Quadrennial Technology Review 2015

Chapter 6: Innovating Clean Energy Technologies in Advanced Manufacturing

Technology Assessments

Additive Manufacturing

Advanced Materials Manufacturing

Advanced Sensors, Controls, Platforms and Modeling for Manufacturing

Combined Heat and Power Systems

Composite Materials

Critical Materials

Direct Thermal Energy Conversion Materials, Devices, and Systems

Materials for Harsh Service Conditions

Process Heating

Process Intensification

Roll-to-Roll Processing

Sustainable Manufacturing - Flow of Materials through Industry

Waste Heat Recovery Systems

Wide Bandgap Semiconductors for Power Electronics

U.S. DEPARTMENT OF ENERGY

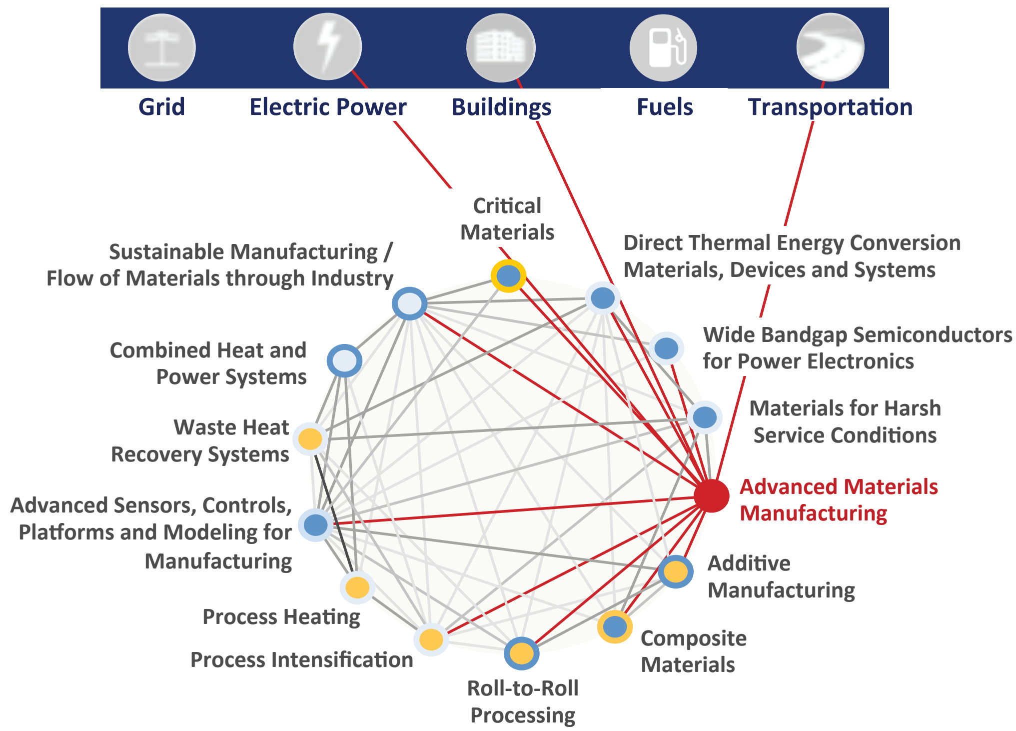
Quadrennial Technology Review 2015

Advanced Materials Manufacturing

Chapter 6: Technology Assessments

NOTE: This technology assessment is available as an appendix to the 2015 Quadrennial Technology Review (QTR). Advanced Materials Manufacuturing is one of fourteen manufacturing-focused technology assessments prepared in support of Chapter 6: Innovating Clean Energy Technologies in Advanced Manufacturing. For context within the 2015 QTR, key connections between this technology assessment, other QTR technology chapters, and other Chapter 6 technology assessments are illustrated below.

Connections to other QTR Chapters and Technology Assessments



Representative Intra-Chapter Connections

- **Additive Manufacturing**: material formulations for additive techniques
- **Roll-to-Roll:** thin- and thick-film substrate production; multilayer alignment
- **Sustainable Manufacturing / Materials for Harsh Service Conditions:** materials to increase durability or facilitate re-use; materials genome techniques for new materials development
- **Advanced Sensors, Controls, Platforms and Modeling for Manufacturing:** computational modeling to support advanced materials development; controls and sensors to support advanced manufacturing techniques
- **Wide Bandgap Semiconductors:** low-cost, commercial-scale production methods for wide bandgap materials

Representative Extra-Chapter Connections

- **Electric Power:** materials genome techniques to develop materials for use in carbon capture and storage (CCS) applications; advanced electricity generation technologies—fossil, nuclear, renewable
- **Buildings:** Advanced building envelope materials
- **Transportation:** Predictive design, modeling, and simulation for vehicle product development
- **Grid**: materials for power flow controllers, solid state transformers, and advanced conductors
- **Fuels**: catalysts for hydrogen production; materials for hydrogen storage; materials for well drilling; materials for high temperature, highly corrosive (acids, water vapor) environments for biomass gasification or other thermal processing

Introduction to the Technology/System

Accelerating Materials Discovery and Development

This technology assessment examines new computational, experimental, and data tools and their application to the research, development, demonstration, and deployment (RDD&D) of new materials and their integration into energy technology systems. These capabilities offer the potential to accelerate the development of advanced energy technologies that can help meet the onrushing energy-linked economic, security, and environmental challenges described in Chapter 1 and its Supplemental Information on energy challenges.

Conventional materials development typically progresses through an iterative cycle of experimentally producing and testing variations of a material until the desired properties for the specific use are achieved. Then the material must go through steps to ensure its performance and lifetime in the technology system under expected conditions, certify it for use, scale-up production (while maintaining its desirable properties), manufacture the technology system, and deploy it. It can take 10-20 years or more for a new material to advance from initial discovery of the material, through its development, to initial commercialization. Advanced computational design of materials and systems, high-throughput experimental testing of material properties, Big Data analytical tools, and other capabilities examined in this assessment have the potential to significantly reduce the time and cost to develop a new material and integrate it in an energy technology.

The following discussion begins with an assessment of these new computational, experimental, and data tools and their advance; then examines a range of applications for them and the potential resulting benefits; next considers programmatic aspects of supporting RDD&D in this arena; and finally closes with a brief of some of the risks and uncertainties facing ongoing development and use of these new capabilities.

Technology Assessment and Potential

Computational, Experimental, and Data Tools

The science and engineering challenges of developing, verifying, and validating advanced computational, experimental, and data tools to aid in materials development are substantial. Materials must be modeled across a broad range of spatial and temporal scales. Spatial scales vary from clusters of atoms (10^{-9} meters) to complete engineered systems (10 meters or more)—a range of ten orders-of-magnitude.[1] The temporal scale ranges even more, from roughly 10^{-12} seconds at the atomic level to 10^{9} seconds for the 30-year life of a power plant component (a difference of more than 20 orders-of-magnitude).[2] Examples of length and time scales used in materials development and modeling are given in Table 6.B.1, from work by LeSar.[3]

Table 6.B.1 Length and time scales used in materials development and modeling.[4]

Unit	Length Scale (m)*	Time Scale (s)	Mechanical Theory
Complex Structure	10^{+3}	10^{+6}	Structural Mechanics
Simple Structure	10^{+1}	10^{+3}	Fracture Mechanics
Component	10^{-1}	10^{+0}	Continuum Mechanics
Grain Microstructure	10^{-3}	10^{-3}	Crystal Plasticity
Dislocation Microstructure	10^{-5}	10^{-6}	Micro-mechanics
Single Dislocation	10^{-7}	10^{-9}	Dislocation Dynamics
Atom	10^{-9}	10^{-12}	Molecular Dynamics
Electron Orbital	10^{-11}	10^{-15}	Quantum Mechanics

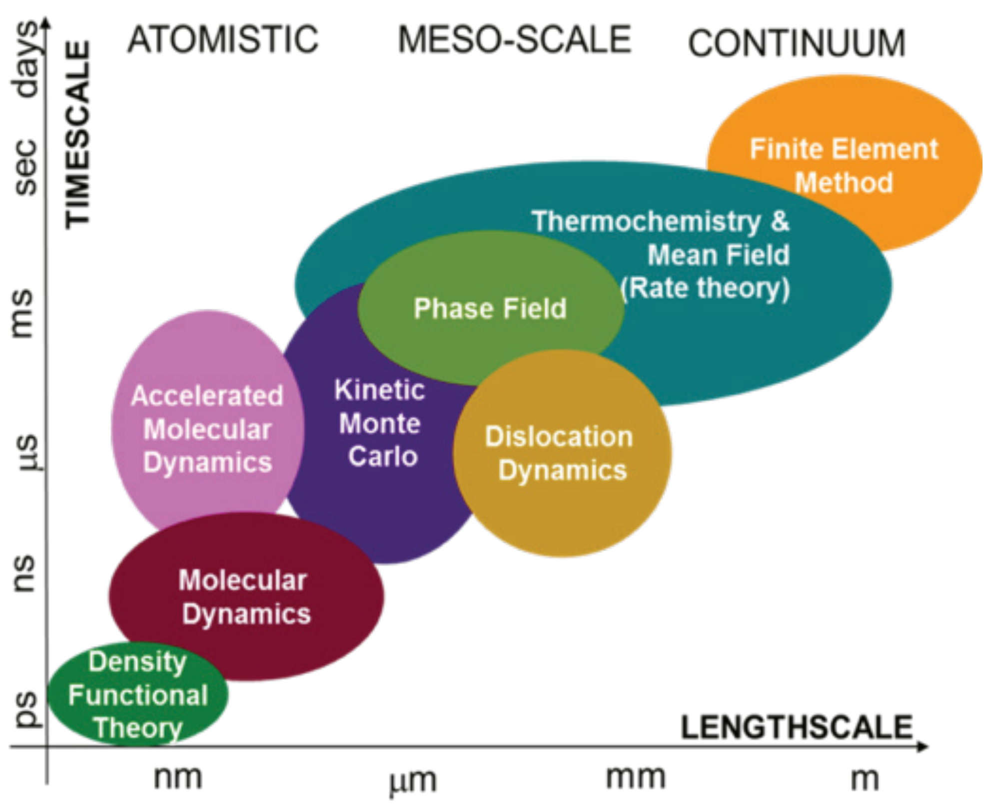
*For scale, the Bohr radius is 5.29x10-11 meters, and typical atomic radii are 10x10-11 to 50x10-11 m (or 0.1 to 0.5 nm).

Individual existing models cannot predict behavior and properties across this broad range of spatial and temporal scales. For example, modeling the inter-atomic binding strength of iron atoms does not capture the complex grain structure necessary to maximize the performance of high-strength steel. Understanding the meso-scale transition from atomic-level modeling to macro-scale performance is critical.[5] Similarly, modeling the picosecond dynamics of atoms does not address how the properties of the bulk material will change over a 30-year component lifetime under extreme stress and corrosion conditions.[6] A variety of models are used for these different scales, including density functional theory; molecular dynamics; kinetic Monte Carlo; thermochemistry and mean field [rate] theory; macroscopic finite element models; and more, as sketched in Figure 6.B.1.[7] Advances are being made in developing capabilities that begin to span these broad scales and a number of successes have been described in recent studies,[8] but much remains to be done.[9]

Advances in scientific theory, modeling, simulation, high performance computing, algorithms, software, data analysis, and experimental techniques are merging to create the ability to design and engineer materials and systems more rapidly and at lower cost than traditional approaches. This portends a period of dramatic change in the processes for scientific and engineering RDD&D. The multi-agency Materials Genome Initiative (MGI), launched in 2011, has the development of such capabilities as its central focus. The goal of the MGI is to achieve a 50% reduction in the time required to discover, develop, manufacture, and deploy a new material, and to do so at a fraction of the cost of conventional approaches.[10,11] Some of the many agencies, universities, national labs, and industries involved in advancing these technologies are listed in documentation from the MGI, National Academy of Sciences, and other organizations and agencies.[12] The following examines the applications and the technical elements of this emerging capability within the over-arching framework of the MGI.

Figure 6.B.1 Models bridging the spatial and temporal scales from atomic to large structures.[13]

Credit: Marius Stan



Integrated Computational Materials Engineering (ICME)[14] is an emerging discipline that integrates computational predictive-modeling tools with system-level computational engineering design optimization and manufacturing design techniques to provide a unified design and manufacturing process to accelerate development of materials into engineering systems. These capabilities align with the goals of the Materials Genome Initiative. The top-down computational system engineering focuses on determining what material capabilities are required to meet system-level performance needs; the bottom-up computational materials discovery, design, and development focuses on identifying the material and determining how to produce it for the system.

The MGI framework incorporates the full spectrum from discovery science to deployment of new technologies: (a) Systems Modeling and Simulation; (b) Predictive Theory and Modeling and Born Qualified; (c) Digital Manufacturing and Design; (d) Advanced Experimentation and Model Verification and Validation; (e) Uncertainties in Models and Physical Systems; (f) Data and Data Analytics; and (g) Demonstrations. These capabilities offer opportunities for significantly accelerating RDD&D, and are briefly examined below.

(a) **Systems Modeling and Simulation.** From a top-down perspective, computational modeling and simulation of an energy technology or system is an important step in determining the requirements for the materials and components within the system, and for evaluating operations, safety, and performance. In energy supply, an example of such modeling and simulation is the Consortium for the Advanced Simulation of Light Water Reactors (CASL),[15] as described in Chapter 9: Enabling Capabilities for Science and Energy. CASL is developing detailed models of reactors to evaluate their operational and safety performance and optimize operations. Another example is the Atmosphere-to-electrons (A2e) initiative in the DOE wind energy program to develop computational tools to explore every step of wind generation, from large-scale atmospheric winds through the wind farm to individual turbines and to the electricity that is generated.[16] Such modeling is also done in vehicle lightweighting and many other areas. More broadly, systems modeling capabilities have been extensively used in the aerospace, defense, transportation, and other sectors.[17] Advanced computing capabilities for modeling, simulation, and other purposes are important across every energy sector. The results of such modeling, conducted iteratively with computational materials development, can help identify requirements for materials design.

(b) **Predictive Theory and Modeling and Born Qualified.** At the other end of the scale from systems modeling is bottom-up predictive materials modeling. Extensive work on the computational modeling of materials has been conducted for decades at national labs and universities, substantially supported by the DOE Office of Science, and more recently it is beginning to be conducted by industry.[18] Advanced computing is increasingly able to characterize new materials and materials processes, as well as complex chemical systems and processes.[19] High performance computing can now enable simulations of matter at scales from a few atoms to millions of atoms with increasing fidelity.[20] An important next step now underway is extending these computational and other capabilities from the atomic level into the meso-scale, where many material performance characteristics are determined and key functionalities of the materials are designed in.[21] This upscaling from an atomic quantum mechanical level to the meso- and macro-level is essential to support engineering development and characterization of large, complex engineered systems. Models identified above—molecular dynamics, kinetic Monte Carlo, etc.—extend capabilities across portions of the meso-scale. These capabilities need further development to advance their performance and support accelerated development of new materials and capabilities.

Evaluating the characteristics of a material from first principles computational analysis enables searching a large space for materials with the desired characteristics. High-throughput computational approaches range from systematically testing all of the potential materials in an area[22] to using computational approaches such as genetic algorithms.[23] Approaches to streamline such searches would reduce computational overheads.

Further development is needed on foundational tools and technologies in this arena that are beyond the reach of any particular company but that can support the broad swath of industry. The MGI identified the importance of developing these computational tools and data systems in forms usable by the engineering community, and linking them to engineering design and manufacturing tools.[24] This, as for the other capabilities described by the MGI, will require networks of experts to provide the needed expertise to the new user, as well as broader workforce development. Open platform approaches can be important contributors to the development and extension of a broad range of capabilities. An important example is the nanoHUB run by the Network for Computational Nanotechnology with support from the National Science Foundation.[25]

Significantly extending predictive theory and modeling would include developing the capability to computationally design functional materials with sufficient fidelity that the material is qualified to meet performance standards for various applications—"Born Qualified"[26]—before it is ever produced, and that the production process is scalable and well-characterized. It would also characterize the material's (and component's) performance under expected operating conditions over its lifetime. This will require substantial further development of computational modeling capabilities and validation of their performance across performance parameters such as material strength, hardness, ductility, corrosion resistance, catalytic activity, or others depending on the specific applications of the material. Achieving this would significantly accelerate the design, development, manufacturing, and introduction of new materials, avoiding the development cycle of repeated testing and then looping back into further development that can take years at high costs. This will require substantial advances in computational modeling at the meso-scale. This will also require substantial attention to regulatory issues for meeting requirements. Advancing these capabilities into applied technology programs at national laboratories, universities, and industry has the potential to significantly advance technology capabilities wherever advanced materials are needed, which includes most areas of energy technology.[27] The new DOE Energy Materials Network[28] will address some of the key aspects of these issues.

(c) **Digital Manufacturing and Design**. With top-down modeling and simulation and bottom-up predictive theory and modeling of materials, developing capabilities for computational manufacturing is also important. Since materials design and manufacturing design are intrinsically integrated, digital capabilities can accelerate modern design, manufacturing, and product support to reduce cycle time and improve productivity and quality. Factories of the future will be networked, data-driven systems that use automation, advanced metrology and sensing, and control systems to improve productivity and competitiveness. As for other capabilities noted above, extending this to medium and small enterprises through the development of foundational tools, networks of experts to provide support to the new user, and workforce development are important. Such efforts are beginning with the launch of new Manufacturing Innovation Institutes,[29] particularly the Digital Design and Manufacturing Institute (DDMI).[30] Others announced for manufacturing innovation include the Lightweight Innovations for Tomorrow (LIFT) Institute[31] and the Institute for Advanced Composites Manufacturing Innovation (IACMI).[32] A broad array of potential benefits for industrial competitiveness are expected from very high performance (exascale) computing.[33]

(d) **Advanced Experimentation and Model Verification and Validation**. Capabilities are needed for the synthesis, characterization, manufacturing scale-up, and performance validation of new materials. Further, capabilities such as *in situ* metrology,[34] real-time process characterization, and process control are needed. Experimentation (high throughput and otherwise) will always continue to be a critical part of the material RDD&D and validation process; this includes development of improved synthesis and characterization tools and capabilities, as well as the associated expertise. In many cases (such as for functional materials interfaces), existing computation and simulation tools have known weaknesses in predicting characteristics and performance. Traditional experimentation can also be very slow or expensive in these cases. Synergistic development of computational and experimental capabilities is needed to accelerate the discovery and development of new materials systems and products.

An important aspect of computational materials development is validation that the model accurately represents the intended design and the physical world. Experimental analysis of the material modeled is thus essential.

Fundamental experimental capabilities to support experimental validation and other needs include world-class light sources, neutron sources, and nanoscale science facilities, and are examined in detail in Chapter 9: *Enabling Capabilities for Science and Energy*. These can provide high resolution (spatial and temporal) analysis of atomic-scale and larger structures and dynamics of materials, chemicals, and chemical processes, and can be tightly integrated with theoretical analysis and with high performance computational modeling to validate and advance the modeling simulations.[35] These facilities serve the critical role of supporting both discovery science and applied science and technology. Such experimental studies can validate predictive materials science and chemistry to meet specific needs, and can be used to accelerate the product development cycle, address national energy challenges, and improve economic competitiveness.[36,37]

Also supporting accelerated materials discovery and development are high-throughput laboratory advances, such as combinatorial chemistry[38,39] and the use of robotics and software to operate laboratory equipment, record and analyze the data, curate the data, and support other activities.[40] For example, the Joint Center for Artificial Photosynthesis (JCAP) Hub (see Chapter 7: *Advancing Systems and Technologies to Produce Cleaner Fuels*) has adapted inkjet printer technology for the rapid preparation and analysis of huge numbers of catalyst samples for combinatorial chemistry.[41] Laboratory automation is moving forward in some areas, such as biology and genetics, where there is large investment by the pharmaceutical industry[42] and improving lab efficiency can provide significant labor and financial savings.

As new computational, experimental, and data tools are developed to accelerate materials RDD&D, additional specialized skillsets will be needed. Training the next generation of researchers in the development and effective use of these tools will be a critical priority for academic institutions and laboratories.

(e) **Uncertainties in Models and Physical Systems**. There are many different uncertainties in systems and materials models, as well as the actual physical systems. It is important to characterize, quantify, and track these uncertainties at different spatial and temporal scales in order to assess overall component and system performance and cost. For models, uncertainties are inherent in numerical solution methods, and numerical error can potentially be amplified as calculations are carried through a sequence of models. Panchal et al. provides a particularly useful review of uncertainty in ICME, including sources of uncertainty and issues of quantifying uncertainty, understanding the propagation of uncertainty through linked models, mitigating uncertainty, and managing uncertainty.[43] For materials, uncertainties include the materials' measured parameters, the processing of the material, and the operating conditions of the material. Of particular note is that the failure of a material will typically begin from a localized point due to a combination of microstructural failure and an extreme event. Further, many material failures occur at the largest flaw; variations and uncertainty in processing and input materials dictate the distribution of largest flaws and hence the distribution of performance characteristics among groups of manufactured components. Uncertainty analyses need to consider such stochastic effects to adequately characterize material performance over time.

(f) **Data and Data Analytics**. Identifying materials with the right properties for a particular application has often been handled by searches across large databases of material properties, including materials informatics approaches with data mining and visualization and combinatorial search.[44] Going forward, the predictive modeling, Born Qualified, systems simulation, design, and demonstration tools described above will generate large volumes of data, amplified by the verification and validation of these computational results using high throughput experimentation and measurement. Altogether, this will require extensive digital data management and curating, and collaboration on standards setting and definition.[45] Some of this can be set up directly, but there is also the challenge of working across numerous and diverse data sources, many of which follow different approaches and reporting protocols. In addition to such data heterogeneity, other challenges in Big Data that have been identified include: data ownership and access, cost and ease of data maintenance, data validation and quality control, data ontologies, data security, developing and maintaining long-term data repositories, and others.[46] Computational systems can be used to address some of these challenges.[47] For example, software can be used to aggregate huge quantities of materials data and then use these data to develop machine-learning models of materials behavior. These models could then guide research in academia and industry towards advanced materials with the desired capabilities. Deep learning tools can have significant benefits for discovery science.[48] Building broad capabilities for such data tools could have substantial benefits for extracting diverse data sets from across energy system engineering and related materials science and other issues. This will also be important for managing uncertainty in the data and extracting key information to provide useful feedback to help improve high-fidelity simulations. Issues of interoperability then become important for making effective use of this data.[49]

Data issues also arise in many other areas, from energy resources to grid integration. Chapter 3: *Enabling Modernization of the Electric Power System* described the explosion of data from grid sensors. Ways to parse this data for faster-than-real-time analysis of impending events are needed. Data mining technologies are also needed, for example, in wind resource assessment to improve integration of wind power into the grid.[50]

(g) **Demonstrations**. Demonstrations of energy technologies can pose particular challenges when the necessary scale is large. For example, full-scale demonstrations of fossil power with carbon capture and storage (CCS), nuclear, concentrated solar power, and others can cost billions of dollars.[51] Some of the difficulty and cost of achieving full scale performance might be addressed through computational techniques such as predictive materials modeling, systems simulation, and integrated computational materials engineering, which can potentially provide extensive information on the performance of materials and the systems themselves. Vehicle simulations, for example, are used to characterize crashworthiness of vehicles, allowing a much broader range of designs to be tested and saving substantial time and cost by reducing the amount of prototyping and physical testing needed. For energy supply technologies, simulation may also reduce the design-test time, enable a wider exploration of the design space, and may allow some of the scale-up demonstration stages to be reduced or bypassed. Even with these potentially substantial savings in time, large-scale demonstrations will still be necessary, and these will require significant investments of time and capital.

One approach that can substantially reduce the development time to produce a demonstration system at scale is additive manufacturing (see Technology Assessment 6A, *Additive Manufacturing*). Not only can this technology be used to manufacture parts with designs not attainable by conventional manufacturing methods, additive manufacturing can also reduce the time to develop and review initial prototypes, accelerate the process of getting a design ready for production, and enable rapid iterative prototyping. However, additive manufacturing itself requires extensive computational support to model systems and to understand the dynamics of the process, for example, the non-equilibrium dynamics of deposition. Open source access to data, designs, and software packages is an important contributor to the current rapid advance of additive manufacturing. Some developers are now providing open access to their patents.[52] These open source approaches may already be having an impact on innovation and the acceleration of technology development, and may be an important contributor to accelerating energy RDD&D in the future.

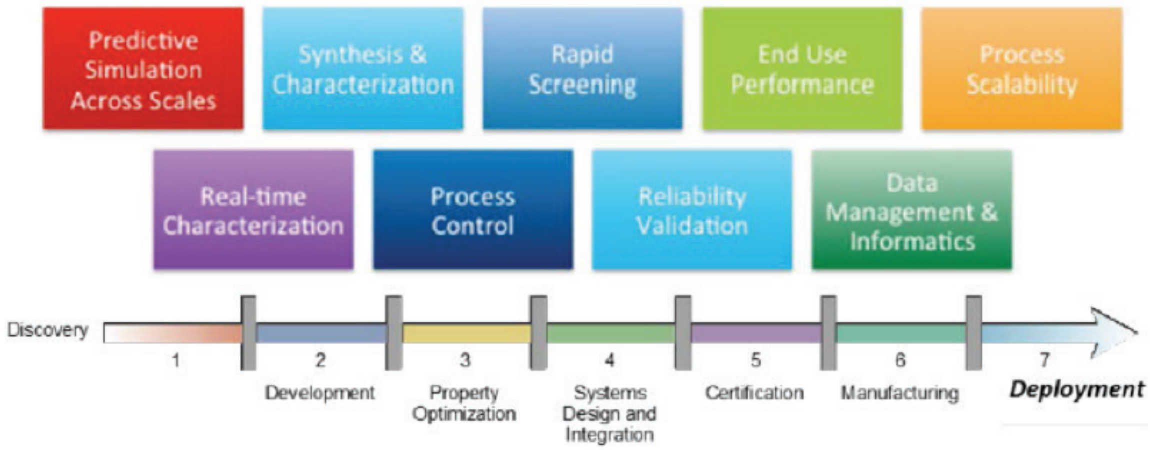
Application to the Advancement of Energy Materials. As the above capabilities are further developed, there are many energy technologies that could benefit from the MGI framework of predictive modeling and development of materials. Material needs for energy technologies can be grouped in a variety of ways. A practical grouping might include:

- **Structural Materials**, such as lightweight materials for vehicles, high temperature materials for thermal power plants, radiation resistant materials for nuclear power, and corrosion resistant materials for energy conversion processes. See the *Materials for Harsh Service Conditions Technology Assessment* (6H) for further details on materials needs and challenges in these areas.
- **Functional Materials and Interfaces for Energy Conversion**, such as high-efficiency photovoltaics that make use of earth-abundant materials; wide bandgap semiconductors for power electronics in electricity transmission and distribution systems (high voltage direct current, power flow controllers, solid state transformers, etc.), electric vehicles, industrial motor drive, and solid state lighting; sensors for applications ranging from high temperature down-hole geothermal use, to *in situ* industrial process control, to building climate control; energy conversion materials for waste heat recovery, including thermoelectric materials; and catalysts for applications ranging from direct solar production of hydrogen to clean-up of vehicle exhaust. For an in-depth exploration of some of these technologies, see the QTR 2015 technology assessments on *Solar Power Technologies* (4P), *Wide Bandgap Semiconductors for Power Electronics* (6N), *Waste Heat Recovery Systems* (6M), and *Direct Thermal Energy Conversion Materials, Devices, and Systems* (6G).
- **Functional Materials for Separations or Isolation**, such as membranes for fuel cells, batteries, air dehumidification, and water purification; porous materials for hydrogen storage and carbon capture; seals and environmental isolation materials that protect equipment from extreme conditions such as high temperature, acidity, moisture, etc.; coatings and lubricant systems; and more. See the QTR 2015 technology assessments on *Fuel Cell Electric Vehicles* (8B), *Carbon Dioxide Capture Technologies* (4E), and *Process Intensification* (6J) for further discussion of specific materials challenges in these areas.
- **New Paradigm Materials Manufacturing Processes**, including cross-cutting manufacturing technologies with energy impacts such as net shape processing, additive manufacturing, roll-to-roll manufacturing, powder metallurgy, intelligent casting, and more. Two of these technologies are further investigated in the QTR 2015 technology assessments on *Additive Manufacturing* (6A) and *Roll-to-Roll Processing* (6K).

The approaches outlined here, summarized in Figure 6.B.2, offer pathways to significantly accelerate the development and manufacturing of advanced energy technologies for the United States. Some aspects of each of these capabilities are under development, but additional work is needed to develop comprehensive, seamless, and robust integrated tool sets for broad adoption in and use by the research community and industry. These advances will involve extensive multi-physics, multi-scale, multi-disciplinary RDD&D work across many institutions and will need rigorous verification, validation, and uncertainty quantification. Successfully doing this will drive a fundamental paradigm shift in which computational, experimental, and data tools will accelerate the discovery, development, and optimization of new materials and systems to meet national and global energy challenges and enhance U.S. economic competitiveness. This opportunity space is broad and is only beginning to be mapped by public and private efforts; systematic analysis is critical to determine priorities and guide investments.

Figure 6.B.2 Tools and techniques for accelerated development and manufacturing of advanced materials and energy technologies.[53] Although the figure suggests that this is a linear process from Discovery to Deployment, in practice it is not at all linear and there are numerous feedback loops, reversals, additions of new technologies and processes from other sources, and many other non-linear aspects.

Credit: Adapted from Reuben Sarkar, EERE, and the Materials Genome Initiative Strategic Plan



Advanced Materials Manufacturing

Advanced materials manufacturing (AMM) refers to major innovations in the properties, manufacturing processes, and market applications of materials vital to the U.S. economy, including metals, polymers, ceramics, composites, and coatings, and builds on the computational, experimental, and data tools for RDD&D described above. The objective for AMM is to develop and validate new materials systems for specific end uses. In particular, next generation materials can be thought of as those that hold promise for step-change impacts in the economic, engineering, and environmental performance of materials across their entire life cycles (i.e., extraction, manufacturing, use and reuse, and end-of-life) as compared to historical performance improvement rates within specific materials classes. Furthermore, materials innovations can occur at many different scales, including improved structural properties at the nanometer scale, novel surface geometries at the micrometer scale, and creation of new materials markets and applications at the global scale. Key examples include new catalysts for more profitable and sustainable fuels and chemicals, advanced surface coatings and geometries for improving materials durability and reducing friction, lightweight metal alloys and composites for more fuel efficient vehicles, and net-shape and near-net-shape techniques for less wasteful and more profitable materials processing. As part of its 2011 Innovation Impact Report, The Minerals, Metals & Materials Society (TMS) (on behalf of the DOE Advanced Manufacturing Office [AMO]) estimated that 54 such materials innovations could save the United States over 2.8 quadrillion British thermal units (quads) of energy—roughly 3% of total U.S. primary energy use—with associated cost savings estimated at $65 billion across the U.S. economy (based on cost data available at the time of publication).[54,55] Innovations in materials thus hold great potential for improving the nation's energy security and economic competitiveness.

Given the vast landscape of different materials, markets, and end use sector applications (e.g., infrastructure, consumer products, transportation, appliances, and so on), it is helpful to discuss next generation materials in terms of specific innovation opportunity areas, building from the broad categories defined above of:

(a) Structural Materials;

(b) Functional Materials and Interfaces for Energy Conversion;

(c) Functional Materials for Separations or Isolation; and

(d) New Paradigm Materials Manufacturing Processes.

Table 6.B.2 summarizes examples of key innovation opportunities within these categories, based on the findings of a panel of experts on breakthrough materials innovation areas convened by TMS for its 2011 *Innovation Impact Report*,[56] with updates arising from the case studies presented in this assessment and expert inputs from QTR reviewers. The representative materials innovations listed under each category were further informed by expert data collected by Oak Ridge National Laboratory (ORNL). Table 6.B.2 also shows the potential segments of the U.S. energy-economic system that could be impacted by innovations in each category.

Quantifying the potential energy, emissions, and economic benefits of next generation materials is difficult for several reasons. First, the rapid pace of innovation and the myriad classes and applications of materials targeted by such innovations create an enormous opportunity space that is intractable to analyze as a whole. Second, the nascent state of many materials innovations means that credible data on their performance are not yet available. Third, when such data are available, they are often at the lab or pilot scale, and therefore difficult to extrapolate to industrial scale conditions. Fourth, materials innovations can have significant life cycle effects—including changes in the types and structures of raw materials supply chains, changes in application product performance, and changes in viable end-of-life options—which makes benefits analysis an uncertain and analytically challenging exercise. Therefore, this technology assessment focuses on providing quantitative data for specific case studies within materials innovation categories drawn from the literature rather than attempting to derive (highly uncertain) estimates of the potential societal benefits of innovation categories as a whole. However, the qualitative summary of impacted economic segments in Table 6.B.2 underscores the broad reach and importance of next generation materials for improving the economic and environmental performance of the U.S. economy.

Table 6.B.2 Materials innovation categories and sectors of likely impact. Areas marked with an "X" indicate opportunities identified in the 2011 TMS Opportunity Analysis for Materials Science and Engineering report;[57] areas marked with an "O" indicate additional opportunities identified by DOE since that report was published.

		Energy Extraction and Generation					Energy Storage		Energy Use	
Category	**Subcategories**	**Solar**	**Wind**	**Nuclear**	**Oil & Gas**	**Coal**	**Batteries**	**Fuel Cells**	**Industry**	**Transportation**
Structural Materials	Low carbon cements		O	O	O				X	
	Composite materials	X	X		X	X	X		X	X
	Lightweight metals	X	X		X	X	X		X	X
	Phase-stable materials			X	X	X			O	
Functional Materials for Energy Conversion	Catalysts				X	X	X	X	X	X
	Thermoelectric materials	X				X			X	X
	Wide bandgap semiconductor materials	O	O						O	O
	Photovoltaic materials	X								
Functional Materials for Separations or Isolation	Separation membranes				X	X	X	X	X	X
	Coatings and surface treatments	X	X	X	X	X	X	X	X	X
	Seals and environmental isolation materials			O	O		X	X	X	X
New Paradigm Materials Manufacturing Processes	Net-shape processing	O	X	X	X	X			X	X
	Magnetic field processing								X	X
	Additive manufacturing	X	O				O	O	X	X
	Roll-to-roll processing	O			O		O	O	O	O
	Next-generation metals processing			O	O				X	X

Performance Advances

Ongoing innovation and focused research on materials are leading to steady improvements in their engineering, economic, and market performance in various applications. Table 6.B.3 summarizes identified performance targets for various materials innovation categories that would lead to substantial national energy and economic benefits. Additional insights for many of these categories are highlighted in the rest of this section, and/or in other Technology Assessments.[58]

Table 6.B.3 Examples of performance targets for consideration

Category	Subcategories	Example performance targets
Structural Materials	Low carbon cements	25% reduction in CO_2 emissions from cement industry by 2030.[59]
	Composite materials	Carbon fiber production costs reduced by 25% within 5 years and 50% within 10 years; carbon fiber embodied energy reduced by 50% within 10 years and 75% within 10 years; 80% recyclability of fiber-reinforced composites within 5 years.[60]
	Lightweight metals	Magnesium die castings with less than 5% porosity by volume; advanced high strength steel with a tensile strength of 1500 MPa; aluminum sheet with a tensile strength of 300 MPa and uniform elongation of 15%, within 5 years.[61]
	Phase-stable materials	Materials with temperature stability exceeding 1300°F at 5,000 psi pressure (to enable advanced ultra-supercritical steam turbines); irradiation-resistant steels for a lifespan of up to 80 years (for nuclear power).[62]
	Multi-material joining	Fastener-free dissimilar material joining technologies with high reliability, joint strength, and ease of use—particularly for lightweight materials (e.g., composites and lightweight metals).[63]
Functional Materials for Energy Conversion	Catalysts	For fuel cell catalysts: Long-term durability (>5,000 hours) under dynamic loading in fuel cell vehicles; less than 40% loss in initial catalytic mass activity after 30,000 cycles between 0.6 and 1.0 V; less than 30 mV loss in performance at 0.8 A/cm2 after 30,000 cycles between 0.6 and 1.0 V, by 2020.[64] For chemicals production: Greater than 91% selectivity and expanded feedstock capabilities by 2020, leading to more efficient conversions and greater applications to bioprocesses.[65]
	Thermoelectric materials	Materials with a thermoelectric figure of merit (ZT) of 2 and above, leading to greater conversion efficiencies compared to existing commercial materials with $ZT \approx 1$.[66]
	Wide bandgap semiconductor materials	Wide bandgap semiconductor-based devices with drain-source breakdown voltage exceeding 1200 V, a current rating exceeding 100 A, and an operating junction temperature spanning −55°C to 150°C (−67°F to 302°F).[67]
	Photovoltaic materials	Flat-plate modules with efficiencies of 25% by 2030 and 40% by 2050; solar panel operational lifetime of 35 years by 2030.[68]

Table 6.B.3 Examples of performance targets for consideration, continued

Category	Subcategories	Example performance targets
Functional Materials for Separations or Isolation	Separation membranes	5x-10x improvements in scale and flux for ceramic, metallic, polymeric, and composite membranes by 2020.[69]
	Coatings and surface treatments	Greater thermal stabilities for higher temperature applications; higher wear resistant and more reparable coatings; 5x improvement in material durability by 2020.[70]
	Seals and environmental isolation materials	Sealant materials with thermal stability of 1830°F (e.g., for use in high-temperature thermoelectric devices).[71]
New Paradigm Materials Manufacturing Processes	Net-shape processing	20% improvement in energy efficiency of powder metallurgy by 2020[72]
	Magnetic field processing	Higher field (>9 tesla), larger bore size (>6 inches) magnet technology designs to enable treatment of larger scale industrial components.[73]
	Additive manufacturing	Buy-to-fly ratio of 2 to 1 for additive manufacturing by 2020.[74]
	Roll-to-roll processing	Process rate of 100 feet per minute (e.g., for membrane electrode assembly manufacturing); sensor and metrology technologies for continuous in-line measurement.[75]
	Next-generation metals processing	Primary metal production energy intensity of 20 kWh/kg, 27 kWh/kg, and 35 kWh/kg for aluminum, magnesium, and titanium respectively (to achieve parity with steel). These targets represent reductions of approximately 64%, 39%, and 65% over current technologies for the three materials.[76]
	Energy/feedstock conversion technologies for industry	Hydrocarbon biofuel production with GHG emissions reduction of at least 50% compared to petroleum-derived fuel.[77]

Beyond these potential advances, we note that the theoretical strength of most materials is about ten times the strength of the same materials as applied in commercial practice. New advances in material design and manufacturing could result in materials that approach these theoretical strength levels, providing game-changing lightweighting and performance advantages.[78] For example, recent research on nanoparticle dispersion in magnesium alloys has yielded materials with record-breaking strengths.[79]

Potential Impacts

The potential positive impacts of AMM on the U.S. economy are vast, and can be realized across different stages of the materials life cycle. As discussed above, analyses of the life cycle benefits of AMM are complex, and quantitative data to support these analyses for the myriad material innovations underway are scarce. However, the following examples underscore the potential benefits of AMM.

Structural Materials

Higher performance structural materials include a broad range of opportunities across metals, polymers, ceramics, and composites that improve strength and engineering performance in various applications, potentially leading to both energy and economic benefits across the U.S. economy. Examples of benefits of high performance materials in this category include:

- Advancements in high-strength, lightweight materials for automotive applications such as magnesium alloys, aluminum alloys, high strength steels, and polymer matrix composites can lead to energy savings in the U.S. transportation sector through lighter weight bodies, chassis, and drivetrains and more efficient engines. For example, a 10% reduction in vehicle mass can lead to 6-8% improvement in vehicle fuel economy.[80]
- Cement calcining processes contribute significantly to the greenhouse gas (GHG) emissions footprint of the U.S. manufacturing sector. Novel substitute materials for producing cement, including magnesium silicates or carbonates, and/or carbon-cycling processes, such as the Calera® or Calix® processes, can reduce or eliminate GHG emissions from calcining. These technologies could provide a pathway towards lower-carbon alternatives to traditional cement (one of the world's largest volume materials) to make progress toward national GHG emissions reduction targets.[81]
- Advanced, phase-stable materials that can withstand the harsh operating environment of an advanced ultra-supercritical steam turbine could increase the energy efficiency of U.S. electricity generation. As an example, a 1% reduction in fuel consumption by U.S. gas and steam turbine power plants could save an estimated 348 TBtu of energy.[82] The potential for high-temperature phase-stable materials to improve gas and steam turbine efficiency is further discussed in the *Materials for Harsh Service Conditions* Technology Assessment.

Functional Materials for Energy Conversion

Materials that convert energy from one form to another can provide energy benefits by enabling unused or underutilized energy sources to be harnessed for useful purposes. Examples of benefits of high performance materials in this category include:

- If high-ZT thermoelectric materials that convert waste heat into electricity at an efficiency of 15% could be applied to 1.5 quads of unrecovered waste heat in selected energy-intensive U.S. industries each year, it is estimated that U.S. manufacturers could save more than $3.6 billion in annual energy costs (according to one report).[83] As part of the 2015 QTR, a detailed evaluation of the potential of thermoelectrics is presented in the *Direct Thermal Energy Conversion Materials, Devices, and Systems* Technology Assessment.
- Wide bandgap semiconductor devices have higher switching frequencies than their silicon-based counterparts, enabling the use of smaller inductors and capacitors in power circuits, and resulting in weight, volume, and cost reductions. Wide bandgap devices also provide higher power density and can reduce energy requirements as a result of their high efficiency.[84]
- Photovoltaic materials can be used to harness the direct and diffuse components of solar radiation to generate electricity, displacing energy generated through fossil fuel combustion and reducing greenhouse gas emissions and air pollutants.[85]

Functional Materials for Separations or Isolation

Functional materials for separations or isolation influence every sector of the U.S. economy, from coatings that protect structural steel in buildings and bridges, to surface treatments and/or modifications to improve the performance of drives, pistons, and bearings in vehicles and machinery, to membranes that assist chemical separations. AMM improvements in these types of materials could lead to benefits such as:

- Improved coatings that reduce corrosion-related losses and costs in the U.S. petroleum refining, chemicals, and pulp and paper industries by 10% would save these three U.S. industries about $1 billion each year for their domestic operations.[86]

- Surface treatments and coatings for reduced friction losses in the engine, drivetrain, and fuel systems enabled by advancements in tribology and computational design could reduce the fuel used by U.S. cars, light trucks, and heavy-duty vehicles by 3-5%, or 0.5 to 1.5 million barrels of petroleum per day.[87]
- Novel surface morphologies can influence the hydrophobicity of materials, thereby reducing drag in solid-liquid interactions. Applications of this new class of materials include reducing drag in marine transport vehicles and drag friction in fluid transport pipes. Additionally, such materials hold promise for harvesting of water from fog, which might be used as a source of water in various world regions. In one study, a wettable mesh harvested 3-10 liters per square meter of mesh per day from fog.[88,89]

New Paradigm Materials Manufacturing Processes

Energy-efficient, advanced materials manufacturing processes provide an opportunity to advance the state-of-the-art and competitiveness of industry for several reasons. First, novel materials innovations may require entirely new production processes, such as a shift from sputtering-based coating applications to colloid-based applications for new energy efficient electrochromic window coatings.[90] Second, improvements to high-volume processes for producing metals, polymers, and other bulk materials in a more energy- and materials-efficient fashion can reduce both the operating costs and the energy, resource, and waste footprints of U.S. industry. For example, next generation metals industry processes, including intelligent casting, improved controls, blank geometry optimization, and inert atmosphere melting can substantially reduce yield losses in the production of metal products. Third, next-generation manufacturing processes such as nanofabrication, roll-to-roll processing, and additive manufacturing may lead to dramatic improvements in manufacturing flexibility, lead time, and productivity while also opening up opportunities for new materials innovations to support the processes (e.g., advanced powders for additive manufacturing). Next generation manufacturing processes could lead to benefits such as:

- Roll-to-roll processing tools and equipment often use less energy (per unit area of manufactured product) for a much shorter duration relative to conventional manufacturing. In addition, roll-to-roll manufacturing enables new products that cannot be fabricated using other methods. For example, electrochromic windows fabricated via roll-to-roll methods could save nearly 2 quads of energy annually if installed in all residential and commercial buildings.[91]
- Next generation catalysts and process pathways for production of olefins, ammonia, methanol, and other commodity chemicals such as catalytic crackers, catalytic oxidative dehydrogenation, and electrolysis could reduce the energy intensity of commodity chemicals production by 20%-40% by 2050.[92]

Additional opportunities are reviewed in separate Technology Assessments, including the *Composite Materials Manufacturing* Technology Assessment (6E), the *Roll-to-Roll Processing* Technology Assessment (6K), and the *Additive Manufacturing* Technology Assessment (6A).

Energy Efficient Metals Processing

The processing and manufacture of metals represents a significant opportunity to advance energy efficiency, productivity, and competitiveness. The 45-year steady rise in the use of remelted scrap to produce steel in the U.S. (now at 59% of all production[93]) has recently been challenged by the practical limitations of arc furnace technology to supply clean steel. Overall energy use is dependent upon a number of factors, including product mix.[94] Many high performance steel applications (such as automotive) require cleanliness levels that cannot be met from pure scrap remelting. Mini-mills have responded by including cleaner ore-based iron in the charge mix, which results in higher energy consumption because of the additional energy required to reduce iron oxide to iron. This trend has motivated increased production capacity of alternative ironmaking processes such as direct reduced iron, which uses natural gas and takes advantage of its current low cost. Technologies based on alternative ironmaking methods (e.g., flash ironmaking[95] and molten oxide electrolysis) have the potential to achieve an estimated 20% energy reduction. New methods of scrap segregation could provide an alternate solution.

Integrated aluminum mini-mills are emerging, enabled by advances in rapid automated chemical analysis and sorting methods for aluminum. Large reductions in energy consumption (up to 85%)[96] are possible by using scrap-based remelting instead of ore-based primary production. However, the problem has been to control the composition to the tolerances needed for specific grades, because the scrap supply is a mix of different grades of aluminum. DOE supports the technology advances needed in this area through the ARPA-E METALS program.

Recently, novel electrolytic processes have emerged in manufacturing, enabled by advances in electrode materials, ion transport materials, and catalytic materials as well as solvents such as molten salts and ionic liquids. These hold the promise of reducing the energy consumption for producing a range of metals from their ores (iron, aluminum, magnesium, titanium, and critical materials). These advances are supported by ARPA-E[97] and the Small Business Innovation Research (SBIR) program.[98]

Processes to produce metals with significant amounts of nanocarbon (several weight percent graphene and nanotubes) are emerging. These materials have demonstrated on-the-order-of a 50% increase in electrical conductivity and on-the-order-of a 10-fold increase in thermal conductivity at the lab scale, which has potential for improved energy efficiency over a wide range of commercial applications. Cost, scalability, and product consistency are challenges that are being addressed.

Case Studies for Benefits of Advanced Materials Research

Table 6.B.4 summarizes several case studies of advanced materials research areas funded through public-private partnerships, along with quantitative estimates of benefits. While the potential energy and economic benefits of materials innovation can vary widely and are highly case specific, the quantitative data in Table 6.B.4 underscore the life cycle savings that might be realized across the U.S. economy through AMM.

Table 6.B.4 Case studies of advanced materials research benefits

Category	Subcategory	Description of Example Technology	Benefits
Functional Materials for Energy Conversion	Coatings and Surface Treatments	A novel catalytic coating is being developed for ethylene crackers, which greatly reduces coke formation in furnace coils. Less coke formation contributes to longer run times and lower decoking frequency, leading to savings in energy use and corresponding air pollutant emissions.[99]	■ 15-25% energy reduction (fuel savings) might be achieved in the ethylene cracking process. ■ Energy savings for the U.S. petrochemicals sector as a whole would range from 4%-6%.
Functional Materials for Separations or Isolation	Separation Membranes	A novel ceramic membrane technology has been developed to replace rubber-based polymer membranes for separating volatile organic compounds from air at fueling stations.[100]	■ Prevents fuel vapor escape from a gasoline storage tank, thereby potentially saving 180 million gallons of gasoline per year domestically.
New paradigm materials manufacturing processes	Net-shape processing	An improved lost foam casting process has been engineered by General Motors which more accurately measures the size and shape of sand used in casting and better characterizes rheological properties to reduce casting defects.[100,101]	■ First funded by DOE in 1989 and commercialized in 2004, this technology had saved an estimated 2.3 TBtu of cumulative energy in the United States as of 2009. ■ Significantly reduces aluminum and sand scrap rates during production of the complex General Motors L61 engine. ■ Increases labor productivity and reduces materials costs compared to conventional sand casting.
New paradigm materials manufacturing processes	Energy/ feedstock conversion technologies for industry	New process technologies have been developed to yield semi-crystalline polylactide particles derived from biomass feedstocks that have improved physical properties, thereby offering a viable replacement to fossil-fuel-derived polymers.[102]	■ Consumes up to 68% less energy in the form of fossil resources compared with producing products from petroleum. ■ Competes in a market based on price and performance, with a better environmental profile than today's plastics. ■ Reduces the nation's dependence on foreign resources and oil for products such as clothing, food packaging, and carpets.

Program Considerations to Support R&D

A high-profile United States activity related to AMM is the Materials Genome Initiative (MGI), identified above. The MGI is a U.S. Federal government multi-stakeholder initiative designed to develop an infrastructure to accelerate and sustain domestic materials discovery, development, and deployment, primarily through funding of research in the areas of computational tools, experimental tools, data management, and collaborative networks.[103]

One approach central to MGI is the Integrated Computational Materials Engineering (ICME) modeling platform, as noted above. The ICME discipline is focused on the development of multi-scale modeling of materials systems to capture the connections between structure, properties, processes, and performance. The need for ICME to accelerate the development and deployment of AMM was stressed in a 2008 U.S. National Research Council report, and further underscored in a 2013 study on ICME implementation in key U.S. industries.[104,105] The European Commission is aggressively funding capacity and network building for ICME, while in the United States a number of conferences have been held and roadmaps developed to promote ICME leadership domestically.[106,107]

An example of a DOE investment in advanced materials manufacturing is the Critical Materials Institute (CMI). The CMI is one of four U.S. DOE Energy Innovation Hubs, with a primary mission to develop, demonstrate, and deploy technologies to ensure greater security and production efficiencies for materials that are critical to national competitiveness and clean energy technologies.[108] The Institute brings together experts from many national labs, universities, and companies for joint research with $120 million in funding commitments to date.

In addition, funding programs and collaboration networks have been established to facilitate progress in particular materials and/or process domains, including public-private U.S. Manufacturing Innovation Institutes focused on additive manufacturing, battery materials, and composites.[109] A key aspect of these initiatives is a sharp focus on high impact materials innovation opportunities, including efforts to overcome the development and adoption barriers discussed in the previous section.

Opportunity Areas and Investment Needs

Advances in basic and applied science are needed if the availability and performance of AMM is to be accelerated, given that performance advancements often rely on improved fundamental understanding of materials properties, chemistry, and physics. This research requires leading edge equipment for materials imaging, synthesis, manipulation, and measurements, all of which can require substantial capital investments. Ongoing support would be needed for staffing research teams and the (sometimes) lengthy experimental and computational processes that can lead to materials breakthroughs. Large scale collaborative public-private partnerships, such as the National Network for Manufacturing Innovation Institutes,[110] shared user facilities such as the Advanced Light Source at Lawrence Berkeley National Laboratory, and the High Performance Computing for Manufacturing program[111] can facilitate collaborations while maximizing the reach of public and private investments in capital equipment. Such initiatives can also require strong commitments to collaboration and shared agendas for research priorities across private companies, universities and research labs, and federal, state, and local government agencies. Chapter 9 and its Supplemental Information appendices provide extensive details on user facilities and basic science issues.

Further development of computational methods, tools, and databases that enable better understanding and prediction of materials properties and processing attributes also depend on investment and new collaborations. Advancements in collaborative databases of materials and process properties, manufacturing process simulations, and methods for predicting performance are all important for successful AMM. Additionally, the Integrated Computational Materials Engineering (ICME) approach seeks to formalize and institutionalize a methodology for developing and linking models and data for multi-scale simulation of materials performance.

Because general ICME methods can apply to any materials innovation category, they can help accelerate discovery and optimization of materials affecting every sector of the U.S. economy.[112]

Materials breakthroughs at the laboratory scale can face major barriers related to manufacturing process scale-up and eventual market acceptance, which can significantly limit a material's potential for large-scale impact on the nation's energy and economic systems. Market readiness programs, pilot and demonstration projects, and extension efforts are some of the mechanisms used to help usher such technologies through the so-called "valley of death" between proof of concept and market adoption. For small businesses, the SBIR program was designed to address this need. Public-private collaborations to demonstrate materials innovations, energy technologies, and manufacturing processes are some of the ways for testing ideas, learning by doing, and proving technologies in controlled trials. Such activities can help overcome the initial market reluctance and perceived risk that often inhibits the adoption of novel technologies.

Table 6.B.5 summarizes major RDD&D opportunity areas for selected materials innovation category, based on expert elicitation and conclusions in the 2011 *Innovation Impact Report*.[113] While not exhaustive, Table 6.B.5 provides an overview of targeted opportunities that could lead to significant national benefits.

Table 6.B.5 Representative RDD&D areas for consideration in selected AMM innovation categories.[114]

		Key RDD&D Activities (Examples)		
Category	**Subcategories**	**0-2 years**	**2-5 years**	**5-10 years**
Structural Materials	Composite materials	Out-of-autoclave curing processes; automated panel lay-up forming to improve production rates	More energy efficient fiber manufacturing processes; high-volume production technologies	Low-cost fiber feedstocks
	Lightweight metals	Low-cost improved processing for metal-based composite casting; improved wear resistance; custom optimized hybrid/gradient metallic systems	New alloy designs with higher retention for better recyclability; improved damage detection techniques; corrosion resistance of aluminum and magnesium	Nanostructurally precise manufacturing of materials for 10X strength increases that approach the theoretical limits
	Phase-stable materials	High-strength, low alloy steels; corrosion resistant zirconium alloys with reduced hydrogen pickup	Stress, corrosion, and cracking resistant stainless steel; high pressure steels; irradiation resistant steels; physics-based models for lifetime prediction	Alternate fuel cladding materials; oxidation and corrosion resistant refractory alloys; materials databases for ICME
	Multi-material joining	Development of design and fatigue data for low-cost, mass-production joining processes, particularly for automotive applications	Surfaces with controlled porosity for direct bonding of polymers or elastomers to improve adhesion; nondestructive evaluation techniques to evaluate bond quality	Integrated computational materials engineering process model for solid-solid joining that incorporates residual stresses, diffusion, microstructure evolution, and mechanical properties

Table 6.B.5 Representative RDD&D areas for consideration in selected AMM innovation categories, continued

		Key RDD&D Activities (Examples)		
Category	**Subcategories**	**0-2 years**	**2-5 years**	**5-10 years**
Functional Materials for Energy Conversion	Catalysts	Laboratory-scale integration of catalysts in membranes	Large-scale integration of catalysts in membranes; predictive modeling	Identification of catalysts for alternate feedstocks; development of atomically precise enzyme-like catalysts
	Thermoelectric materials	Thermoelectric polymers for weight optimized components	Highly conductive materials compatible with additive manufacturing, polymer designs with integrated circuits	Capacitance materials compatible with additive manufacturing to enable structurally integrated energy storage; oxidation barrier coatings
Functional Materials for Separations or Isolation	Separation membranes	Investigation of tradeoffs between flux and stability in membrane systems; real-world degradation studies	High-flux, dense ceramic membranes; enhanced selectivity in polymers to reduce thickness	Development of strong, 1-molecule-thick membranes with atomically precise pore structures for energy efficient desalination and other separation applications
	Coatings and surface treatments	Development of high-wear resistant coatings; in-situ defect monitoring	Identification of materials for high temperature, conductivity, and oxidation resistance; low-cost laser processing; high accuracy non-planar surface treatments	Ultra-high temperature thermal barrier coatings for oxy-combustion turbines
New Paradigm Materials Manufacturing Processes	Net-shape processing	Innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components	Room temperature formability for non-ferrous alloys; nanomaterial tooling; direct consolidation of titanium powder; high magnetic field metal casting; Use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components	Processes for simultaneous improvements of shape and materials properties; use innovative joining methods to improve dimensional control and enable forged and formed components to replace machined components
New Paradigm Materials Manufacturing Processes	Additive manufacturing	Automated spark plasma sintering; closed-loop hardware/software for improved yields; development of families of polymer nano-filled compounds; new inks and slurries for direct writing systems	Continuous process for production of titanium powder; increased process throughput; new inks and slurries for direct writing systems; new file formats; larger chambers for metals deposition; improved sensing and control of surface quality and residual stresses	Large-scale printed energy storage batteries; techniques to integrate additive manufacturing systems seamlessly into existing manufacturing infrastructure and operations

Table 6.B.5 Representative RDD&D areas for consideration in selected AMM innovation categories, continued

		Key RDD&D Activities (Examples)		
Category	**Subcategories**	**0-2 years**	**2-5 years**	**5-10 years**
New Paradigm Materials Manufacturing Processes	Next-generation metals processing	Improved instrumentation for aluminum reduction cells	New electrode materials for aluminum reduction cells; continuous process for titanium powder; titanium molten metal delivery system; novel membranes for more efficient electrochemical processes; atomically precise catalysts for more efficient reactions at the electrodes	Direct reduction of iron ore using electrolytic hydrogen; novel electrochemistry processes for aluminum or magnesium production; continuous casting processes for high-end alloys; advanced scaling of melt facilities; low-cost, high-property magnesium system for high-volume casting or sheet production

Risk and Uncertainty, and Other Considerations

As with any research area, investments in AMM developments are not without substantial risks and uncertainties. Given that many materials innovations are based on the discovery of fundamental new structures, interactions, and properties at the laboratory scale, there is always a significant risk that such discoveries may not ultimately translate into new products that can be manufactured at levels of acceptable cost or meet other performance requirements. The development of integrated computational tools and models that can help predict materials and market performance can help reduce these risks.

The materials innovation processes described in this technology assessment require ongoing support for capital equipment for experiments, measurements, and testing, as well as pilot facilities for production; these costs can pose a significant challenge for many companies and research institutions. Further, as noted above, given that materials development often requires more than a decade of work, it can be very difficult for companies and research organizations, particularly smaller ones, to maintain ongoing research activities. Mechanisms to help address these challenges need to be considered, ranging from various kinds of RDD&D supports, to collaborations, to resource sharing of leading edge tools and expertise from the national laboratories.

The strong coupling between energy prices and markets for new materials across all materials innovation categories—such as high-strength lightweight materials for vehicles, materials for clean energy applications, and new processes for reducing manufacturing energy use and waste in key materials industries such as iron and steel and chemicals—also poses risks. Energy price increases can encourage greater efficiency and the corresponding demand for novel, more energy efficient, materials and processes; energy price decreases can discourage demand for improved energy efficiency technologies. The potential value of these new computational, experimental, and data tools for RDD&D, and their potential to accelerate the RDD&D process and help address pressing national economic, environmental, and security challenges both strongly motivate pursuit of these advances and the search for mechanisms that can help address these risks, and encourage the ongoing and accelerated development of these capabilities.

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"The workshop concluded that emerging capabilities in predictive modeling and simulation have the potential to revolutionize the development of new materials and chemical processes. Coupled with world-leading materials characterization and nanoscale science facilities, this predictive capability provides the foundation for an innovation ecosystem that can accelerate the discovery, development, and deployment of new technologies, including advanced energy systems. Delivering on the promise of this innovation ecosystem requires the following:

- **Integration of synthesis, processing, characterization, theory, and simulation and modeling**. Many of the newly established Energy Frontier Research Centers and Energy Hubs are exploiting this integration.
- **Achieving/strengthening predictive capability in foundational challenge areas.** Predictive capability in the seven foundational challenge areas described in this report is critical to the development of advanced energy technologies.
- **Developing validated computational approaches that span vast differences in time and length scales**. This fundamental computational challenge crosscuts all of the foundational challenge areas. Similarly challenging is coupling of analytical data from multiple instruments and techniques that are required to link these length and time scales.

- **Experimental validation and quantification of uncertainty in simulation and modeling**. Uncertainty quantification becomes increasingly challenging as simulations become more complex.
- **Robust and sustainable computational infrastructure, including software and applications**. For modeling and simulation, software equals infrastructure. To validate the computational tools, software is critical infrastructure that effectively translates huge arrays of experimental data into useful scientific understanding. An integrated approach for managing this infrastructure is essential.
- **Efficient transfer and incorporation of simulation-based engineering and science in industry**. Strategies for bridging the gap between research and industrial applications and for widespread industry adoption of integrated computational materials engineering are needed."

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[46] National Research Council, "Big Data in Materials Research and Development: Summary of a Workshop," National Academies Press, 2014. http://www.nap.edu/catalog.php?record_id=18760 . One characterization of the data challenge within this workshop was the 4 V's – "Volume, Velocity, Variety, Veracity".

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See: Shanan E. Peers, Ce Zhang, Myron Livny, Christopher Re., "A Machine Reading System for Assembling Synthetic Paleontological Databases," PLOS One, Dec. 1, 2014

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Acronyms

AMM	Advanced Materials Manufacturing
AMO	Advanced Manufacturing Office (of the U.S. Department of Energy)
CASL	Consortium for the Advanced Simulation of Light Water Reactors
EMN	Energy Materials Network
ICME	Integrated Computational Materials Engineering
MGI	Materials Genome Initiative
ORNL	Oak Ridge National Laboratory
TMS	The Minerals, Metals, and Materials Society
SBIR	Small Business Innovation Research

Glossary

Additive manufacturing	The process of producing three-dimensional objects directly from computer-aided design (CAD) model data, usually by adding material layer upon layer. Also called “3D printing.”
Born Qualified	The capability to design a material using predictive theory and modeling with sufficient predictive power that the material is qualified to meet performance standards for one or more applications before it is ever produced. “Born Qualified” is a major goal of computational materials design, and will require extension of computational modeling capabilities, validation of predictive models, and improved material property databases.
Energy Materials Network	A U.S. Department of Energy national laboratory-led initiative to reduce the time-to-market for advanced materials innovations critical to clean energy technologies.
Integrated Computational Materials Engineering	Emerging discipline that integrates computational predictive-modeling tools with system-level computational engineering and manufacturing techniques to provide a unified design and manufacturing process to accelerate development of materials into engineering systems.
Magnetic field processing	A thermal processing method involving the use of magnetic fields to manipulate materials at an atomistic level. Magnetic field processing can be used to tailor structures at nanoscales and microscales.
Materials Genome Initiative	Multi-agency government initiative launched in 2011, with goals to reduce the time to discover, develop, manufacture, and deploy a new material by half, and to do so at a fraction of the cost of conventional approaches.
Net-shape processing	A manufacturing technique in which intermediate product forms are very close to the final (net) shape of the product. Net shape processing can result in less waste and reduced machining or surface finishing requirements.
Roll-to-roll processing	A low-cost, high throughput technique for continuous two-dimensional deposition of materials over large areas onto moving webs, carriers, or other substrates. Also known as web processing or reel-to-reel.