U, Dolen M. Current trends and research opportunities in hybrid additive manufacturing. The Int J of Adv Man Technology [Internet] 2021 Jan [cited 2024 Jul 29];113:623-648. Available from: https://doi.org/10.1007/s00170-021-06688-1

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testing and quality assurance protocols must be established for parts manufactured using hybrid techniques.

Convergent manufacturing allows for quicker development and production of prototypes and end-use components. By combining additive and subtractive processes in one setup, it reduces the overall manufacturing time and streamlines the production workflow. Through the combination of multiple processes, new materials can be fabricated that are not possible through traditional manufacturing approaches. For example, with functionally graded materials (FGMs) the composition or structure and hence properties are gradually and smoothy varied over the component's volume. This makes it possible to produce complex geometries with multiple functionalities—a result that is impossible to achieve with traditional methods alone. Multifunctionality and process combination allows for the integration of sensors and electronics directly into metal and ceramic parts, creating "smart" components that can monitor their own health and the environment around them. Convergent manufacturing can create interpenetrating lattice structures with optimized properties as a function of location (e.g., ceramic matrix composites with optimized material fractions for improved toughness).

To foster the adoption of convergent manufacturing methodologies, industry stakeholders should consider strategic investments in R&D and form partnerships with academic and research institutions. Further development of standards and best practices for hybrid manufacturing will also be crucial in overcoming current barriers and encouraging widespread adoption.

R&D efforts in convergent manufacturing technologies focused on HEMs are needed to demonstrate applicability of new components. Critical investments in specific convergent manufacturing platforms are required to enable HEM research and component production and demonstrations targeted in the 2025–2030 timeframe. Near-term opportunities exist for hybrid additive/subtractive technologies for component repair because large portions of the platform manufacturing technologies already exist. In contrast, more complex processes and methodologies, including additive manufacturing for powder metallurgy, location-specific materials property control, ceramic/metallic systems manufacturing, and composite technology integration, require more development. System-level capabilities must first be established, with an end application in mind.

Near-Net Shape (NNS) Processing

Lower the cost of AMTs for high temperature alloys (C16)

Develop additive manufacturing of components for high-temperature applications (C22)

Evolution in energy systems has historically been driven by the coupling of innovations in materials and manufacturing science, which inherently leads to increasingly harsh operating conditions, and to higher system efficiencies. Nickel-based superalloys, refractory alloys, ceramics, and CMCs are the HEMs of choice for next-generation energy systems operating at high temperatures. However, due to materials manufacturing limitations and/or lack of ability to manufacture increasingly complex geometries, traditional manufacturing is facing limitations in defining next-generation energy systems.

In recent years, powder bed fusion additive manufacturing (PBF-AM) has shown the potential to successfully process refractory alloys, which were once only fabricable through solid-state metallurgical processing techniques, such as PM-HIP. The novelty in additive manufacturing techniques is the ability to fabricate geometries in a layerby-layer process and provide unique thermal signatures tailored for site-specific application. This can mitigate the problems associated with densifying the material and unlock the ability to fabricate significantly more novel and complex geometries that cannot be manufactured through traditional technologies for the necessary material families of interest. However, not all conventional materials are feasible for processing through 3D printing. Thus, materials discovery and innovation, as well as innovations in manufacturing technologies for high temperature HEMs, are essential. National Landscape of High-Impact Crosscutting Opportunities for Next Generation Harsh Environment Materials and **122** Manufacturing Process Research, Development, and Demonstration / January 16, 2025



Figure 22. Turbine blade made via arc-wire directed energy deposition (a) with the 17-4 stainless steel wire used to make it. (b). Gas-atomized Fe-based glassy alloy powders (c) consolidated into a tool using powder metallurgy.

Efforts have been made to design HEMs for processing with additive manufacturing (AM), utilizing the unique thermal signatures of existing AM methods. Additionally, advancements in the data science of in situ AM process monitoring, and smart manufacturing have provided a basis for developing the processing science as well as component certification and qualification. However, despite these materials and manufacturing innovations, acceleration in their adoption is not occurring rapidly.

During the COVID-19 pandemic, both domestic and global supply chains became increasingly strained. This led to difficulty in obtaining replacements for what were once common components of energy systems, such as steel turbine blades for steam turbines. As a result, AM methods have been explored for their capability to replace traditionally manufactured components to reduce lead times. However, where there was once an extreme urgency to seek alternative manufacturing solutions, a gradual return of the traditional approach to manufacturing the components is occurring. This is a direct result of a lack of confidence in the economics and scalability of AM processes and in the maturity and consistency of the materials being manufactured through these processes. The AM community has not yet compiled large historical data sets on performance that are available for traditionally processed materials to build human trust in these new manufacturing processes.

The availability of HEM feedstocks for advanced manufacturing processes will influence the extent to which industry adopts and manufactures components from emerging HEMs. This is true for both domestic and global supply chains. In many instances, either the ability to manufacture the feedstocks does not exist, or scaling their manufacture is not economical due to low market demand for these materials. Additionally, a robust domestic supply chain does not yet exist for advanced manufacturing.

Historically, 20 to 30 years are required to bring a new material and manufacturing process to full commercialization for high-risk high-reward components such as those found in the energy systems' harshest environments. This timeline must be shortened. Therefore, innovative solutions leveraging existing efforts for materials and manufacturing acceleration are necessary to ensure a matriculation in the 2030–2035 timeframe.

Among the efforts currently underway in the research arena that could directly impact the advanced manufacturing of high temperature HEMs are: 1) Data science and mod-sim tools targeting the rapid development of the advanced manufacturing processing science for new HEMs. These will enable the rapid generation of machine tool pathing

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and layer slicing which is a significant hurdle in transitioning from prismatic to complex geometries such as those found in harsh environment energy systems. 2) Development of next-generation advanced manufacturing systems that are designed for scalability and production. 3) Adoption of the digital twin and digital factory concepts as an approach for the certification and qualification of components manufactured by advanced means, while also utilizing the digital data as a means for quality control.

However, one major factor slowing current advancements in additive manufacturing of HEMs is the siloing effect of intellectual property in materials development, manufacturing processes, and scale-up to component geometries. This results in disconnected research efforts, dividing the elements (materials, data sciences, manufacturing, component design/performance, etc.) which must be linked and occur in unison to result in rapid development and deployment. Due to the diversity of energy problems requiring HEM manufacturing solutions, we should select and support crosscutting high-impact opportunities, which can motivate and incentivize industry to consider investing in and capitalizing on the advantages additive manufacturing can bring.

If these efforts are successfully pursued, they will empower the development of next-generation energy systems that can utilize HEMs to achieve the ambitious energy and emissions metrics the federal government has set. These efforts can help spur the development of domestic supply chains for materials and manufacturing, enabling the United States to remain globally competitive and at the forefront of emerging technologies.

Scale-up of large component manufacturing including forging of pressure vessel via methods such as DED-AM, PM-HIP). (C3)

Employ nondestructive evaluation (NDE) methods for large part analysis (porosity, internal cracks, grain structure/size). (C2)

Enable near net shaping of hard, brittle, high temperature ceramics using unique die design or 3D printed preforms and pressure transfer media in EFAS (C71)

The increasing performance pressures on HEMs can be alleviated by either the development of new materials (metallic alloys, ceramics, composites) or substantial improvements in component designs, or a combination of the two. Near-net shape (NNS) processing significantly reduces scrap generation as well as prototype design and validation times.^{286,287} The extreme operating conditions that HEMs are expected to withstand often require novel materials, frequent repairs, or replacements, which makes these materials more vulnerable to supply chain disruptions. A robust domestic supply chain is critical for energy generation, national security, and global economic competitiveness. NNS processes like powder metallurgy—hot isostatic pressing (PM-HIP), powder bed fusion (PBF), and directed energy deposition (DED)—can enable robust domestic supply chains and create the next-generation workforce for energy sectors like wind, hydropower, and nuclear, as well as the aerospace, oil and gas, and transportation sectors. For example, PM-HIP is being used to fabricate pressure vessels for nuclear reactors.²⁸⁸ Wire-arc directed energy deposition can be used to make large-scale hydropower components and first wall/blanket panels for fusion reactors. Figure 1a shows power generation turbine blades made using electron beam PBF²⁸⁹ and

²⁸⁶ Tang HP, Qian M, Liu N, Zhang XZ, Yang GY, Wang J. Effect of Powder Reuse Times on Additive Manufacturing of Ti-6Al-4V by Selective Electron Beam Melting. JOM [Internet]; 2015 Mar [cited 2024 Jul 29]; 67(3):555–63. Available from: <u>https://doi.org/10.1007/s11837-015-1300-4</u>

²⁸⁷ Yang S, Min W, Ghibaudo J, Zhao YF. Understanding the sustainability potential of part consolidation design supported by additive manufacturing. J Clean Prod. [Internet]. 2019 Sep; [cited 2024 Jul 29];232:722–38. Available from: https://doi.org/10.1016/j.jclepro.2019.05.380

 ²⁸⁸ Lou X, Gandy D. Advanced Manufacturing for Nuclear Energy. JOM [Internet]. 2019 Jun [cited 2024 Jul 29];71(8): 2834–6. Available from: https://doi.org/10.1007/s11837-019-03607-4

 ²⁸⁹ Adair D, Kirka M, Ryan D. Additive Manufacture of Prototype Turbine Blades for Hot-Fired Engine
 Performance Validation Trials. In: Proc ASME Turbo Expo 2019 Turbomach Tech Conf Expo. [Internet] 2019
 June 17-21; Phoenix, AZ. 2019 [cited: 2024 Jul 31]. Available from: https://doi.org/10.1115/GT2019-90966

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Figure 1b shows a prototype geometry for a HIP can made using hybrid manufacturing at ORNL. The HIP can was subsequently filled with powders and then densified.



Figure 23. (a) Inconel 738 turbine blade made using electron beam PBF and (b) prototype HIP can made using hybrid manufacturing.

NNS processing for sustainable HEM manufacturing faces technical, infrastructure, and economic constraints. The currently available materials that are suitable for NNS are a small fraction of those available for traditional processing. Even the ones that are amenable to NNS processing were tuned for thermal conditions experienced in traditional manufacturing processes. For example, currently used metallic alloys are not always suitable for the unique thermal conditions encountered in processes like PBF or DED and the final material properties may not meet the desired specifications. The development of new materials that take advantage of the extreme processing conditions encountered in NNS can result in properties far superior to traditionally processed materials. For example, AI-Ce based alloys made using laser-PBF have demonstrated creep strength superior to existing high temperature aluminum alloys.²⁹⁰ Large-scale NNS parts often suffer from residual stresses that can impact their dimensional tolerances and subsequent usability.²⁹¹ Infrastructure availability is another key challenge since the size of the components that can be made via technologies like PM-HIP and wire-DED are limited by the size of the HIP that can be used for densification and post-processing. Additionally, new materials are often evaluated based on trial-and-error approaches with guidance from data analytics and modeling. However, such an approach is economically unviable for large-scale parts in the absence of reliable models to guide the manufacturing process.

These key constraints should be addressed to develop domestic supply chains for HEMs manufactured using NNS processing:

 Novel materials design: Design new materials that are tailored for the thermo-mechanical conditions encountered in different NNS processes, with a focus on extreme operating conditions such as high temperatures, corrosive environments, high radiation fluxes, and high wear rates. Use of computational thermodynamics coupled with advances in AI will be important to screen rapidly through a seemingly infinite combination of chemistries.

²⁹⁰ Bahl S, Wu T, Michi RA, An K, Yu D, Allard LF, et al. An additively manufactured near-eutectic Al-Ce-Ni-Mn-Zr alloy with high creep resistance. Acta Mater [Internet]. 2024 [cited 2024 Jul 29];268:119787. Available from: <u>https://doi.org/10.1016/j.actamat.2024.119787</u>

²⁹¹ Lee Y, Feldhausen T, Fancher CM, Nandwana P, Babu SS, Simunovic S, et al. Prediction of residual strain/stress validated with neutron diffraction method for wire-feed hybrid additive/subtractive manufacturing. Addit Manuf. [Internet]. 2024 Jan [cited 2024 Jul 29];79:103920. Available from: https://doi.org/10.1016/j.addma.2023.103920

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- Feedstock availability: Develop new supply chains for ensuring feedstock availability for the newly developed HEMs. Pilot scale feedstock processing will be critical to evaluate and screen for desired HEMs prior to production at scale.
- New platform technologies: Materials development and processing are intertwined and should not be treated as disjointed efforts. Therefore, there is a need to develop new platform technologies that can enable NNS processing or even net shape processing of HEMs at different size scales.
- Reliable computational models: Most of the existing models are descriptive in nature. However, for largescale NNS processes, reliable predictive models are critical to minimize scrap generation. Challenges such as distortion from residual stresses in fusion-based AM and powder consolidation during PM-HIP, should be addressed with the help of reliable computational models.
- Infrastructure: NNS processes can make large-scale parts, but the scale is often limited by the scale of
 post-processing operations like HIP in the case of metallic materials. The size of PM-HIP components for
 nuclear applications is limited by the size of available HIP systems. Further, transportation infrastructure
 is critical for manufacturing and assembly of parts across different geographic regions.
- Materials testing: Materials testing is critical to understand the performance of NNS HEMs. As we explore
 new paradigms, it is critical that we can test these new materials. For example, high temperature tensile
 test capabilities under vacuum environments may be needed to understand material performance
 decoupled from oxidation-induced degradation.

New manufacturing methods like NNS processing advance the development of new materials and offer an opportunity to significantly reduce material development cycle times while developing new manufacturing platforms. The prototyping capabilities of NNS processes, coupled with advances in thermodynamic models and machine learning, provide new avenues for the development of HEMs for NNS processing. Development of new materials and NNS processes also provides technical and economic incentives to develop new and resilient domestic supply chains. Additionally, NNS processing of HEMs will create opportunities for development of new infrastructure, such as HIP systems, furnaces, and efficient transportation, for the adoption of HEMs for energy generation.

Addressing challenges in NNS processing of HEMs requires integration of materials research, modeling, feedstock processing, design of robust manufacturing systems, and data analytics. For successful deployment of NNS processing, collaborative efforts between relevant industry sectors, academia, and national laboratories are critical. These collaborations will enable the development of sustainable and resilient supply chains necessary for energy generation, transportation, and national security infrastructure. For mainstream adoption of NNS processes to manufacture HEMs, there must be a primary focus on new materials discovery and validation via pilot scale systems. In tandem, more reliable computational models should be developed and validated. The knowledge can then be transferred for scaling up and generating relevant property datasets important to relevant industries.

Developing NNS processes for HEMs is an ambitious aim. In the timeframe between 2025 and 2030, the focus should be materials discovery, pilot scale feedstock development, and framework development for predictive models. Between 2030 and 2035, the focus should shift to fabricating mission critical components using HEMs to demonstrate and understand lifecycle performance, followed by deployment to relevant industry sectors.

Materials Sustainability

Develop materials and components operating in harsh environments with circularity in terms of recycling. *(C7)*

Product and material circularity involves increasing recirculation of products and materials in the economy for as long as possible while minimizing life cycle environmental impacts. For HEMs—materials that are robust, highly

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processed, and high in embodied energy—increasing circularity is critical for maximizing sustainability.^{292,293} If the circularity of HEMs is built into the supply chain during the development stage, many of the challenges in the reuse and recycling of HEMs can be greatly reduced.²⁹⁴

When used in harsh environments, recycled materials must withstand high temperatures, pressures, corrosive environments, mechanical wear, and other extreme conditions, ^{295,296,297} while aligning with DOE emissions/energy goals. The cascade use model of circularity illustrates the options available for minimizing the overall life cycle impact of HEMs. In order of desirability, the options include reuse/repair, remanufacturing, recycling, and recovery, with the overall objective of minimizing or eliminating solid waste disposal while maximizing the intrinsic value of HEMs.²⁹⁸ Figure 24 illustrates the relative value of each of these circular economy options within the cascade use model.

 ²⁹² Cremonesi A, Grobert N, Gumbsch P, Piketty L, Montelius L, Vandeputte K, et al. Materials 2030 manifesto: systemic approach of advanced materials for prosperity – a 2030 prospective [Internet]. 2022 Feb 7 [cited: 2024 Jul 31]. Available at: https://research-and-innovation.ec.europa.eu/document/download/fa1f3f35-7cac-49c7-a212-366879848f4c_en?filename=advanced-materials-2030-manifesto.pdf
 ²⁹³ Burinskienė A, Lingaitienė O, Jakubavičius A. Core elements affecting the circularity of materials. Sustainability

²⁹³ Burinskienė A, Lingaitienė O, Jakubavičius A. Core elements affecting the circularity of materials. Sustainability [Internet]. 2022 Jul 8 [cited 2024 Jul 31];14(14):8367. Available from: <u>https://www.mdpi.com/2071-</u> 1050/14/14/8367

²⁹⁴ Silvestroni L, Rueschhoff LM, Acord K, Castro R, Powell, C, et al. Synthesis of far-from-equilibrium materials for extreme environments. MRS Bulletin [Internet]. 2022 Nov [cited 2024 Jul 29]; 11: 1143-1153. Available from: https://doi.org/10.1557/s43577-022-00454-8

²⁹⁵ Fox R., Lalena JN, Snyder W. Materials for harsh environments: 2020 virtual workshop summary report [Internet]. 2021 Mar 31 [cited: 2024 Jul 31]. Available from: <u>https://www.energy.gov/eere/ammto/articles/materials-harsh-environments-2020-virtual-workshop-summary-report</u>

²⁹⁶ Prameela SE, Pollock TM, Raabe D, Meyers MA, Aitkaliyeva A, Chintersingh KL, et al. Materials for extreme environments. Nature Reviews Materials [Internet]. 2023 Feb 1 [cited 2024 Apr 28]; 8(2): 81–8. Available from: <u>https://www.nature.com/articles/s41578-022-00496-z</u>

²⁹⁷ Al-Azawii MMS, Alhamdi SFH, Braun S, Hoffmann JF, Calvet N, Anderson R. Thermocline in packed bed thermal energy storage during charge-discharge cycle using recycled ceramic materials - Commercial scale designs at high temperature. J of Energy Stor [Internet]. 2023 Aug 1 [cited 2024 Jul 31]; 64:107209–9. Available from: <u>https://doi.org/10.1016/j.est.2023.107209</u>

 ²⁹⁸ Faisal NH, Rajendran V, Prathuru A, Hossain M, Muthukrishnan R, Balogun Y, et al. Thermal spray coatings for molten salt facing structural parts and enabling opportunities for thermochemical cycle electrolysis.
 Engineering Reports [Internet]. 2024 Jun 14 [cited 2024 Jul 31]; Available from: https://doi.org/10.1002/eng2.12947

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Figure 24. Cascade use model for circular economy identifying economic values.

Generally, the highest value circularity option for HEMs is to repair and/or reuse the part and extend the service life of the original component, followed closely by remanufacturing. For instance, a high temperature heat exchanger part might be pulled from service after a certified lifetime for a given application, then analyzed and refurbished for a second service in a lower temperature class of service. In this way, the loss of up to 90% of the embodied energy used to originally produce the part can be avoided.

The existing state of HEMs circularity is limited for several reasons. First, the service life of HEMs tends to be long and the materials themselves are relatively new,²⁹⁹ so a large portion of HEMs are still in service. Second, even after these materials come out of service, the resulting volume is extremely small compared to high-volume materials such as steel, aluminum, and glass. Finally, the elemental composition of HEMs is highly varied. Limited availability combined with a highly variable raw material content makes it difficult and expensive to identify, sort, and classify recycled HEMs.³⁰⁰

The future state is to improve the sustainability of HEMs by establishing repair, remanufacturing, recycling supply chains for HEMs. Unlike virgin raw materials, even relatively pure recycled materials have some level of impurities that can have a significant impact on final product properties. It has taken many decades to establish the recycling supply chains for steel and aluminum. In addition to sorting and classification, recycled materials must be well characterized as essentially new and different raw materials. There also exists some domestic companies that use pyrometallurgical operations (i.e., re-melting, vacuum refining) to recycle nickel-based superalloys. However, pyrometallurgical techniques lose elements to slag and evaporation and have high energy consumption. Therefore, the U.S. needs further development and scaling of hydrometallurgical and hybrid/combined recycling methods that can better recover individual and rare elements (i.e., have greater selectivity), produce recycled products of greater purity, consume less energy, and are thus more cost-effective. Lastly, processes must be established for incorporating recycled materials into useful products. By including circularity in the development of HEMs, the supply chain development time will be substantially reduced.

Next Steps:

 ²⁹⁹ Was GS, Petti D, Ukai S, Zinkle S. Materials for future nuclear energy systems. J. Nuclear. Physics [Internet].
 2019 Dec [cited 2024 Jul 29];527:151837. Available from: https://doi.org/10.1016/j.jnucmat.2019.151837
 ³⁰⁰ Hardee H. Advanced materials emerge as challenging new frontier for aircraft recycling [Internet]. Flight Global. 2023 [cited 2024 Jul 31]. Available from: https://www.flightglobal.com/airframers/advanced-materials-emerge-as-challenging-new-frontier-for-aircraft-recycling/153420.article

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- Define metrics for sustainability of HEMs.
- Include circularity considerations (e.g., design for ease of recirculation, recycling) in the future development of new HEMs.
- Create testing and simulation methods/tools for predicting long-term material behavior in different environments.
- Develop an end-to-end framework for cascade use model of HEMs circularity.

Ceramics with Complex Geometries, High Entropy Alloy Manufacturing & Advanced Manufacturing Integration/Joining Techniques

Develop AMTs to make complex structures using HEMs (C18)

Creating complex structures using harsh environment materials involves careful engineering to ensure durability and functionality. Some examples include aerospace components, oil and gas equipment, chemical processing plants, power generation systems, and marine structures. Each application requires a detailed understanding of the specific environmental challenges and operational requirements to select the most suitable materials and design structures to withstand the intended conditions. Advanced manufacturing techniques such as additive manufacturing (3D printing) and precision machining play crucial roles in fabricating these complex structures with harsh environment materials, which can be seen Figure 25.

Technical constraints in the application of complex structures made of harsh environment materials encompass a range of challenges that impact design, manufacturing, and performance:

- Manufacturing complexity: Creating intricate complex structures from harsh environment materials such as titanium alloys or ceramic composites involves complex machining, shaping, and joining processes due to their high hardness and brittleness.³⁰¹
- Thermal management and corrosion resistance: Managing thermal expansion and heat dissipation in structures exposed to high temperatures (e.g., in aerospace or power generation) remains a challenge, requiring innovative cooling strategies and materials like superalloys or corrosion-resistant steels with high temperature stability.³⁰²
- Cost and scalability issues: Harsh environment materials can be expensive and complex structures may require sophisticated manufacturing processes. Balancing performance requirements with cost constraints while ensuring scalability for mass production can be challenging.³⁰³
- Sustainable material usage: The demand for eco-friendly manufacturing processes and recyclable materials requires advancements in sustainable material development, processing techniques, and waste reduction strategies.³⁰⁴

Future goals for complex structures made of harsh environment materials aim to achieve crosscutting benefits across multiple application spaces by focusing on:

³⁰¹ Bin Rashid A, Haque M, Islam M, Rafi M, Chowdhury P. Breaking boundaries with ceramic matrix composites: a comprehensive overview of materials, manufacturing techniques, transformative applications, recent advancements, and future prospects. Advances in Mat Sci and Eng [Internet]. 2024 May 17 [cited 2024 Aug 30];2024:1–33. Available from: <u>https://doi.org/10.1155/2024/2112358</u>

³⁰² Careri F, Khan RHU, Todd C, Attallah MM. Additive manufacturing of heat exchangers in aerospace applications: a review. App Therm Eng [Internet]. 2023 Nov 25 [cited 2024 Aug 30];235:121387. Available from: https://doi.org/10.1016/j.applthermaleng.2023.121387

³⁰³ Song W, Yang J, Liang J, Lu N, Zhou Y, Sun X, et al. A new approach to design advanced superalloys for additive manufacturing. Additive manufacturing [Internet]. 2024 Mar 1 [cited 2024 Aug 30];84:104098–8. Available from: <u>https://doi.org/10.1016/j.addma.2024.104098</u>

³⁰⁴ Cann JL, De Luca A, Dunand DC, Dye D, Miracle DB, Oh HS, et al. Sustainability through alloy design: Challenges and opportunities. Progress in Mat Sci [Internet]. 2021 Apr [cited 2024 Aug 30];117:100722. Available from: <u>https://doi.org/10.1016/j.pmatsci.2020.100722</u>

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- Multifunctionality: Developing structures with integrated functionalities like structural strength, thermal management, and self-healing capabilities to benefit industries such as aerospace, automotive, and renewable energy.^{305,306}
- Sustainability: Emphasizing sustainable material usage, manufacturing processes, and end-of-life strategies to reduce environmental impact and promote a circular economy.^{307,308}
- Digital integration: Incorporating digital twins and AI-driven analytics for real-time monitoring, predictive maintenance, and data-driven decision making to enhance efficiency and reliability.³⁰⁹
- Cost efficiency: Optimizing material sourcing, manufacturing techniques, and supply chains to reduce costs without compromising quality or performance.³¹⁰



Figure 25. a) Al-Ce alloy impeller; b) side and c) top view of a geothermal rotor prototype optimized for advanced manufacturing.

Capability enhancements such as advanced material design, integrated digital design and precision manufacturing techniques, and advanced characterization are necessary to achieve the desired targets.³¹¹ The pursuit of advanced materials and manufacturing techniques for complex structures using harsh environment materials offers benefits such as improved performance, durability, and sustainability across industries like aerospace, automotive, and

³⁰⁵ Mostafaei A, Ghiaasiaan R, Ho I-Ting, Strayer S, Chang KC, Shamsaei N, et al. Additive manufacturing of nickel-based superalloys: A state-of-the-art review on process-structure-defect-property relationship. Prog in Mat Sci [Internet]. 2023 Jul 1 [cited 2024 Aug 30];136:101108–8. Available from: https://doi.org/10.1016/j.pmatsci.2023.101108

³⁰⁶ Osada T, Kamoda K, Mitome M, Hara T, Abe T, Tamagawa Y, et al. A Novel design approach for self-crackhealing structural ceramics with 3D networks of healing activator. Sci Reports [Internet]. 2017 Dec 19 [cited 2024 Aug 30];7(1). Available from: <u>https://doi.org/10.1038/s41598-017-17942-6</u>

³⁰⁷ Abokersh MH, Norouzi M, Boer D, Cabeza LF, Casa G, Prieto C, et al. A framework for sustainable evaluation of thermal energy storage in circular economy. Renewable Energy [Internet]. 2021 Sep [cited 2024 Sep 4];175:686–701. Available from: https://doi.org/10.1016/j.renene.2021.04.136

³⁰⁸ Gunasekara SN, Barreneche C, Inés Fernández A, Calderón A, Ravotti R, Ristić A, et al. Thermal energy storage materials (TESMs)—what does it take to make them fly? Crystals [Internet]. 2021 Nov 1 [cited 2023 Jun 16];11(11):1276. Available from: <u>https://doi.org/10.3390/cryst11111276</u>

³⁰⁹ Kalidindi SR, Buzzy M, Boyce BL, Dingreville R. Digital twins for materials. Frontiers in Mat [Internet]. 2022 Mar 16 [cited 2024 Sep 4];9. Available from: <u>https://doi.org/10.3389/fmats.2022.818535</u>

³¹⁰ Yilmaz S, Theodore M, Ozcan S. Silicon carbide fiber manufacturing: cost and technology. Composites Part B: Engineering [Internet]. 2024 Jan 1 [cited 2024 Sep 4];269:111101–1. Available from: https://doi.org/10.1016/j.compositesb.2023.111101

³¹¹ Levashov EA, Mukasyan AS, Rogachev AS, Shtansky DV. Self-propagating high-temperature synthesis of advanced materials and coatings. International Materials Reviews [Internet]. 2016 Oct 25 [cited 2024 Sep 4];62(4):203–39. Available from: https://doi.org/10.1080/09506608.2016.1243291

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energy. The improved performance enabled by more complex part geometries can lead to beneficial impacts such as increased product reliability, reduced maintenance costs, and enhanced competitiveness in global markets. Success in advanced materials and manufacturing of complex structures using harsh environment materials can be measured through metrics such as increased component lifespan, reduced failure rates, and improved energy efficiency, leading to tangible cost savings and enhanced performance for end-users. U.S. industries—such as power generation, distribution, chemical manufacturing, and aerospace—will benefit directly from developments in this sector.^{312,313}

R&D activities with target years from 2025 to 2030 are crucial from a failure analysis perspective to meet goals effectively. Early initiation of R&D activities allows for systematic exploration of material properties, manufacturing processes, and design considerations. This proactive approach enables the early identification and mitigation of potential failure modes, reducing the risk of costly failures during product development or operational phases.³¹⁴ Also, optimized material selection is critical to ensure that the chosen materials align with durability, reliability, and safety goals to minimize failure risks. Sometimes data-driven approaches empower engineers and analysts to make informed decisions, prioritize design improvements, and allocate resources effectively to address potential failure scenarios. Lastly, establishing R&D frameworks aligned with industry standards, regulations, and safety protocols ensures that products meet required quality, reliability, and safety standards.

In-Situ Repair Techniques

Develop in situ repair and mitigation for component/plant life extension (C120)

Aging infrastructure is a topic of increasing concern as power plants age. The majority of energy base load is provided by large nuclear and hydropower plants built many decades ago. As these power plants age, cost and frequency of repairs increase. High direct costs are associated with removing energy generation components, such as turbines, for repair. High indirect costs are associated with outages for component repair. Many repairs are made with processes that are more than 50 years old. In many cases, metal components are repaired with fusion welding, which results in warping and microstructural degradation that reduces performance and increases the frequency of repair.

Improved manufacturing methods and processes such as cold spray can be leveraged to effectuate in-situ repairs that improve performance and service life. The U.S. Department of Defense (DoD) has invested heavily in developing portable high pressure cold spray over the last few decades. Cold spray is growing increasingly common for repair in DoD and in the aerospace sector, yet it is relatively unknown in the energy sector. Identifying more candidate technologies and doing needed technology maturation will enable modern in situ repair capability, which can improve the economics and robustness of energy infrastructure and allow in situ repair technologies to be advanced for energy infrastructure.

Anticipated outcomes of this focus area include development of technologies that:

- Avoid capital expenses associated with energy generation component replacement.
- Reduce direct cost in repair of energy generation components.
- Reduce indirect costs associated with plant outages.
- Provide improved economics and increased robustness of energy infrastructure.
- Provide crosscutting benefits such as increased competitiveness of domestic manufacturing, enabling superior designs for new energy infrastructure.

https://doi.org/10.1016/j.jeurceramsoc.2022.01.058

³¹⁴ Zhang L, Wang Y, Lv J, Ma Y. Materials discovery at high pressures. Nature Reviews Materials [Internet].
2017 Feb 21 [cited 2024 Sep 4];2(4). Available from: <u>https://doi.org/10.1038/natrevmats.2017.5</u>

³¹² Sisco K, Plotkowski A, Yang Y, Leonard D, Stump B, Nandwana P, et al. Microstructure and properties of additively manufactured Al–Ce–Mg alloys. Scientific Reports [Internet]. 2021 Mar 26 [cited 2024 Sep 4];11(1). Available from: https://doi.org/10.1038/s41598-021-86370-4

³¹³ Cramer CL, Ionescu E, Graczyk-Zajac M, Nelson AT, Katoh Y, Haslam JJ, et al. Additive manufacturing of ceramic materials for energy applications: Road map and opportunities. Journal of the European Ceramic Society [Internet]. 2022 Jul [cited 2024 Sep 4];42(7):3049–88. Available from: https://doi.org/10.1016/j.javaraapapa.2022.01.058

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Challenges associated with in-situ repair include:

- Access to repair area
- Remote locations
- Degradation associated with current structural repair techniques (warping and microstructural degradation associated with arc welding)
- Environmental hazards
- Environmental sensitivities
- Increasing scarcity of skilled trade workers
- Lack of industry standards for application and quality assurance for field application of technologies of interest
- Lack or low TRL of field portable equipment for newer technologies.

The target metric criteria for this work are "developed ability to repair components instead of replacing them." To achieve this goal and the anticipated outcomes listed above, the following capabilities need to be developed:

- Application-specific material system and process development
- Codification and quality assurance
- Equipment miniaturization and robotics to support in-situ repair in confined spaces
- Field portability to enable in-situ repair at remote locations
- Improved processes for structural repair of metals
- Improved processes for structural repair of composite turbine blades
- Automation to reduce hazards to humans and decrease plant outage time.

Anticipated benefits and market impacts include:

- Improved performance and service life of new and existing components
- Enable favorable economics for maintaining existing energy infrastructure
- Enable improved economics for emerging energy infrastructure
- Delay/eliminate capital expenses associated with replacement of components.
- Provide resilience against climate change through retention of water resources for agriculture and societal use
- Decrease dependency on foreign manufacturing
- Increased competitiveness of domestic manufacturing.

Metrics to quantify successful development of in-situ repair for capital energy generation components include:

- Net-present value calculations for deferment/elimination of capital expense from actual repairs and project repairs
- Percent improvement calculation compared to traditional methods for power generation efficiency, repair interval, and reduction in downtime for repair
- Reported cost saving and projected cost saving associated with developed techniques
- Percent improvements in material properties from laboratory testing
- Percent improvements in performance service life from field data.

The scheduled R&D activities advance existing dimensional restoration and coating techniques by performing application-specific process development to meet stakeholder needs. Subsequently, new processes are developed to expand types of achievable repairs beyond the reach of current technology. Manual repair and telerobotic application must first be done to inform design scope for equipment miniaturization and AI/ML enabled path planning and qualification of robotic repairs.

Near term (2025–2030):

- Dimensional restoration
- Wear and corrosion-resistant coatings
- Manual and telerobotic repair
- NDE and codification.

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Long Term (2030-2035):

- Structural repair for metals
- Structural repair for composites
- Repair automation
- Small form factor robotic repair with AI/ML-enabled path planning and quality assurance
- NDE and codification.

Due to low profit margins in the current energy market, aging nuclear and hydropower facilities may lose economic viability if capital components (such as turbines) fail. Similarly, as newer solar and wind facilities age and cease to receive government incentive, continued economic viability could be at risk without advancement in repair technology. This focus area protects the resilience and economic viability of electricity generation.

3D Printing Cementitious Materials

Develop novel cementitious materials for applications in geothermal wells. (C95)

The development and processing of cementitious materials for use in harsh environments is a vital area of research, crucial for both current and future energy technologies. From geothermal well bore casings to the bases of offshore floating wind turbines, concrete remains the most cost-effective and scalable option for building the durable infrastructure essential for energy systems.^{315,316,317}



Figure 26. a) 3D Printing of cementicious material through material extrusion; 3D printing of alternative cements (PVAenhanced Ca(OH)₂ slurries) with (b) and without (c-e) tire-waste additives.

To date, the industry has primarily focused on energy optimization and the use of blended cements, achieving some notable but limited progress.³¹⁸ According to the Portland Cement Association, these efforts have culminated in an approximately 11% reduction in greenhouse gas emissions from 2019 to 2024. These savings include 0.7 gigatons per year from traditional methods such as enhancing energy efficiency, utilizing alternative fuels, and substituting clinker, complemented by 1.3 gigatons per year from emerging technologies like carbon capture and storage,

³¹⁵ Scrivener K, et al. Eco-efficient cements: Potential economically viable solutions for a low-CO₂ cement-based materials industry. [Internet] United Nations Environment Programme (FR); 2017. [cited: 2024 Jul 31]. Available from: <u>https://wedocs.unep.org/bitstream/handle/20.500.11822/25281/eco_efficient_cements.pdf</u>

³¹⁶ Haleem A, Javaid M. Additive manufacturing applications in industry 4.0: a review. J of Ind Integration and Management [Internet]. 2019 Oct 4 [cited 2024 Aug 1];04(04):1930001. Available from: https://www.worldscientific.com/doi/abs/10.1142/S2424862219300011

 ³¹⁷ Timperley J. Q&A: Why cement emissions matter for climate change? [Internet]. Carbon Brief; 2018. [cited 2024 Aug 1]. Available from: <u>https://www.carbonbrief.org/qa-why-cement-emissions-matter-for-climate-change</u>
 ³¹⁸ Naskar AK, Bi Z, Li Y, Akato SK, Saha D, Chi M, et al. Tailored recovery of carbons from waste tires for enhanced performance as anodes in lithium-ion batteries. RSC Adv [Internet]. 2014 [cited 2024 Jul 31]; 4:38213. Available from: <u>https://doi.org/10.1039/c4ra03888f</u>

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carbon-cured concrete, and additive manufacturing (see Figure 34).³¹⁹ These emerging technologies require dedicated research in the development of an integrated approach combining both low carbon cementitious materials, as advanced high performance substitutes to traditional Portland cements, and novel processing techniques. Examples of novel techniques include advanced precast molds, which enable the replacement of hydraulic binder with aerial binder, and 3D printing.^{320,321} The envisioned research actions include three areas: materials development, calcination alternatives, and infrastructure optimization.

Carbon-capture materials development through mineralization:

- Carbon-neutral cementitious binders enabled through advanced processing: Enable low-carbon cementitious materials (LCCMs acting as Portland cement substitutes) through the replacement of hydraulic binder (i.e., ordinary Portland cement with or without additives) with aerial binder such as Ca(OH)₂. Since LCCMs are cured with the diffusion of CO₂, there is need for advanced processing techniques like 3D printing and advanced precast molds which retain the cost and strength evolution profiles of Portland cement while minimizing material use. For building construction applications, rapid stiffening/hardening can be achieved through varied additives, including commercially available polymers such as PVA and polyethyleneimine (PEI) at ambient temperature or temperature-activated polymerization at the point of deposition.
- *Carbon-capture mineralization*: In addition to leveraging the lime cycle for carbon neutrality, abundant Mgand Ca-bearing minerals (wollastonite, olivine, serpentine, pyroxene, etc.) can be efficiently converted to carbonates in gas-liquid-solid environments with alkali-glycinate as the aqueous solvent and *p*CO₂ of 1 atm.³²² These powders can be incorporated as negative-carbon additives to the LCCMs, sequestering CO₂. Also, amino acids can potentially be utilized to pre-concentrate CO₂ as carbonates to promote continued mineralization.
- *Recycling of high-carbon bearing materials such as waste tires*: While about 45% of tire waste is reused as tire-derived fuel chips, reusing tire-waste byproducts as additives to LCCMs will provide carbon-reuse and improve viscosity and durability .^{323,324,325,326}
- *Bio-mineralization*: Incorporating bacteria and or enzymes in cementitious materials is known to promote carbon-induced mineralization, leading to self-healing properties that increase the materials' durability

³¹⁹ Kaplan MF. Nuclear radiation and the properties of concrete. Nonlinear Structural Mechanics Research Unit [Internet]. 1983 Aug [cited 2024 Aug 1];15(17). Available from:

https://inis.iaea.org/search/search.aspx?orig_q=RN:15052206

 ³²⁰ Francey S, Tran H, Berglin N. Global survey on lime kiln operation, energy consumption, and alternative fuel usage. Tappi J [Internet]. 2011 Aug [cited 2024 Jul 31];19-26. Available from: <u>http://doi.org/10.32964/TJ10.8.19</u>
 ³²¹ Timperley J. Q&A: Why cement emissions matter for climate change? [Internet]. Carbon Brief; 2018 Sept 13
 [cited 2024 Aug 1]. Available from: <u>https://www.carbonbrief.org/qa-why-cement-emissions-matter-for-climate-change</u>

³²² Czigler T, Reiter S, Schulze P, Somers K. Laying the foundation for zero-carbon cement. [Internet]. McKinsey & Company; 2020 May 14 [cited 2024 Jul 31];9p. Available from:

https://www.mckinsey.com/industries/chemicals/our-insights/laying-the-foundation-for-zero-carbon-cement

³²³ Jonkers HM. Self-Healing Concrete: A Biological Approach. In: van der Zwaag S, editor. [Internet]. Springer; 2007 [cited 2024 Jul 31]; 100. Available from: <u>https://doi.org/10.1007/978-1-4020-6250-6_9</u>

 ³²⁴ Le Pape Y, Ghosh D, Sant G, Mattus CH, Tajuelo Rodriguez E, Post B. Development and Characterization of
 3D-Printed Cementitious Systems for Innovative Nuclear Systems. [Internet] Oak Ridge National Laboratory;
 2020 Mar [cited: 2024 Jul 31]; ORNL/TM-2020/1450. Available from: https://tcr.ornl.gov/wp-content/uploads/2020/10/M3TC-20OR0403012.pdf

³²⁵ Li Y, Paranthaman MP, Akato K, Naskar AK, Levine AM, Lee RJ, et al. Tire-derived Carbon Composite Anodes for Sodium-ion Batteries. J Power Sources [Internet]. 2016 Jun 1 [cited 2024 Jul 31];316:232-238. Available from: <u>https://doi.org/10.1016/j.jpowsour.2016.03.071</u>

³²⁶ Gadikota G, Park AHA. Accelerated carbonation of Ca-and Mg-bearing minerals and industrial wastes using CO2. In: Carbon Dioxide Utilisation. [Internet] Elsevier; 2015 [cited 2024 Jul 31];115-137. Available from: <u>https://doi.org/10.1016/B978-0-444-62746-9.00008-6</u>

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and decrease maintenance and repair.^{327,328,329} Innovative self-healing properties coupled with integrated sensors could be a promising solution for early detection problems, monitoring real-time conditions, and autonomous repairing, thereby helping to reduce operation and maintenance (O&M) costs.

Alternatives to calcination:

- *Electrochemical conversion*:³³⁰ While more energy-intensive than traditional calcination, electrochemical conversion when coupled with renewable electricity is cheaper and allows carbon capture.
- Sub-atmospheric calcination:³³¹ Literature suggests higher CaCO₃ decomposition rates.
- *Oxygen-enhanced combustion*:³³² Capturing oxygen from the air using a membrane and performing calcination in pure oxygen will increase the calcination performance.

Infrastructure optimization toward climate resilience:

- *Topological structural optimization for material use reduction:* Additive manufacturing technologies change the design strategies of concrete infrastructure. Adapted Building Information Modeling (BIM) and design methods³³³ are expected to reduce the volume of materials needed to obtain comparable structural performance.
- Integrated smart cementitious HEM structures: The structural resilience of critical infrastructures needs novel construction technologies, including health-monitoring and self-healing capabilities.

Success will be measured through the development of novel cementitious HEMs and processing technologies that reduce the environmental impacts relative to Portland cement-based concretes while retaining or enhancing the performance, durability, and cost of traditional concretes in use today for these demanding applications. It is expected that there will be significant advancements over traditional concretes in some of the most extreme environments—for example, in nuclear containment shielding where many of the long-term durability concerns arise from the differential strains between the cement binder and aggregates, induced by radiation triggered expansion, that lead to cracking and failure.³³⁴ In LCCMs the chemical composition of the aggregates can be nearly identical to the binder, reducing this concern. Other such auxiliary benefits are expected in many of the other harsh environment applications, like offshore wind where chloride penetration is a threat to conventional reinforced concrete.

 ³²⁷ Derby R. Climate Change. [Internet] Government Relations Portland Cement Association; 2019 [cited 2024 Jul 31];4. Available from: http://www2.cement.org/DC/Climate_Change.pdf

³²⁸ Scrivener KL, John MV, Gartner EM. Eco-efficient cements: Potential economically viable solutions for a low-CO2 cement-based materials industry. [Internet] United Nations Environment Programme (Paris); 2017. Available from: <u>https://wedocs.unep.org/bitstream/handle/20.500.11822/25281/eco_efficient_cements.pdf</u>

³²⁹ Mittal A, Saxena A, Mohapatra B. Oxygen Enrichment Technology—An Innovation for Improved Solid Fuel Combustion and Sustainable Environment. In: Sangwan K, Herrmann C, editors. Enhancing Future Skills and Entrepreneurship [Internet]. 2020 Jul 28 [cited: 2024 Jul 31];13-19. Available from: <u>https://doi.org/10.1007/978-3-030-44248-4_2</u>

³³⁰ Custelcean R, Williams NJ, Garrabrant KA, Agullo P, Brethomé FM, Martin HJ, et al. Direct air capture of CO2 with aqueous amino acids and solid bis-iminoguanidines (BIGs). Ind Eng Chem Res [Internet]. 2019 Nov 26 [cited 2024 Jul 31];58:23338-23346. Available from: https://pubs.acs.org/doi/10.1021/acs.iecr.9b04800

³³¹ Naskar AK, Paranthaman MP, Bi Z. Pyrolytic Carbon Black Composite and Method of Making the Same. U.S. Patent 9,441,113 B2, issued September 13, 2016.

³³² Ellis LD, Badel AF, Chiang ML, Park RJ-Y, Chiang Y-M. Toward electrochemical synthesis of cement - An electrolyzer-based process for decarbonating CaCO3 while producing useful gas streams. Proc Natl Acad Sci. [Internet]. 2020 [cited 2024 Jul 31]; Jun;117(23):12584-12591. Available from: https://doi.org/10.1073/pnas.1821673116

³³³ Plaza MG, Martínez S, Rubiera F. CO₂ Capture, Use, and Storage in the Cement Industry: State of the Art and Expectations. Energies [Internet]. 2020 Oct 30 [cited 2024 Jul 31];13(21):5692. Available from: https://doi.org/10.3390/en13215692

³³⁴ Sant G, Vance KE, Balonis M. Enhanced carbonation and carbon sequestration in cementitious binders. U.S. Patent 10,968,142 B2, issued April 6, 2021.

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3.5 Focus Area 5: Materials and Process Development Acceleration Tools Recommendations

The action plan table below lists several details that should inform funding strategies for next generation materials and process development investments utilizing mod/sim acceleration tools. The action plan table also describes the roadblocks with the existing state of the art and challenges to be addressed with mod/sim technologies. Specific opportunities with associated timelines follow the action plan.

Neglecting this R&D could have adverse implications across various energy technologies

Critical need not addressed: Without the availability and the utilization of advanced physics-based, highperformance computing, and multiscale materials and manufacturing process modeling and simulation capabilities, as well as modern machine learning methods for data mining, future innovation in HEMs will be extraordinarily delayed and immensely more costly. Exploration of the vast compositional spaces for multi-component material systems via a direct design approach would necessitate more extensive use of less effective and less efficient trialand-error or empirical-based techniques involving one chosen materials system at a time in solving technical challenges. Likewise, for process optimization, without ML for accurately predicting results, the Design of Experiments (DoE) would be the only tool to assess the influences of different treatments and process parameters.

Action Plan for Focus Area 5

Table 11. Action Plan for Materials and Process Development Acceleration Tools.

Scope						
Technologies for material and manufacturing process	Tools such as multi-scale physics-based deterministic methods (e.g., ICME) and data-driven stochastic methods (e.g., artificial intelligence and machine learning) need greater utilization to speed up innovation in materials and process design. In-situ measurements and characterization methods will also be utilized to facilitate the exploration and design of advanced materials to meet application requirements, using both traditional direct design (given the material, find its properties) and inverse design (given the properties find a suitable material) approaches					
development acceleration tools	Process development acceleration tools such as the same multi-scale physics-based deterministic and data-mining stochastic methods called for with materials design can be used together with a suite of smart manufacturing digital tools (e.g., sensors and digital twins) to monitor, optimize, and adjust operational parameters in real time, particularly with self-learning or autonomous closed-loop control systems, in order to more efficiently achieve production of components having the desired properties.					
Technologies of Interest: Deterministic and probabilistic computational and data driven methods; coupled approac						
Roadblo	ocks	Challenges to pursue				
 Material properties highly sensitive to processing environment and operational parameters as well as feedstock purity Limited material property databases for physics-based approaches Defect- and dopant-induced functionalities can be particularly difficult to model with deterministic methods. By its function follows form nature, deterministic approaches generally exclude a wide range of other potentially more useful solutions. Vast materials/phase landscape to explore for data mining approaches Mod/sim holistic design approaches require experimental validation, cost analyses, uncertainty analyses, and multi- elisative entimination 		 Develop high-throughput screening, better global optimization routines and generative models to narrow vast search space with data mining Greater utilization of bridging (multi-scale/multi-step) approach (e.g. ICME) deterministic methods Experimental validation of mod/sim results Validated model-based qualification/certification approaches 				
	Stakeholders and P	otential Roles				
Stakeholder	Role					

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Product Manufacturers/Suppliers	•	Explore (mod/sim), design, synthesize, and fabricate advanced materials with enhanced properties with improved performance in demanding service applications. Innovate in material properties, performance modeling and testing, experimental validation, manufacturing qualification, and field application certification.
End Users/Original Equipment Manufacturers (OEMs)	•	Validated mod/sim-based qualification and certification pathways will shorten advanced material deployment timeframes

Table 12. Challenges identified for FA5 with potential impact and effort (pace of TRL advancement) needed.

ID	Impact Score	Challenge Title	Location	Metric Target	TRL	TRL/5 years	Application Space
C38	1130	Develop advanced manufacturing process- informed material design for extreme environment materials	UR	Reduce manufacturing \$ and time by 50%	2	3	
C36	964	Develop advanced manufacturing process development with novel in-situ measurements for extreme environment materials	UR	50% \$ and lead time reduction with potential performance improvements	2	3	
C37	819	Develop rapid materials characterization and testing in support of advanced materials for extreme environment	UR	50% reduction in characterization time	3	2.5	
C78	424	Acquire comprehensive understanding of materials behavior in harsh environments at different time and length scales	UR	25% improvement in materials performance	3	2.5	
C15	307	Demonstrate HEMs in relevant Harsh environment conditions to validate manufacturing routes	LR	Demonstrate process informed qualification	4	2	
C47	271	Integrate comprehensive data analytics and modeling and simulation for material design and selection for extreme environment materials	UR	Shorten development time by 25%	5	1.5	
C19	174	Design and synthesis of new materials with unique properties and behavior of a variety of harsh operating environments	UR	Multifunctional/cross- cutting novel materials	2	3	
C80	173	Develop molten salt (particularly FLiBe and Chloride salts) component testing for material compatibility with molten salt reactors, fusion, solar, and thermal storage to enable higher temperature operation	LL	OT > 700-750°C, 6" dia. Parts	4	2	
C84	85	Demonstrate modeling and Simulation of HEMs to expedite qualification	UR	Demonstrate mod/sim qualification	2	3	
C86	68	Develop high temperature WHR materials to capture heat from high temp processes (Iron blast furnace or aluminum smelting) and use this for drying or preheating via HT heat exchanger.	UL	OT > 400°C	3	2.5	
C134	8	Qualify new materials in codes & standards, including additional materials to ASME Section III Division 5	UL	Incorporate more real- world conditions	2	3	

Data Analytics and Model Simulation

Develop advanced manufacturing process development with novel in-situ measurements for extreme environment materials (C36)

Development of scalable manufacturing systems and processes for materials for harsh environments is essential for ensuring national economic prosperity, reducing emissions, supporting the development of alternative energy technologies, and numerous defense applications. Critically, HEMs are required to exhibit exceptional performance in environments which may include but are not limited to high temperatures, irradiation, corrosive mediums, and severe tribological loading. Materials systems suitable for these environments, both monolithic and multi-material composites, are by their very nature extremely difficult to process (high melting temperature, brittleness, impurity-

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sensitivity, etc.). Therefore, there is not only a need to identify novel systems with improved performance, but also to establish manufacturing routes that enable the fabrication of cost-effective, high-integrity components from these materials. Furthermore, advanced manufacturing techniques such as additive manufacturing, EFAS, powder metallurgy, and subtractive processes offer additional flexibility in controlling resulting material structure (microstructure), properties, shape, and surface texture. These qualities impact aggregate component performance and, hence, optimization of the manufacturing process itself opens opportunities to further bolster the performance of HEMs.



Figure 27. a) In-process AI anomaly detections and post-manufacture inspection results overlayed on an image of the physical component; b) harsh environment materials manufacturing modeling ties together information from numerous modalities for effective decision making and process/material optimization.

In the past decade, advanced manufacturing routes have demonstrated the viability of fabricating complex geometries from difficult-to-process HEMs ranging from refractory metals to advanced ceramics.^{335,336} Historically these kinds of materials, while exhibiting exceptional intrinsic properties, have been used sparingly due to processing difficulties. Today, an opportunity exists to leverage manufacturing advances to develop novel high-performance HEM technologies. While ongoing research focuses on the processing of HEMs via various routes (AM, sintering, PM, subtractive, deposition processes, etc.), it is also essential to concurrently establish HEM-focused analytics, simulation, and modeling tools to support these efforts. ORNL has demonstrated remarkable success in the powder bed AM space with the in-situ processing monitoring tool *Peregrine.*³³⁷ Additional development upon this foundation may be necessary for other manufacturing routes, HEM-specific materials, and novel sensing technologies. AM is particularly well suited for process monitoring due to layer-by-layer access to the entire component; however, there are opportunities to develop similar capabilities in other processes via different

³³⁵ Ledford C, Fernandez-Zelaia P, Graening T, Campbell Q, Rojas JO, Rossy AM, Kato Y, et al. Microstructure and high temperature properties of tungsten processed via electron beam melting additive manufacturing, Int J Refract Met Hard Mater [Internet]. 2023 Jun [cited 2025 Jul 29];113:106148. Available from: https://doi.org/10.1016/j.ijrmhm.2023.106148

³³⁶ Mostafaei A, Elliott AM, Barnes JE, Li F, Tan W, Cramer CL, Nandwana P, et al. Binder jet 3D printing— Process parameters, materials, properties, modeling, and challenges, Prog Mater Sci [Internet]. 2021 Jun [cited 2025 Jul 29];119:100707. Available from: <u>https://doi.org/10.1016/j.pmatsci.2020.100707</u>

³³⁷ Snow Z, Scime L, Ziabari A, Fisher B, Paquit V. Machine learning enabled sensor fusion for in-situ defect detection in L-PBF. [Internet] Oak Ridge National Laboratory; 2023 Dec [cited 2024 Jul 29]; report. Available from: https://www.ornl.gov/publication/machine-learning-enabled-sensor-fusion-situ-defect-detection-l-pbf

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data modalities: machining (cutting forces and tool wear³³⁸), sintering (optical shrinkage measurements³³⁹), thermoset processing (spectroscopy³⁴⁰), chemical vapor deposition (spectroscopy³⁴¹), etc. In addition to process monitoring, the maturation of HEM technologies requires the establishment of robust manufacturing design and optimization tools. For instance, while multi-material systems (dissimilar joints, coatings, etc.) have shown promise in various HEM applications, their design and fabrication is often laborious and time consuming.³⁴²

Physics-based numerical simulation of processing, deformation, thermodynamics, and materials performance under harsh conditions are essential for understanding the key driving manufacturing physics.³⁴³ However, perhaps even more importantly, it is essential to establish computationally efficient surrogate models to be used in design tasks (see Figure 27). Furthermore, recent advances in AI, especially generative AI, offer opportunities for developing HEM-specific design and optimization tools.³⁴⁴

Constraints include:

- Wide range of processing modalities: fusion-based AM, stir friction welding, cold spray, sintering, PVD/CVD, deformation-based processes, powder metallurgy, powder metallurgy HIP, etc.
- Wide range of materials systems: refractory metals, carbon-carbon, ceramics, polymers, coatings, multimaterials solutions.
- Complexity of data sources/modalities across various manufacturing processes: images, time series, spectral data, categorical data, etc. Need for storage/retrieval/security infrastructure.
- Complex physics codes require computational resources often not available outside of academia or national labs.
- Design and optimization problems can be extremely complex and challenging, given multiple material length scales and coupled optimization (feedstock materials, base material, coating system, surface treatments, composite structure, etc.). Evaluation of computationally expensive physics codes is too time consuming for quantitative optimization. Sources of uncertainty in properties, process control, feedstock, tooling, etc.
- Difficulty in assessing in-service HEMs' performance. Essential feedback for manufacturing optimization.
- Feedstock considerations: Supply chain and security in general, plus material-specific issues (e.g., sensitivity to oxygen and downstream manufacturing/material impact).
- Fundamental physical multi-material and systems limitations (e.g., thermodynamic/structural/manufacturing compatibilities; formation of deleterious phases in interfaces; build-up of stresses across interfaces; and access to large furnaces and pressure vessels).
- Limitations of existing infrastructure that currently supports processing of non-HEMs (machine capabilities, sensor limitations, etc.).

 ³³⁸ Liang SY, Hecker RL, Landers RG. Machining process monitoring and control: the state-of-the-art, J Manuf Sci Eng [Internet]. 2004 Jul [cited 2025 Jul 29];126:297–310. Available from: https://doi.org/10.1115/1.1707035
 ³³⁹ Baber J, Klimera A, Raether, F. In situ measurement of dimensional changes and temperature fields during sintering with a novel thermooptical measuring device, J Eur Ceram Soc [Internet]. 2007 [cited 2025 Jul 29];27(2-3):701–705. Available from: https://doi.org/10.1016/j.jeurceramsoc.2006.04.043

³⁴⁰ Antonucci V, Giordano M, Cusano A, Nasser, Nicolais, L. Real time monitoring of cure and gelification of a thermoset matrix, Compos Sci Technol [Internet]. 2006 Dec 18 [cited 2025 Jul 29];66:3273–3280. Available from: https://doi.org/10.1016/j.compscitech.2005.07.009

 ³⁴¹ Choy KL., Chemical vapour deposition of coatings. Prog Mater Sci [Internet]. 2003 [cited 2025 Jul 29];
 48(2):57–170. Available from: <u>https://doi.org/10.1016/S0079-6425(01)00009-3</u>

³⁴² Kannan JJR, Lee Y, Pierce D, Unocic K, Fillingim, Feldhausen, Rossy AM, et al. Additive manufacturing as a processing route for steel-aluminum bimetallic structures. Mater Des [Internet]. 2023 Jul [cited 2025 Jul 29]; 231:112003. Available from: <u>https://doi.org/10.1016/j.matdes.2023.112003</u>

³⁴³ Cheng J, Fernandez-Zelaia P, Hu X, Kirka Z. Effect of microstructure on fatigue crack propagation in additive manufactured nickel-based superalloy Haynes 282: an experiment and crystal plasticity study. J Mater Sci [Internet]. 2022 Feb 22 [cited 2024 Jul 29]; 57(2022):9741–9768. Available from: <u>https://doi.org/10.1007/s10853-022-06957-8</u>

³⁴⁴ Fernandez Zelaia JP, Cheng J, Mayeur JR, Ziabari AK, M.M. Kirka, Digital Polycrystalline Microstructure Generation Using Diffusion Probabilistic Models. Materialia [Internet]. 2024 Mar [cited 2024 Jul 29];33:101976. Available from: https://doi.org/10.1016/j.mtla.2023.101976

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• HEM component processing expense.

Opportunities:

- Digital frameworks that are agnostic of manufacturing process and physics simulations. Process/material specific simulations can 'plug' into a sufficiently flexible framework, as well as data collection, storage, processing, etc. Tools with embedded analysis methods for different manufacturing and data modalities (e.g., time series analysis for machining forces, imaging for additive, imaging for machining tool wear, spectroscopy analysis for CVD and polymer processing, non-contact optical measurements for sintering).
- Establish, distribute, and use surrogate models for simulating processes (deformation for forging/machining, deposition for CVD, thermodynamics for coatings, melting/solidification for AM/joining) and evaluating relevant higher order HEM properties (finite element for creep, fatigue, corrosion, tribology, etc., and thermodynamic calculations for thermal stability and corrosion) based on national laboratory computing resources.
- Develop rapid model calibration capabilities and data fusion between model and experiments to address difficult, time consuming, and computationally expensive physics-based model calibration.
- Leverage advances in generative-AI technologies for solving inverse problems, microstructural design, process optimization, shape optimization, materials selection, multi-materials systems optimization, etc. ML/AI for combining process models with performance models and enabling efficient design.
- Use risk-based flaw-tolerant-type qualification/certification approaches for intelligent performance assessment of as-fabricated components from in-situ and ex-situ qualification data. Can be used for significant cost and materials savings. (Such approaches ask whether, for example, a certain defect density, shape discrepancy, or coating thickness is acceptable.)

Success will be measured through the establishment of licensed research software that has demonstrated effectiveness in the manufacture of HEMs. While focused on energy applications, the methods and framework may benefit HEMs used in other industry domains such as transportation, defense, aerospace, etc.

In the near term (2025–2030), analytics and mod-sim capabilities will be developed for targeted advanced manufacturing routes, along with some crosscutting efforts for key shared capabilities (e.g., generative AI for optimization, calibration capabilities, and surrogate performance capabilities). Subsequent work (2030–2035) will focus on establishment, validation, and verification of material- and process-agnostic tools.

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Process-Informed HEMs Design

Develop advanced manufacturing process-informed material design for extreme environment materials (C38)

While metallurgical research has been largely focused on optimization of the microstructure at the component level, traditional additive manufacturing methods have emphasized shape or topology optimization. Key innovations and acceleration in harsh environment materials development are expected to arise by bridging these two fields.

Indeed, innovations in alloys for harsh environments through additive manufacturing are happening at an increasing pace.^{345,346,347,348,349} Example processing based strategies that are now applied to fabricate harsh environment materials through powder metallurgy and additive manufacturing include dispersion hardening, grain refinement, nanoparticle strengthening, in-situ alloying, and gaseous (e.g., nitrogen) alloying. New paradigms for concurrent process-materials-product design are emerging. One recent example is the development of large-scale high pressure die casting, also called Gigacasting, by Tesla Motors.³⁵⁰

Often, there is a tradeoff between processability and the ability of the material to resist harsh environment conditions. Studying the development of thermal and residual stresses under *operando* conditions (through X-rays, neutrons,³⁵¹ electrons, etc.) can provide insight that allows breaking of processability-material property tradeoffs. *Operando* characterization and modeling-simulation based approaches are significant tools that will accelerate process-informed materials design.

Process-informed HEMs design, however, suffers from number of constraints:

- How to scale processing technologies from the laboratory to industrial is often unknown and this lack of knowledge is a relevant bottleneck that can prevent commercialization of promising process-informed HEM designed materials.
- For powder-based processing technologies like LPBF or powder metallurgy (PM), feedstock control and pedigree of powder becomes of utmost importance. Changes in powder suppliers can lead to unwarranted changes in the performance or processability of HEMs.
- Even when using the same powder supplier, changing LPBF machines (even under equivalent processing conditions) can have disproportionate influence on the performance or processability of HEMs. Weak links in harsh environments (e.g., melt pool boundaries in creep loading conditions) can be sensitive to fine details of powder pedigree and machine settings and characteristics.

³⁴⁵ Pollock TM, Clarke AJ, Babu SS. Design and tailoring of alloys for additive manufacturing. Metallurgical and Materials Transactions A [Internet]. 2020 Oct [cited 2024 Jul 25];51:6000-6019. Available from: <u>https://doi.org/10.1007/s11661-020-06009-3</u>

³⁴⁶ Michi RA, Plotkowski A, Shyam A, Dehoff RR, Babu SS. Towards high-temperature applications of aluminium alloys enabled by additive manufacturing. International Materials Reviews [Internet]. 2021 Jul [cited 2024 Jul 25];67(3):298-345. Available from: <u>https://doi.org/10.1080/09506608.2021.1951580</u>

³⁴⁷ Smith TM, Kantzos CA, Zarkevich NA, Harder BJ, Heczko M, Gradl PR, Thompson AC, et al. 3D printable alloy designed for extreme environments. Nature [Internet]. 2021 Jul [cited 2024 Jul 25];617(7961):513-518. Available from: <u>https://doi.org/10.1038/s41586-023-05893-0</u>

³⁴⁸ Qu Z, Zhang Z, Liu R, Xu L, Zhang Y, Li X, Zhao Z, et al. High fatigue resistance in a titanium alloy via nearvoid-free 3D printing, Nature [Internet]. 2024 Feb [cited 2024 Jul 25];626(8001):999-1004. Available from: <u>https://doi.org/10.1038/s41586-024-07048-1</u>

³⁴⁹ Ren J, Zhang Y, Zhao D, Chen Y, Guan S, Liu Y, Liu L, et al. Strong yet ductile nanolamellar high-entropy alloys by additive manufacturing, Nature [Internet]. 2022 Aug [cited 2024 Jul 25];608(7921):62-68. Available from: <u>https://doi.org/10.1038/s41586-022-04914-8</u>

³⁵⁰ Kuehmann C. Concurrent design of materials and systems. The Bridge [Internet] National Academy of Engineering; 2024 Mar 29 [cited: 2024 Jul 31];54(1). Available from: <u>https://www.nae.edu/313284/Concurrent-Design-of-Materials-and-Systems</u>

³⁵¹ Plotkowski A, Saleeby K, Francher CM, Haley J, Madireddy G, An K, et al. Operando neutron diffraction reveals mechanisms for controlled strain evolution in 3D printing. Nat Comms [Internet]. 2023 Aug 16 [cited: 2024 Jul 31];14:4950. Available from: <u>https://doi.org/10.1038/s41467-023-40456-x</u>

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- With the ready availability of enormous amounts of control and post-fabrication data, a constraint is the lack of development of adequate information processing paradigms (both physics-based and machine learning) to effectively and efficiently optimize and accelerate materials design and production.
- The timeline for harsh environment materials development and qualification is several decades, even with the application of ICME methodologies.³⁵²

Process-informed HEMs design offers several salient opportunities, including:

- Rapid development of new harsh environment capable materials that takes advantage of new and emerging advanced processing techniques. An example would be new dispersion strengthened alloys that take advantage of rapid solidification conditions in additive manufacturing. These alloys can replace precipitation hardened alloys that are applied in commercial HEMs (see Michi et al. for example processinformed high temperature aluminum alloys).³⁵³
- Concurrent materials-process-product design.
- Use of advanced manufacturing to develop HEMs with > 2–5x mechanical properties of current generation HEMs.
- Use of advanced manufacturing to develop materials with equivalent response at elevated homologous temperature (fraction of melting temperature, T/T_M) and with improved corrosion response in harsh environments.
- Use of advanced manufacturing to develop materials with characteristics that make them resistant to multiple harsh environments.
- Develop harsh environment materials with improved circularity; for example, use of recycled feedstock material to upcycle scrap.
- Develop data analytics/modeling tools that accelerate materials and process development for harsh environment applications.

The R&D pathway will begin in the 2025 to 2030 timeframe with intense development of process-informed HEMs with 2–5x improvements in mechanical properties relevant for the specific applications over current generation HEMs under similar conditions. Because process improvements will be developed concurrently in this 2025–2030 period, individual plans for HEM development should be aware of and possibly flexible with respect to those developments. From 2030 to 2035, the priority shifts to possible qualification, including code qualification, of process-informed HEMs.

Success will be measured by the extent to which new HEMs and processes are commercialized because of their improved cost, properties, and/or overall performance and energy savings. In many cases, alloys with increased temperature limit³⁵⁴ can be a common bottleneck for higher energy utilization efficiency. Such alloys will benefit multiple sectors, including the power generation, transportation, materials development, foundries, and aerospace industries.

Demonstrate HEMs in relevant Harsh environment conditions to validate manufacturing routes (C15)

Since high entropy alloys (HEAs) were first proposed in 2004,³⁵⁵ they have attracted much interest as potential candidates for HEMs. Compositions associated with HEAs are in the centers (e.g., corresponding to near equimolar

³⁵² Kuehmann CJ, Olson GB. Computational materials design and engineering. Mat Sci and Technol [Internet].
2009 Apr 1 [cited: 2024 Jul 31];25(4). Available from: https://doi.org/10.1179/174328408X371967

³⁵³ Michi RA, Plotkowski A, Shyam A, Dehoff RR, Babu SS. Towards high-temperature applications of aluminum alloys enabled by additive manufacturing. International Materials Reviews [Internet]. 2021 Jul [cited 2024 Jul 25];67(3):298-345. Available from: <u>https://doi.org/10.1080/09506608.2021.1951580</u>

³⁵⁴ Kennedy RL. ALLVAC® 718PLUSTM, superalloy for the next forty years. Loria EA, editor. TMS [Internet]. 2005 [cited 2024 Jul 30];718(625). Available from:

https://www.tms.org/superalloys/10.7449/2005/Superalloys 2005 1 14.pdf

³⁵⁵ Yeh JW, Chen SK, Lin SJ, Gan JY, Chin TS, Shun TT, Tsau CH, et al. Nanostructured high-entropy alloys with multiple principal elements: novel alloy design concepts and outcomes, Advanced Engineering Materials [Internet]. 2004 May [cited 2024 Jul 24]; 6: 299–303. Available from: <u>https://doi.org/10.1002/adem.200300567</u>

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constituent concentrations) of multinary (high-order/multi-component) phase diagrams and this allows increased flexibility in terms of selecting HEA constitutions, provided process-informed design can be utilized in physically obtaining these phases. High entropy materials have four features in common: (1) high entropy effect, (2) severe lattice distortion effect, (3) sluggish diffusion effect, and (4) cocktail effect.

Many interesting metallurgical phenomena and properties such as unprecedented fracture toughness have been reported in HEAs.^{356,357} In 2015, high entropy stabilization was first reported for and expanded to a mixture of oxides.³⁵⁸ Several other high entropy ceramics, including oxides, carbides, silicates and nitrides have now since reported. These ceramic systems have proven useful as HEMs, including as thermal barrier coatings, wear resistant coatings, and environmental barrier coatings (EBCs) (see Figure 28).³⁵⁹

³⁵⁶ Cook DH, Kumar P, Payne MI, Belcher CH, Borges P, Wang W, Walsh F, et al. Kink bands promote exceptional fracture resistance in a NbTaTiHf refractory medium-entropy alloy. Science [Internet]. 2024 Apr [cited 2024 Jul 24];384(6692):178–184. Available from: <u>https://doi.org/10.1126/science.adn2428</u>

³⁵⁷ Liu D, Yu Q, Kabra S, Jiang M, Forna-Kreutzer P, Zhang R, Payne M,et al. Exceptional fracture toughness of CrCoNi-based medium-and high-entropy alloys at 20 kelvin. Science [Internet]. 2024 Apr [cited 2024 Jul 24];378(6623):978–983. Available from: <u>https://doi.org/10.1126/science.abp8070</u>

 ³⁵⁸ Rost CM, Sachet E, Borman T, Moballegh A, Dickey EC, Hou D, Jones JL, et al. Entropy-stabilized oxides. Nat Comms [Internet]. 2015 Sept [cited 2024 Jul 24]; 6: 8485. Available from: https://doi.org/10.1038/ncomms9485
 ³⁵⁹ Oses C, Toher C, Curtarolo S. High-entropy ceramics. Nature Reviews Materials. [Internet]. 2020 Feb [cited 2024 Jul 24]; 5: 295–309. Available from: https://doi.org/10.1038/s41578-019-0170-8

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Figure 28. a) Examples of harsh environments with applications (b-e) for high entropy ceramics.

High entropy ceramics suffer from several constraints/roadblocks:^{360,361}

- Much mechanical property data on high entropy ceramics is limited to hardness and elastic modulus. Fracture toughness, room and high temperature strength, creep, and fatigue data must be generated from robust design of these materials.
- Processing routes to reach good densification are not developed.
- More entropy characterization must be performed to validate the high entropy nature of these ceramics.
- Dynamic oxidation information for this class of materials is limited.
- Sample size is limited.

High entropy ceramics offer several new opportunities:

³⁶⁰ Nisar A, Zhang C, Boesl B, Agarwal A. A perspective on challenges and opportunities in developing high entropy-ultra high temperature ceramics. Ceramics International [Internet]. 2020 Nov [cited 2024 Jul 24];46:25845–25853. Available from: https://doi.org/10.1016/j.ceramint.2020.07.066

³⁶¹ Xiang H, Xing Y, Dai F-Z, Wang H, Su L, Miao L, Zhang G, et al. High-entropy ceramics: present status, challenges, and a look forward, J of Adv Ceram [Internet]. 2021 Apr [cited 2024 Jul 24];10:385–441. Available from: <u>https://doi.org/10.1007/s40145-021-0477-y</u>

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- Computational approaches, including thermodynamic and density functional theory predictions, along with application of machine learning techniques, are well-equipped for the development of new high entropy ceramics.
- Multiphase high entropy ceramics can be explored in addition to single phase high entropy ceramics.
- Databases of high entropy ceramics, including mechanical, thermal, and functional properties, can be developed.
- Machine learning approaches predict oxidation of high entropy ceramics.

Success will be measured through harsh environment applications where high entropy ceramics are able to be commercialized as coatings or bulk materials. High entropy materials in general represent a crosscutting opportunity in energy generation and utilization. Industries that would benefit include the coatings and protection industries, power equipment providers, service and repair companies, and hydrogen power system organizations.

Rapid Materials Characterization

Develop rapid materials characterization and testing in support of advanced materials for extreme environment (C37)

Materials and process development acceleration tools such as high throughput processing, physics-informed multiscale modeling and simulation, *in-situ* measurement, digital twins, AI/ML, automation, and other smart manufacturing techniques are among the focus areas of this landscape. Rapid testing capabilities must be supplemented with rapid materials characterization capabilities to reduce risk for the high levels of investment traditionally required to develop and qualify materials for harsh environments. Capabilities of interest include *in-situ*, *ex-situ*, high throughput, and *operando* characterization.³⁶² Integration of high throughput and automated testing with advanced AI techniques will lead to rapid materials characterization modalities that will significantly accelerate materials and process development.

Rapid characterization of materials is being implemented with a variety of techniques, such as mechanical testing.³⁶³ Additive processing techniques such as directed energy deposition are particularly amenable to high throughput synthesis and characterization.^{364,365,366} In addition, high throughput characterization can benefit process optimization schemes, as shown in Figure 29 for process-parameter optimization:

³⁶² Jenks C, Ho Nyung Lee, Lewis J, Kagan C, Nealey P, Braun P, et al. Basic Research Needs for Transformative Manufacturing. [Internet]. Department of Energy; 2020 Mar 9 [cited 2024 Jul 30]; Available from: <u>https://www.osti.gov/servlets/purl/1618267</u>

³⁶³ Heckman NM, Ivanoff TA, Roach AM, Jared BH, Tung DJ, Brown-Shaklee HJ, Huber T, et al. Automated highthroughput tensile testing reveals stochastic process parameter sensitivity. Mat Sci & Eng: A [Internet]. 2020 Jan [cited 2024 Jul 25]; 772: 138632. Available from: <u>https://doi.org/10.1016/j.msea.2019.138632</u>

³⁶⁴ Vecchio KS, Dippo OF, Kaufmann KR, Liu X. High-throughput rapid experimental alloy development (HT-READ). Acta Materialia [Internet]. 2021 Dec [cited 2024 Jul 25];221:117352. Available from: https://doi.org/10.1016/j.actamat.2021.117352

³⁶⁵ Couet A. Integrated high-throughput research in extreme environments targeted toward nuclear structural materials discovery. Journal of Nuclear Materials [Internet]. 2021 Dec [cited 2024 Jul 25]; 559: 153425. Available from: <u>https://doi.org/10.1016/j.actamat.2021.117352</u>

³⁶⁶ Wang Y, Goh B, Nelaturu P, Duong T, Hassan N, David R, Moorehead M. Integrated high-throughput and machine learning methods to accelerate discovery of molten salt corrosion-resistant alloys. Adv Science [Internet]. 2022 May [cited 2024 Jul 25]; 9: 2200370. Available from: <u>https://doi.org/10.1002/advs.202200370</u>
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Figure 29. Illustration of a scheme for rapid process-parameter development and analysis implemented at the Zeiss lab at the Manufacturing Demonstration Facility at Oak Ridge National Laboratory.³⁶⁷

Rapid materials characterization suffers from number of constraints:

- High throughput characterization data generated at the lab or coupon scale may not be transferrable in a
 facile manner to commercial or component scale.
- Data generated from rapid characterization techniques does not directly result in improved physical understanding.
- There is a lack of machine learning and AI methodologies that can take advantage of voluminous data generated by rapid characterization techniques.
- Rapid synthesis techniques can be a constraint even in conditions where rapid characterization techniques are available.
- Rapid and accelerated testing for components that require extended life (e.g., tens of thousands of hours of operation for thermoelectric power plant components) can create unforeseen risk associated with differences in microstructural evolution or delayed phase transformations.
- Qualification of components is not readily coupled to rapid characterization schemes.

Rapid characterization techniques offer several salient opportunities, including:

- Extensive characterization is often necessary for commercialization, e.g., generation of a materials card for component design. Rapid characterization enables acceleration of the process.
- Rapid characterization techniques applied to new harsh environment materials can take advantage of new and emerging AI/ML data analytics methodologies; together they can further accelerate materials and process development. One example is the process-parameter development implemented at the Manufacturing Demonstration Facility (MDF) at ORNL.
- Rapid characterization can reduce the development time of new harsh environment materials, historically a slow process. At the very least, rapid characterization can reduce the time needed for new materials to become available for qualification.

³⁶⁷ Ziabari A, Venkatakrishnan SV, Snow Z, Lisovich A, Sprayberry M, Brackman P, Frederick C. Enabling rapid X-ray CT characterisation for additive manufacturing using CAD models and deep learning-based reconstruction. npj Computational Materials [Internet]. 2023 May [cited 2024 Jul 25];9:91, 2023. Available from: https://doi.org/10.1038/s41524-023-01032-5

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• Demonstrated high throughput experimental capabilities integrated with advanced AI techniques can support a digital design and manufacturing infrastructure and increased materials irradiation. Creep testing capability can provide materials to be applied in advanced reactors and other harsh environments.

Success will be measured through new HEMs and processes that are commercialized because of availability of rapid characterization techniques. Coupling of generated data to AI/ML and automated experimental techniques that complement physics-based understanding is key to successful accelerated development of harsh environment materials. Industries that would benefit include materials test equipment companies, software companies that specialize in materials informatics and simulation, AI/ML companies, sample/part testing organizations, and DED based additive machine vendors.

Multi-Scale Behavior and Degradation of Materials

Acquire comprehensive understanding of materials behavior in harsh environments at different time and length scales (C78)

The last few decades have seen tremendous advances in computational materials science and the marriage of this discipline to materials engineering has led to the emergence of ICME.³⁶⁸ Multi-scale materials modeling is a hallmark of ICME methodologies, and such approaches are gradually beginning to evolve from aspirational activities to characterize complex phenomena spanning from the atomistic scale to macroscopic scale behavior.³⁶⁹ Establishing links between multiple scales is often time- and resource-intensive. An alternate approach is to find the most relevant scale(s) for the problem of interest. Indeed, Yip and Short describe the mesoscale (illustrated in Figure 30 between micro and macro scale) where modeling, simulation, and experimental capabilities can have the highest impact in bridging scientific discoveries at the microscale and technological applications at the macroscale.³⁷⁰



³⁶⁸ National Research Council. Integrated computational materials engineering: a transformational discipline for improved competitiveness and national security. [Internet] National Academies Press; 2008 [cited 2024 Jul 30]. Available from: <u>https://nap.nationalacademies.org/catalog/12199/integrated-computational-materials-engineeringa-transformational-discipline-for-improved-competitiveness</u>

³⁶⁹ Van Der Giessen E, Schultz PA, Bertin N, Bulatov VV, Cai W, Csányi G, Foiles SM. Roadmap on multiscale materials modeling. Modelling and Simulation in Mat Sci and Eng [Internet]. 2020 Mar [cited 2024 Jul 25];28,043001. Available from: <u>https://doi.org/10.1088/1361-651X/ab7150</u>

³⁷⁰ Yip S, Short MP. Multiscale materials modelling at the mesoscale, Nature Materials [Internet]. 2013 Sept [cited 2024 Jul 25];12:774-777. Available from: <u>https://doi.org/10.1038/nmat3746</u>

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Figure 30. Complexity-capability map as represented by Yip and Short, showing that the separation between scientific studies and discoveries at the microscale and technological innovations at the macroscale can be bridged by modeling, simulation, and experimental capabilities at the mesoscale (represented by mesoscale science or MSS).

Technologies where materials degradation is relevant can benefit through the application of multi-scale modeling approaches. In this context, materials degradation broadly refers to reduction in the ability of a material to perform at a desired level in-service due to environmental exposure. Corrosion and microstructural evolution are salient examples of processes that lead to materials degradation. In general, multiscale approaches have been more successful in modeling microstructural evolution³⁷¹ compared to corrosion processes.³⁷² AI/ML approaches are being applied to enhance the understanding of materials degradation to enhance and supplement the understanding gained from physical multi-scale models.³⁷³

Multi-scale behavior and degradation of materials suffers from several constraints:

- Existing multi-scale models often lack resolution to design corrosion-resistant systems that are effective.
- Numerical strategies for linking multi-scale models for corrosion and other multiscale materials degradation processes must evolve.
- As multi-scale models for corrosion are created, the uncertainty in models at lower scales can propagate to larger scales; gaps in experimental characterization must be filled, especially at lower scales.
- Qualification of new materials in codes and standards can be time and resource prohibitive.
- Developmental HEMs must demonstrate performance in relevant harsh environment(s) to validate manufacturing routes.

Multi-scale behavior and degradation of materials also offer several salient opportunities:

- Design and development of degradation-resistant materials is a crosscutting energy generation and utilization opportunity.
- Higher temperature materials can enable longer operating lifetime and greater efficiency. New materials must be tested in representative conditions and at relevant time and length scales. A specific example in the case of CSP is long-term generation data in relevant environments. Long-term test programs, material down-selection studies with industry, and cost share for fabrication trials are all opportunities.
- Material degradation understanding can support advanced non-LWR material selection, lifting assessments, licensing, inspection, and operation.
- Qualification of new materials in codes and standards, including additional materials to ASME Section III Division 5. Acceleration of qualification is relevant.
- Development of CMC materials for thermal energy storage.

Success will be measured through the number of technologies that are commercialized in the next decade through understanding multi-scale behavior and degradation of materials. As noted earlier, picking the right scale to bridge scientific discovery to technological application will help manage the problem in certain cases. Although energy OEMs will benefit if success is realized, other kinds of firms relevant to this landscape that will benefit most are power generation companies and computational and simulation engineering firms that provide improved modeling capabilities.

³⁷¹ Vaithyanathan V, Wolverton C, Chen LQ. Multiscale modeling of precipitate microstructure evolution. Physical Review Letters [Internet]. 2002 Mar [cited 2024 Jul 25];88:125503. Available from: https://doi.org/10.1103/PhysRevLett.88.125503

³⁷² Gunasegaram DR, Venkatraman MS, Cole IS. Towards multiscale modelling of localised corrosion. International Materials Reviews [Internet]. 2013 Dec [cited 2024 Jul 25];59:84-114. Available from: https://doi.org/10.1179/1743280413Y.000000024

³⁷³ Nash W, Drummond T, Birbilis N. A review of deep learning in the study of materials degradation, npj Materials Degradation [Internet]. 2018 Nov [cited 2024 Jul 25];2:37. Available from: <u>https://doi.org/10.1038/s41529-018-0058-</u>

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Research sequence will be materials development of multi-scale models for HEMs in the 2025–2030 timeframe and code qualification and licensing in the subsequent 2030–2035 timeframe.

Novel High-Performance Materials for Crosscutting Applications

Design and synthesis of new materials with unique properties and behavior of a variety of harsh operating environments (C19)

High temperature alloys are among the most crosscutting materials that enable a variety of energy technologies. Two common attributes for harsh environment applications for alloys include creep or high temperature deformation resistance and oxidation resistance.

Figure 29, adapted from Evans and Wilshire,³⁷⁴ compares common alloy systems by their respective upper temperature limits for oxidation resistance and creep resistance. The refractory alloys Mo and W have superior creep resistance but are deficient in oxidation resistance. In contrast, 12 Cr steels demonstrate a good balance of oxidation and creep resistance, which, along with their affordability, means they are likely the most applied alloys by tonnage in several thermoelectric power plant components. The Ni and Co superalloys are so-called because of their combination of creep and oxidation resistance that is unmatched by other alloys.³⁷⁵ In the last couple of decades, high entropy alloys (HEAs) have received much attention, but they lack creep resistance; the body-centered cubic (BCC) HEAs with good high temperature tensile properties are prone to oxidation.³⁷⁶ Most recently, new HEA concepts have led to co-improvement in room and high temperature properties.³⁷⁷ In the opportunity space shown in Figure 31, new refractory alloys, HEAs, ceramic matrix composites, oxide dispersion steels, etc., can provide an unprecedented combination of creep and oxidation for creep and oxidation resistance. Such novel high-performance materials will have an impact on crosscutting energy technologies.³⁷⁸

https://www.tms.org/superalloys/10.7449/2005/Superalloys_2005_1_14.pdf

³⁷⁴ Evans RW, Wilshire B, editors. Introduction to creep. 1st ed. Institute of Materials, 1993.

³⁷⁵ Pollock, TM, Tin S. Nickel-based superalloys for advanced turbine engines: chemistry, microstructure and properties. Journal of Propulsion and Power [Internet]. 2012 May [cited 2024 Jul 25];22(2):361-374. Available from: <u>https://doi.org/10.2514/1.18239</u>

³⁷⁶ Gorr B, Schellert S, Müller F, Christ HJ, Kauffmann A, Heilmaier M. Current status of research on the oxidation behavior of refractory high entropy alloys. Advanced Engineering Materials [Internet]. 2021 Feb [cited 2024 Jul 25];23:2001047. Available from: <u>https://doi.org/10.1002/adem.202001047</u>

³⁷⁷ Cook DH, Kumar P, Payne MI, Belcher CH, Borges P, Wang W, Walsh F. Kink bands promote exceptional fracture resistance in a NbTaTiHf refractory medium-entropy alloy. Science [Internet]. 2024 Apr [cited 2024 Jul 25];384:178-184. Available from: <u>https://doi.org/10.1126/science.adn2428</u>

³⁷⁸ Kennedy RL. ALLVAC® 718PLUSTM, superalloy for the next forty years. Loria EA, editor. TMS [Internet]. 2005 [cited 2024 Jul 30];718(625). Available from:

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Figure 31. Comparison of common alloy systems in terms of resistance to oxidation and high temperature creep fracture (adapted from Evans and Wilshire).

Novel high-performance materials for crosscutting applications suffer from several constraints:

- Materials development has been a historically slow process. Often, development of new materials is the bottleneck for implementation of new energy technologies such as molten salt reactors.
- Few harsh environment materials simultaneously meet requirements of creep resistance, oxidation resistance, processability, and cost.
- There are additional constraints in terms of moving lab-scale high-performance materials to commercial scale.
- Long-term performance evaluation is challenging and can only be performed on down-selected materials.
- Specific sub-classes of materials may need to be developed for crosscutting applications. For example, different superalloys may be applied for molten salt applications in nuclear reactors than for CSP applications.
- Feedstock development and control remains a constraint for powder processing related applications such as laser powder bed fusion.

Novel high-performance materials for crosscutting applications also offer several opportunities:

- New materials concepts, such as those resulting from HEAs, and advanced manufacturing are exciting
 new avenues leading to the development of new harsh environment capable materials at an accelerated
 rate.
- SiC-based CMC development and use in turbine applications provides new opportunities for applications of these materials in other harsh environments.
- New superalloys for molten salt-based energy technologies may be used in a number of other applications.
- Alloys with higher operating temperature in relation to their melting point are another opportunity with crosscutting benefits.
- Development of coatings and graded materials provides crosscutting benefits for resisting multiple harsh environments.
- Design and synthesis of new materials with unique properties and behavior in a variety of harsh operating environments creates opportunities to crosscut activities in multiple DOE program offices.

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Success will be measured through the development and deployment of high-performance materials in crosscutting harsh environment applications. Simultaneously increasing the creep and oxidation resistance of new and existing classes of materials is stated to be a salient crosscutting opportunity across a variety of application spaces.

Industries that will benefit from development of novel high-performing materials include those in power generation, metal alloying, and aerospace. The sequence of events will be materials development of HEMs with crosscutting benefits in the 2025–2030 timeframe followed by possible qualification, including code qualification, in the 2030–2035 timeframe.

HEM Modeling and Simulation

Integrate comprehensive data analytics and modeling and simulation for material design and selection for extreme environment materials (C47)

Harsh environment applications require innovations in materials and process engineering that are accelerated by computational efforts in discovery, prediction, and simulation. Modeling efforts can have critical impacts on understanding processes over a variety of scales, including material microstructure, grain boundaries and interfaces, large-scale stresses and strains, component durability, and degradation predictivity.

Computation can inform many aspects of the industrial process. Current modeling of materials for harsh environments is difficult: classical simulations struggle to handle the large number of variables and heterogenous environments involved, but atomistic simulations based on quantum mechanics are too expensive. Neural network potentials show great promise in bridging this gap, as they can achieve the accuracy of quantum-mechanical simulations and be trained to automatically parameterize the needed potentials at a significantly cheaper cost than full quantum-mechanical simulations.^{379,380} Relevant needs include screening of promising coatings and materials used in HEM components, predicting durability and behavior in the operating environment, and modeling of processes to better understand the mechanisms contributing to failure.

Appropriate models ideally capture the entire range of the harsh environment, including evolution of the environment during device or process operation. To do this, two needs of particular importance must be met: 1) an automatic way to generate training data and create accurate neural network potentials or other machine learning-based potentials, and 2) a coupling to macroscopic variables available from continuum modeling. Thus, research is needed to automatically generate high-quality training data that can be iteratively improved upon and is relevant to practical devices. Establishing approaches to determine which training data is needed to produce an accurate and relevant model is perhaps the most important development needed for effective materials design in this space. Further, data-driven (more precisely, data mining) approaches to optimizing devices and processes are already common with solely experimental data, but computational data is needed to supplement and maximize the power of these approaches.^{381,382}

³⁷⁹ Batatia I, Kovàcs DP, Simm G, Ortner C, Csányi G. MACE: higher order equivariant message passing neural networks for fast and accurate force fields. Adv. Neural Inf. Process. Syst. [Internet]. 2022 [cited 2024 Jul 30];35:11423–11436. Available from: <u>https://doi.org/10.48550/arXiv.2206.07697</u>.

³⁸⁰ Ko TW, Ong SP. Recent advances and outstanding challenges for machine learning interatomic potentials. Nat Comput Sci [Internet]; 2023 Dec [cited 2024 Jul 30];3:998–1000. Available from: <u>https://doi.org/10.1038/s43588-023-00561-9</u>

³⁸¹ Fong AY, Pellouchoud L, Davidson M, Walroth, D, Church C, Tcareva E, Wu L, et al. Utilization of machine learning to accelerate colloidal synthesis and discovery. J. Chem. Phys. [Internet] 2021 Jun [cited 2024 Jul 30];154:224201. Available from: https://doi.org/10.1063/5.0047385

³⁸² Lee C, Kort-Kamp WJM, Yu H, et al. Grooved electrodes for high-power-density fuel cells. Nat Energy [Internet] 2023 May [cited 2024 Jul 30];8:685–694. Available from: <u>https://doi.org/10.1038/s41560-023-01263-2</u>

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Advances in integrated computational materials engineering and data analytics have benefits across technology areas. Computational screening of appropriate materials for coatings and claddings has positively impacted development of components for geothermal drilling, molten salt tanks for concentrating solar, and nuclear reactor vessels. Modeling can inform the design of process conditions for joining, as in the modeling of interface physics in EFAS to optimize temperature profiles and understand grain boundary mobilities. More robust computational methods also stand to improve energy technologies such as electrolyzers, batteries, and fuel cells by better capturing underlying device performance; this is currently complicated by the complexity of multi-material layers and the significant material changes that occur because of electrochemical cycling.³⁸³

Process integrated analytics also play a large role in sensor management, *in situ* process monitoring, and overall monitoring of structural health in harsh manufacturing environments. Modeling and analysis techniques can also bolster development of target metrics and develop computational frameworks that can be translated across application spaces. In considering sensors for industrial environments, the operation of embedded power electronics in harsh environments will improve stability at high temperatures.³⁸⁴

Advances in this space would benefit and impact markets across DOE application spaces. Among others, CSP, geothermal, wind energy, and nuclear systems benefit directly from targeted modeling and computational efforts (e.g., through contributions to reduced failure rate; increased system and component longevity and durability; more rapid advancement of technology development; and contributions to qualification processes or technology readiness timelines). Success can be measured by comparing field performance data, failure rates, and experimentally validated materials properties to outputs of modeling and computational efforts. For example, high temperature alloys identified by a computational screening to be robust against degradation can be validated by corrosion testing. In the realm of materials optimization, success would look like automatic navigation of complex materials design spaces in conjunction with experiments to design better devices at a measurably faster pace than what was previously possible. Various metrics for device performance would show a faster pace of improvement after this modeling approach is developed, if it is successful. The industrial players to be impacted include not only computational materials-informatics and simulation companies, but also semiconductor suppliers and chip manufacturers.

Advancements in the field are proceeding rapidly. With continued investment, the tools currently under development could be mature enough to impact material and device design. Capitalizing on the rapid growth of knowledge around neural network and machine learning approaches in the commercial, national lab, and academic sectors is critical for meeting DOE's climate goals. Integration of computational discovery and learning methods expands the number of strategies available to improve device and component performance, thus advancing the pace of innovation. Additionally, field and component failures that could have been caught by process and system monitoring will negatively impact the viability of these technologies on a commercial scale. Computational efforts should be appropriately scoped toward the technology of interest (i.e., materials screening for early-stage technology and component durability or forecasting schemes for improving longevity in more mature technologies).

For many applications, it will be necessary to precede or work closely alongside technology development to robustly understand, optimize, and predict the future behavior of various systems, components, and processes. Data analytics development for a given process can evolve over time, although frameworks should be developed early to guide process development and further reduce process and operating costs.

³⁸³ Liu H, Li B, Liu Z, Liang Z, Chuai H, Wang H, Nee Lou S, et al. Ceria -Mediated Dynamic Sn0/Snδ+ Redox Cycle for CO2 Electroreduction. ACS Catal. [Internet] 2023 Mar [cited 2024 Jul 30]; 13(7): 5033–5042. Available from: <u>https://doi.org/10.1021/acscatal.2c06135</u>

³⁸⁴ Lee CW, Zakutayev A, Stevanović V. Computational Insights into Phase Equilibria between Wide-Gap Semiconductors and Contact Materials. ACS Appl. Elec. Mat [Internet]. 2024 Apr [cited 2024 Jul 30];6(4):2383-2391. Available from: <u>https://doi.org/10.1021/acsaelm.4c00032</u>

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Demonstrate modeling and Simulation of HEMs to expedite qualification (C84)

The design and deployment of new HEMs by purely experimental means is time, labor, and cost intensive. However, urgent energy needs for new HEMs and the rapidly changing landscape for advanced manufacturing demands increasingly rapid development. Computational modeling and simulation tools offer an approach to accelerate design and adoption timelines in a variety of ways.³⁸⁵ Physics-based modeling approaches offer a window of understanding into the underlying connections between processing, microstructure evolution, and the properties and performance of materials and end-use components. Simultaneously, the emergence and maturation of machine learning and AI has created new ways of evaluating and utilizing data produced both experimentally and computationally. Although it is unrealistic to entirely replace experiments, there are several ways in which models may complement experimental methods to accelerate development. For example, computational thermodynamics tools are frequently used to guide the development and selection of alloy compositions,³⁸⁶ while process models are used to help determine optimal processing conditions.³⁸⁷ These types of approaches are critical for minimizing trial-and-error experimentation. More mature models are valuable for informing component design decisions, or even qualification approaches. In the context of HEMs, it is important that as new materials are development, make meaningful predictions, and accelerate adoption.

While the needs for energy solutions and HEM applications are growing, the computational environment available for supporting modeling and simulation tools is also changing rapidly. Al/ML research and commercial investment has driven deployment and adoption of GPUs, and modern computing resources, especially leadership-class machines available within the DOE complex (e.g., ORNL's Frontier supercomputer³⁸⁸), increasingly contain hybrid CPU/GPU architectures.³⁸⁹ However, rapid advancement in computing is also making large-scale parallel processing increasingly accessible, both for day-to-day engineering applications and for edge-computing in manufacturing environments, where routine simulation and data analysis may be used to build digital twins to aid in qualification.

Modern computing toolsets must therefore be developed to maximally leverage this evolving landscape. The DOEfunded Exascale Computing Project funded development of libraries for performance-portable and scalable use of diverse computing architectures (e.g., libraries such as Kokkos³⁹⁰ and Raja³⁹¹ for parallelization across a variety of

³⁸⁵ Furrer D. Development and industrial application of integrated computational materials engineering. Model Simul Mater Sci Eng [Internet]. 2023 Aug [cited 2024 Jul 25]; 31: 073001. Available from: <u>https://doi.org/10.1088/1361-651X/aced59</u>

³⁸⁶ Kannan R, Nandwana P. Predicting sintering window of binder jet additively manufactured parts using a coupled data analytics and CALPHAD approach. Integrating Mater Manuf Innov [Internet]. 2023 Oct [cited 2024 Jul 25];12:421–429. Available from: <u>https://doi.org/10.1007/s40192-023-00313-7</u>

³⁸⁷ Saunders RN, Teferra K, Elwany A, Michopoulos JG, Lagoudas D. Metal AM process-structure-property relational linkages using Gaussian process surrogates, Addit Manuf [Internet]. 2023 Jan [cited 2024 Jul 25];62:103398. Available from: https://doi.org/10.1016/j.addma.2023.103398.

³⁸⁸ Oak Ridge National Laboratory. Frontier supercomputer debuts as world's fastest, breaking exascale barrier. [Internet] Oak Ridge National Laboratory; 2022 May 30 [cited: 2024 Jul 31]. Available from:

https://www.ornl.gov/news/frontier-supercomputer-debuts-worlds-fastest-breaking-exascale-barrier

³⁸⁹ Khan A, Sim H, Vazhkudai SS, Butt AR, Kim Y. An analysis of system balance and architectural trends based on Top500 supercomputers, in: Int. Conf. High Perform. Comput. Asia-Pac. Reg., ACM, Virtual Event Republic of Korea, [Internet]. 2021 Jan [cited 2024 Jul 25]; pp. 11–22. Available from: https://doi.org/10.1145/3432261.3432263.

³⁹⁰ Trott CR, Lebrun-Grandie D, Arndt D, Ciesko J, Dang V, Ellingwood N, Gayatri R, et al. Kokkos 3: programming model extensions for the exascale era. IEEE Trans. Parallel Distrib. Syst. [Internet]. 2022 Apr [cited 2024 Jul 25]; 33 (2022) 805–817. Available from: https://doi.org/10.1109/TPDS.2021.3097283.

³⁹¹ D.A. Beckingsale, T.R. Scogland, J. Burmark, R. Hornung, H. Jones, W. Killian, A.J. Kunen, O. Pearce, P. Robinson, B.S. Ryujin, RAJA: Portable Performance for Large-Scale Scientific Applications, in: 2019 IEEEACM Int. Workshop Perform. Portability Product. HPC P3HPC, IEEE, Denver, CO, USA, 2019: pp. 71–81. Available from: https://doi.org/10.1109/P3HPC49587.2019.00012.

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CPU and GPU backends). These resources make it significantly easier to develop software tools for diverse computing architectures. With such diversity, many different types of modeling tools will be necessary. Complex physics-based simulation platforms may be developed that can utilize the largest supercomputers for individual calculations, ensembles for training surrogate ML models, or for purposes of uncertainty propagation through process-structure-property linkages. Simplified models may be developed for deployment at the edge in faster-than-real-time calculations to inform process controls or digital twins for qualification.

Modeling and simulation research relevant to HEMs is subject to the following constraints:

- Process-microstructure-property relationships are complex and sometimes unknown. For example, few predictive simulations are available to predict the environmental effects of new alloys. New capabilities must be developed to capture the complex physics relevant to HEM development, especially for the characteristically complex conditions characteristic of advanced manufacturing processes (e.g., additive manufacturing³⁹² or field-assisted sintering and joining) and when spanning many length and time scales.³⁹³
- The complex physics relevant to many HEMs and advanced manufacturing processes requires sophisticated models, resulting in complex, computationally intensive simulations. Because new tools slated for deployment in diverse computing architectures must achieve results that are both fast and accurate, they will likely require the development of new and efficient algorithms and methods.
- For complex models, especially when linked together (e.g., ICME approaches), quantifying and propagating uncertainty is necessary to capture the reliability of model predictions.³⁹⁴ This is especially true as applications mature from early-stage development of new materials toward deployment and qualification of end-use components.
- Model calibration and validation, as well as training of ML/AI models, requires highly pedigreed and curated datasets. Limited data is available for complex materials systems, becoming even scarcer or absent entirely as new material classes are developed.

Success will be measured by accelerated development timelines for HEMs, use of modeling tools for rapid process optimization, and increasing acceptance of model-assisted qualification through implementation of digital twins. These successes will also leverage and help to proliferate adoption of advanced computing architectures for use in data collection, analysis, and complementary modeling in industrial environments.

Commercial software industries that focus on materials and environmental simulation, along with computer assemblers and chip manufacturers, will benefit the most from advancements in modeling and simulation for HEM design and selection. The sequence of events will be early-stage development of simulation tools for HEMs that make substantial use of modern computing architectures in the 2025–2030 timeframe, concurrent with and followed by their incorporation into materials design and process optimization (2025–2035). Later adoption (after 2035) will focus on accelerating materials qualification for energy applications.

³⁹² Sharma S, Joshi SS, Pantawane MV, Radhakrishnan M, Mazumder S, Dahotre NB. Multiphysics multi-scale computational framework for linking process–structure–property relationships in metal additive manufacturing: a critical review, Int. Mater. Rev. [Internet]. 2023 Oct [cited 2024 Jul 25]; 68: 943–1009. Available from: https://doi.org/10.1080/09506608.2023.2169501.

³⁹³ Fish J, Wagner GJ, Keten S. Mesoscopic and multiscale modelling in materials. Nat. Mater. [Internet]. 2021 May [cited 2024 Jul 25]; 20: 774–786. Available from: <u>https://doi.org/10.1038/s41563-020-00913-0</u>.

³⁹⁴ Sankararaman S, Mahadevan S. Integration of model verification, validation, and calibration for uncertainty quantification in engineering systems. Reliab. Eng. Syst. Saf. [Internet]. 2015 Jun [cited 2024 Jul 25]; 138: 194–209. Available from: <u>https://doi.org/10.1016/j.ress.2015.01.023</u>.

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Qualification of PM HEMs for sCO₂ Turbomachinery

Qualify new materials in codes & standards, including additional materials to ASME Section III Division 5 (C134)

Thermal power cycles that operate with supercritical carbon dioxide (sCO_2) will have a crosscutting role in future systems with applications in all kinds of thermoelectric plants, including nuclear power, concentrated solar power, and waste heat recovery. The crosscutting nature of sCO_2 power and propulsion applications is shown in Figure 30. As a working fluid, sCO_2 offers multiple benefits with heat source temperatures between 350°C and 800°C, including compact footprints, good operational flexibility, and potential to lower the LCOE. Several technical challenges exist, however, including material availability for high operating temperatures and pressures, and the durability of turbomachinery components and heat exchangers in sCO_2 .

The choice of material for use in sCO₂ applications is determined by the mechanical and thermal properties of the material, compatibility with sCO₂ environment, and fabrication cost of the power plant. The sCO₂ environment affects the ionic solubility, dissociation, corrosion, oxidation, and creep resistance of the material.³⁹⁵ sCO₂ pressures up to 300 bar and the higher density of sCO₂ (compared to sH₂O) can have a significant impact on the turbine rotor blades and may require the use of higher strength alloys.³⁹⁶ The sCO₂ can dissolve into seal materials, causing decompression. Various classes of structural alloys are employed at different temperatures. For operating temperatures less than 650°C, traditional stainless steel can be employed, but at temperatures higher than 650°C, much more expensive nickel-based or titanium-based alloys are required.³⁹⁷ Carbon ingress is a challenge for Febased alloys but has been reported to be less of a vulnerability for Ni-based alloys.³⁹⁸

 ³⁹⁵ Badescu V, Lazaroiu GC, Barelli L, editors. Power engineering: advances and challenges, part a: thermal, hydro and nuclear power. 1st ed. CRC Press; 2018 Feb. Available from: https://doi.org/10.1201/9781315202105
 ³⁹⁶ Wright IG, Pint BA, Shingledecker JP, Thimsen D. Materials considerations for supercritical CO₂ turbine cycles. Proceedings of ASME Turbo Expo 2013: Turbomachinery Technical Conference and Exposition [Internet].
 ²⁰¹³ Jun [cited 2024 Jul 24] San Antonio, Texas. Available from: http://dx.doi.org/10.1115/GT2013-94941
 ³⁹⁷ Maziasz P, Pint B, Shingledecker J, Evans N, Yamamoto Y, More K, Lara-Curzio E. Advanced alloys for compact, high-efficiency, high-temperature heat-exchangers. Int J of Hydrogen Energy [Internet]. 2007 [cited 2024 Jul 24];32: 3622–3630. Available from: https://doi.org/10.1016/j.ijhydene.2006.08.018
 ³⁹⁸ Pint BA, Pillai R, Lance MJ, Keiser JR. Effect of Pressure and Thermal Cycling on Long-Term Oxidation in CO₂ and Supercritical CO₂. Oxidation of Metals [Internet]. 2020 Nov [cited 2024 Jul 24]; 94: 505–526. Available from: https://doi.org/10.1007/s11085-020-10004-9

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Figure 32. Overview representing a range of sCO₂ power applications and the temperature range of the energy source. ^{399,400}

Qualification of HEMs for sCO₂ turbomachinery suffers from several constraints:

- Most reported studies are limited to low sCO₂ velocity laboratory conditions and are unrepresentative of high velocity operating conditions within practical sCO₂ power systems.
- Heat exchangers must operate with adequate heat conduction for up to 60 years in demanding conditions, including high temperatures and pressures, as well as corrosive, oxidation, carburization/decarburization —all at a reasonable cost.
- Due to the oxygen activities of sH₂O and sCO₂ environments, at temperatures greater than 650°C, superalloys or titanium-based alloys could be required to reduce oxidation propensity and to achieve pressure containment without excessive material thicknesses. However, this would come at a much higher capital cost.
- Testing under more realistic conditions of high velocity flow, stress, and impurities is required. Data reliability, consistency, and reproducibility are of paramount importance.

Qualification of HEMs for sCO₂ turbomachinery offers various opportunities:

At twice the density of supercritical steam, sCO₂ power cycles can achieve ~8–10% higher efficiency at a turbine inlet temperature of 760°C and a 10–20x smaller footprint compared to a steam Rankine cycle. However, due to the cost of high-grade materials, they are less attractive unless used in conjunction with CSP, where solar energy is stored as heat and converted to electricity on-demand using a sCO₂ power cycle.

³⁹⁹ White MT, Bianchi G, Chai L, Tassou SA, Sayma AI. Review of supercritical CO₂ technologies and systems for power generation. Applied Thermal Engineering [Internet]; 2021 Feb [cited 2024 Jul 24] 185: 116447. Available from: <u>https://doi.org/10.1016/j.applthermaleng.2020.116447</u>

⁴⁰⁰ Mendez C, Margarita C, Rochau GE. sCO₂ brayton cycle: roadmap to sCO₂ power cycles NE commercial applications [Technical Report]. Sandia National Laboratories (NV); 2018 [cited 2024 July 24]. SAND-2018-6187. Available from: <u>http://dx.doi.org/10.2172/1452896</u>.

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- ASME code cases are approved for IN740H and Haynes 282 Ni-base superalloys, for use in sCO₂ turbomachinery Longer-term studies on corrosion are needed because both sCO₂ and sH₂O can oxidize Fe, Ni, and Cr under the right circumstances.
- Mechanical property degradation studies (strength and durability) would be beneficial.
- Welding and diffusion bonding of metals and their effect on sCO₂ environment corrosion resistance must be studied.
- Understanding the long-term behavior of coatings and seals in sCO₂ environments is essential.

 sCO_2 power generation represents a crosscutting opportunity in energy generation and utilization. Success will be measured by how quickly sCO_2 technologies can be commercialized. As mentioned earlier, sCO_2 power generation represents a crosscutting opportunity in energy generation and utilization. Industries that would benefit include predominantly those within the power generation sector. Qualification of HEMs for sCO_2 turbomachinery to accelerate sCO_2 process development should begin in 2025.

Molten Salt Corrosion-Resistant Materials Testing

Develop molten salt (particularly FLiBe and Chloride salts) component testing for material compatibility with molten salt reactors, fusion, solar, and thermal storage to enable higher temperature operation (C80)

Molten salt powered energy technologies provide attractive energy solutions in the nuclear, thermal energy storage, and CSP sectors. To reduce the levelized cost of electricity, next-generation CSP plants with higher process temperature and energy efficiency are being developed.⁴⁰¹ For example, NREL researchers have proposed a higher temperature molten salt system combined with a sCO₂ Brayton power cycle.⁴⁰² Molten salt reactors (MSRs) have also been proposed to expand beyond their current role in power generation toward chemical synthesis, particularly for hydrogen generation.⁴⁰³ Production of hydrogen also demands an increase in reactor operating temperature in the range of 800°C–1,000°C. Establishing design strategies for the development of corrosion-resistant structural materials⁴⁰⁴ and accelerated^{405,406} and in-situ⁴⁰⁷ evaluation in a molten salt environment is required to accelerate the adoption of molten salt powered energy technologies. High throughput molten salt corrosion testing is being developed (as shown in Figure 33) for compositionally complex alloys.

⁴⁰¹ Ding W, Bauer T. Progress in research and development of molten chloride salt technology for next generation concentrated solar power plants. Engineering [Internet]. 2021 [cited 2024 Jul 25]; 7(3):334–347. Available from: <u>https://doi.org/10.1016/j.eng.2020.06.027</u>

⁴⁰² Yin JM, Zheng QY, Peng ZR, Zhang XR. Review of supercritical CO₂ power cycles integrated with CSP. Int J of Energy Research [Internet]. 2019 Dec [cited 2024 Jul 25]; 44:1337–1369. Available from: https://doi.org/10.1002/er.4909

⁴⁰³ Forsberg CW. Hydrogen, nuclear energy, and the advanced high-temperature reactor. International Journal of Hydrogen Energy [Internet]. 2003 Oct [cited 2024 Jul 25]; 28(10): 1073–1081. Available from: https://doi.org/10.1016/S0360-3199(02)00232-X

⁴⁰⁴ Pillai R, Sulejmanovic S, Lowe T, Raiman SS, Pint BA. Establishing a design strategy for corrosion resistant structural materials in molten salt technologies. JOM [Internet]. 2023 Jan [cited 2024 Jul 25];75:994–1005. Available from: https://doi.org/10.1007/s11837-022-05647-9

⁴⁰⁵ Couet A. Integrated high-throughput research in extreme environments targeted toward nuclear structural materials discovery. J of Nucl Mat [Internet]. 2022 Feb [cited 2024 Jul 25];59:153425. Available from: <u>https://doi.org/10.1016/i.jnucmat.2021.153425</u>

 ⁴⁰⁶ Wang Y, Goh B, Nelaturu P, Duong T, Hassan N, David R, Moorehead M, et al. Integrated high-throughput and machine learning methods to accelerate discovery of molten salt corrosion-resistant alloys. Adv Sci [Internet].
 2022 May [cited 2024 Jul 25];9:2200370. Available from: https://doi.org/10.1002/advs.202200370

⁴⁰⁷ Wang Y, Olson AP, Falconer C, Kelleher B, Mitchell I, Zhang H, Sridharan K, et al. Radionuclide tracing based in situ corrosion and mass transport monitoring of 316L stainless steel in a molten salt closed loop, Nature Comm [Internet]. 2024 Apr [cited 2024 Jul 25];15:3106. Available from: <u>https://doi.org/10.1038/s41467-024-47259-8</u>

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Molten salt corrosion-resistant materials testing suffers from several constraints:

- For nuclear applications, the number of alloys that are allowed for use in high temperature nuclear components is very limited. Maximum usage temperature of these alloys has increased only at a rate of 2.85°C/year as opposed to aerospace alloys, which have increased their operating temperature by 5°C/year since the 1950s.
- Experimental challenges associated with high throughput testing in corrosive environments include small amounts of salt in high throughput testing schemes, which can lead to saturation, and results that are not representative of reactor or thermal energy storage conditions.
- While static corrosion testing in molten salt environments is acceptable for down-selecting materials, further testing procedures that test salt-material interactions in non-isothermal conditions are required.⁴⁰⁷
- Physics-based or machine learning models to quantify material dissolution in various salt-alloy combinations of interest have limited to no availability.
- Testing under realistic conditions (at higher temperatures) is costly, as is testing to evaluate material compatibility in salt environments of interest.
- Molten salt tank design, manufacturing, and lifetime performance are a concern for molten salt energy storage.

Molten salt corrosion-resistant materials offer several opportunities:

- Design and development of molten salt corrosion-resistant materials is a crosscutting energy generation opportunity (e.g., nuclear energy, thermal energy storage, and concentrated solar power).
- Molten salt reactor designs for chemical synthesis have been proposed. Higher temperature operation is required along with system compatibility between alloys and salts.
- A next-generation molten salt system combined with supercritical (sCO₂) Brayton cycle has been proposed.
- Higher temperature operation, including in hydrogen generation and sCO₂, etc., would be enabled.
- There is renewed private sector interest in molten salt reactor concepts that were developed and demonstrated at ORNL in the 1960s.
- Development of coatings and bulk materials resistant to multiple harsh environments (e.g., molten salt reactor systems and sCO₂ environments).

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Figure 33. A high throughput molten salt corrosion testing setup for complex concentrated alloys developed DED was performed to make arrays of compositionally complex alloys with various concentrations of desired elements.⁴⁰⁶

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4. Conclusion

This landscape focused on five program thrusts selected to maximize both the outcome (impact) and crosscuts (reach) of future efforts with a scope of improving the performance and lowering the manufacturing costs of harsh environments material components, which are used in alternate forms of energy production, efficient energy utilization in the industrial sector, and energy storage technologies. These five focus areas, or thrusts, are:

- FA1: Functional surface technologies
- FA2: Materials integration into energy systems
- FA3: High-performance materials
- FA4: New paradigm materials manufacturing processes
- FA5: Materials and process development acceleration tools.

The advancement of high-impact crosscutting materials and manufacturing RD&D in these five focus areas is pivotal for the progress and sustainability of energy manufacturing technologies. The landscape has therefore outlined four strategic goals and identified the significant opportunities and challenges in the five focus areas, emphasizing the need for robust materials and components that can endure the demands of harsh environments, as well as development of competitive manufacturing processes and component integration into energy systems.

The four strategic goals (SG) are:

- Accelerate the exploration, development, and demonstration of structural and functional highperformance materials (including enabling technologies) engineered for harsh service conditions including materials circularity and sustainability considerations. Structural and functional materials families are entire classes or sub-classes of materials that exhibit exceptional properties and have potential crosscutting interests to DOE.
- Drive improvements to existing manufacturing technologies as well as develop and de-risk competitive novel advanced manufacturing technologies (AMTs) that promise greater process repeatability, reproducibility, cost savings, and sustainability for the production of high-quality HEM components at industrially relevant scales. Similar to the first goal, achieving this goal may involve the use of process development acceleration tools.
- Shorten manufactured HEM qualification and certification times.
- Support targeted HEM/component development and/or their manufacturing for specific high-impact opportunities, working in collaboration with other DOE technology and program offices.

The RD&D opportunities identified in the five focus areas serve to addresses the urgent requirements of the energy sector. In all, 70 opportunities were identified in the landscape. The urgency or timing for addressing each of these challenges was determined by their expected impact, reach, and required effort as measured by the TRL development pace based on their current TRL state, vis-à-vis the RISE analyses. A high impact/reach opportunity requiring a high degree of effort (i.e., one currently at a low TRL) will need to be pursued more aggressively than one with the same impact/reach potential requiring less effort (i.e., one already at a high TRL) in order to enter TRL 8 (TRL 7 completed) by the end of the next decade.

Based on the key takeaways identified throughout the landscape, some of the higher impact, more crosscutting opportunities from the five focus areas can be grouped together into the following five grand challenges, with their relevance to the five focus areas (FA), four strategic goals (SG), and application spaces given in brackets and their urgency (i.e., no-later-than timeframe to begin TRL advancement) indicated in boldface parenthesis. Most AMMTO projects seek to advance the TRL by a one-to-two step increase over a three-year period of performance. Thus, R&D should begin around 2025 for high impact opportunities currently at TRL 3 or lower to enter TRL 8 by 2035. High impact opportunities currently at TRL 5 or higher could begin as late as 2030 to enter TRL 8 by 2035.

Focus Area 1, Functional surface technologies grand challenge:

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Develop materials, coatings, cladding, and manufacturing processes for components exhibiting superior molten salt and liquid metal corrosion resistance, validated/qualified under realistic (real world) conditions of temperature, flow, pressure, and irradiation. [*Also relevant to FA 3 & 4; SG 1, 2, 3 & 4; and to thermoelectric power production, energy storage, industrial applications.*] (2030-2035)

Focus Area 2, Materials integration into energy systems grand challenge:

Improve capabilities to produce FGMs and multi/dissimilar-material integration through advanced joining/bonding techniques, including solid-phase processing like AFSD, FSW, and diffusion bonding (EFAS, HIP) to create systems with superior properties for specific harsh environment applications. [*Also relevant to SG 2 & 4; and all forms of energy production, energy storage, and industrial applications.*] (2030-2035)

Focus Area 3, High-performance materials grand challenge:

Continue to enhance the performance and lower the manufacturing cost of components made from advanced alloys, ceramics, and coatings with superior high-temperature oxidation-, corrosion-, and/or wear-resistance. This would include near net shape (NNS) monolithic and composite components having complex geometries, large dimensions, textured microstructures, or surface engineering for enhanced properties and performance. [*Also relevant to FA 1 & 4; SG 1 & 2; and to thermoelectric power production, industrial applications.*] (2030-2035)

Focus Area 4, New paradigm materials manufacturing processes grand challenge:

Evolve domestic manufacturing capability and feedstock/supply chain capacity to competitively produce ultra-largescale metallic components for service in harsh environment energy and industrial systems, including establishment of community-accepted validation benchmarks to accelerate qualification and certification for AMTs. [*Also relevant* to SG 2 & 3; and all forms of energy production, energy storage, and industrial applications.] (2025-2030)

Focus Area 5, Materials and process development acceleration tools grand challenge:

Progress and utilize enhanced length- and time-scale bridging methods for physics-based (deterministic) processinformed approaches, as well as probabilistic methods like machine learning, with the compilation of large research community accessible microstructure databases on HEMs to predict, design, and control microstructures, properties, and long-term performance of HEM components. [*Also relevant to SG 1, 2 & 3; and all forms of energy production, energy storage, and industrial applications.*] (2025-2030)

The HEM Landscape's RD&D efforts are scheduled to unfold from 2025 to 2035 with a clear focus to align with DOE's energy capacity and efficiency goals. Reaching these goals requires a strategic and coordinated effort among industry, national laboratories, and academia.

The R&D pathways involve methodical approaches to materials development, starting with the identification of potential materials followed by rigorous testing and analysis to optimize processing parameters. Subsequent steps include the manufacturing qualification and field certification of these materials against industry standards and regulatory requirements, ensuring their suitability for deployment in real-world applications.

Data analytics, modeling, and simulation technologies are instrumental in carrying out the activities described in this landscape, as they will provide the tools necessary to understand and predict material behavior, optimize designs, and expedite the qualification process. By integrating these technologies with experimental techniques, researchers can create a synergistic feedback loop that accelerates innovation and reduces development timeframes.

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The successful execution of this RD&D landscape will lead to the commercialization and eventual adoption of new materials and processes that are essential for the continued evolution of the energy sector. These advancements will yield materials with enhanced performance characteristics such as improved processability, cost-effectiveness, and creep, oxidation, corrosion, irradiation, and wear resistance. Furthermore, the development of coatings and functionally graded materials will provide crosscutting benefits for resisting multiple harsh environments.

Ultimately, this detailed RD&D agenda will facilitate the development of sustainable and resilient energy infrastructure, driving economic growth and positioning the United States as a global leader in energy innovation and sustainability. The next generation harsh environment materials and manufacturing process research agenda described in this landscape further promises to deliver transformative high-performance materials and manufacturing technologies that will shape the future of energy production, storage, and efficient utilization.

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Appendix



Figure 34. Description of icons from Figure 1.

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Industry-Informed Deliverables for TRL **TRL Phases R&D** Phases **TRL Definitions** Advancement & Tech Adoption **REE Production - Fully Operational -Fully Transitioned** Actual application of technology in its 9 Monitor and manage system performance **Production Scale** System final form operating under full range of after deployment, gather reports to validate operating conditions. field Techno Economic Analysis (TEA), Technology is proven to work - Actual Integrated Reliability Analysis (RAM), Life Cycle Cost technology is in its final and integrated Readiness Analysis (LCCA), Life Cycle Analysis (LCA), form and is qualified via (Qualified through Supply Chain Analysis (SA), Market Impact 8 testing/demonstrations. Full capability is ADICT) Analysis (MIA), Throughput Analysis, etc. demonstrated and hand off to production [Full Size] is approved. Full-scale, similar (prototypical) critical Final technologies demonstrated in a relevant Configuration 7 environment - Provides insight into full-Prototype Scale [Full Size] scale vs. 1/4th scale system differences. Provide continuous evidence for industry **Demonstrated in** Model/prototype is tested in relevant relevant reports such as Techno Economic Relevant environment - capable of performing all Analysis (TEA), Reliability Analysis (RAM), Environment the required functions of a full system -Life Cycle Cost Analysis (LCCA), Life Cycle 6 [1/4th the size/cost may include prototype in advanced high-Analysis (LCA), Supply Chain Analysis (SA), of Full Size] fidelity test bed. Market Impact Analysis (MIA), Throughput Analysis, etc to meet minimum target metrics Technology components are integrated for industry hand off **Demonstrated with** to represent the final system at lab scale **High Fidelity** - system is tested in a simulated 5 [1/4th the size/cost environment with components of highof Full Size] Lab Scale fidelity critical technology components. Tech advancement from TRL 4 → 5 provides Basic technological components are Integrated integrated and tested to establish evidence (quantitative assessments, Components integrated viability within a laboratory demonstration, certification/test reports) that 4 [1/10th the size/cost environment. Used to determine if R&D components address industry of Full Size] components are able to work as a expectations, requirements, interests, and system to meet metrics. constraints. Tech advancement from TRL 3 → 4 provides Active R&D is initiated. Includes analytical/laboratory-scale studies to evidence (quantitative assessments, **Proof of Concept** physically validate benchmarks and demonstration, certification/test reports) of [1/10th the size/cost 3 provide analytical predictions. verified and validated industry informed **Discovery Scale** of Full Size] Technology/components are expectations, requirements, interests, and identified/screened for viability. constraints. Tech advancement from TRL $2 \rightarrow 3$ provides Application Translation to applied R&D begins. Basic evidence (quantitative assessments, Formulated principles are formulated and observed. demonstration, certification/test reports) of [<<1/10th the 2 Applications are formulated with limited verified and validated industry informed size/cost of Full analytical studies. expectations, requirements, interests, and Size] constraints.

Table 13. Description of TRL phases and associated deliverables and requirements.

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constraints.
