Advanced Reactor Technologies Program

Fast Reactor Structural Materials

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DOE-NE Materials Crosscut Coordination Meeting

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Presentation Outline

- **Introduction of Advanced Reactor Technologies (ART) Advanced Materials R&D Program**
- **Highlight modeling activity of Fast Reactor Structural sub-area**

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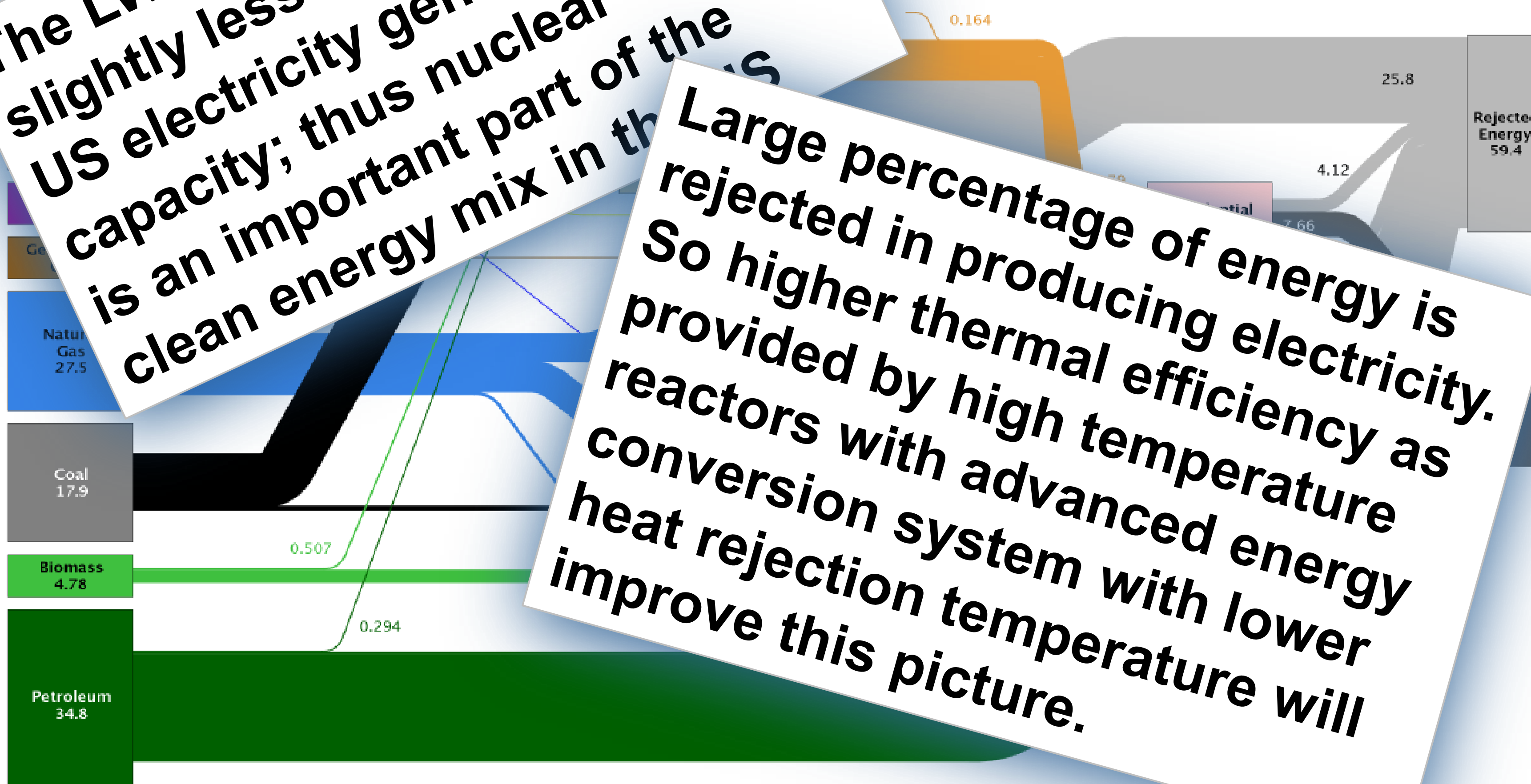
Nuclear E rgy Plays an Important Role in US Electrical Generation

Sankey Diagram D esources (Left) to End-Use Sectors (right). Estimated U llion BTU.

The LWR fleet provides slightly less than 20% of the US electricity generation capacity; thus nuclear energy is an important part of the clean energy mix in th US



Large percentage of energy is rejected in producing electricity. So higher thermal efficiency as provided by high temperature reactors with advanced energy conversion system with lower heat rejection temperature will improve this picture.

DOE Quadrennial Technology Review, September 2015

Advanced High Temperature Reactor Systems

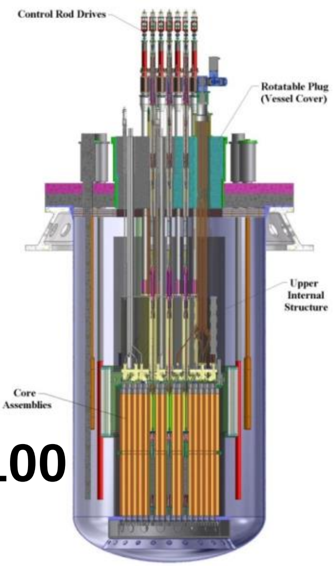
- **Higher thermal efficiency; lower operating pressure; passive safety features**
- **Technologies are at various readiness levels, some are quite mature while others are less so**
- **Various design and operating experience (concepts, test, demonstration, commercial reactors) from the 1940's to the present**
  - High temperature gas-cooled reactors
    - Oak Ridge, Peach Bottom, Fort St. Vrain, GT-MHR, NGNP (USA); Dragon, Magnox, AGR (UK); UNGG, ANTARES (France); AVR, THR (Germany); HTTR (Japan); HTR-10, HTR-PM (China); PBMR (South Africa); GT-MHR (Russia)
  - Sodium-cooled fast reactors
    - BR-5/10, BN-350, BN-600, BN-800, BN-1200 (Russia); Fermi 1, S1G, S2G, EBR I, EBR II, FFTF, CRBR, PRISM (USA); Dourreay (UK); SNR-300 (Germany); Joyo, Monju, JSFR, 4S (Japan); Phenix, Superphenix, Rapsodie, Astrid (France); FBTR, PFBR (India); CEFR, CFR-600 (China); PGSFR (Korea)

Structural Materials Are Critical For Technologies of Advanced Reactors

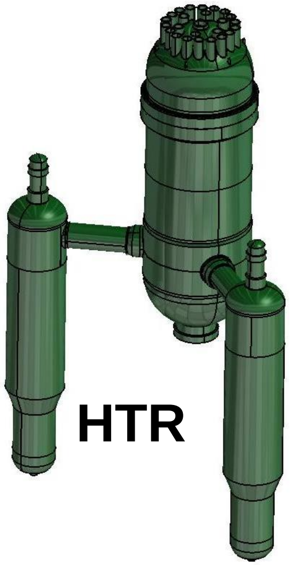
- **Development and qualification of advanced structural materials are critical to the <u>design</u> and <u>deployment</u> of the advanced nuclear reactor systems that DOE is developing**
  - High and Very High Temperature Gas Cooled Reactors (HTGRs and VHTRs)
  - Sodium Cooled Fast Reactors (SFRs)
  - Salt Cooled Reactors
    - MSRs (dissolved fuel) & FHRs (solid fuel)
  - Lead and Lead-Bismuth Cooled Reactors (LFRs)
- **Structural materials must perform over design lifetimes for pressure boundaries, reactor internals, heat transfer components, etc.**

Advanced Materials R&D Activities under Advanced Reactor Technologies Program

- A variety of research and development (R&D) activities in the Advanced Materials area are being conducted to significantly improve
  - Efficiency, safety, performance, and economics of advanced reactor systems
- In addition to the operating temperature range, selection of construction materials for an advanced reactor is critically dependent on the coolant system
  - Due to material compatibility and mass transfer issues
  - Particularly for the lengthy design lifetime desired to reduce the levelized capital cost
- Different construction materials are often required for different advanced reactor systems
- Quality assurance (QA) of data plays a vital role in establishing confidence in the R&D results developed by the ART Program
- Data are generated to the ASME NQA-1 quality level or its equivalent



AFR-100



HTR

Advanced Materials Program Elements Break Down Along Reactor Environments

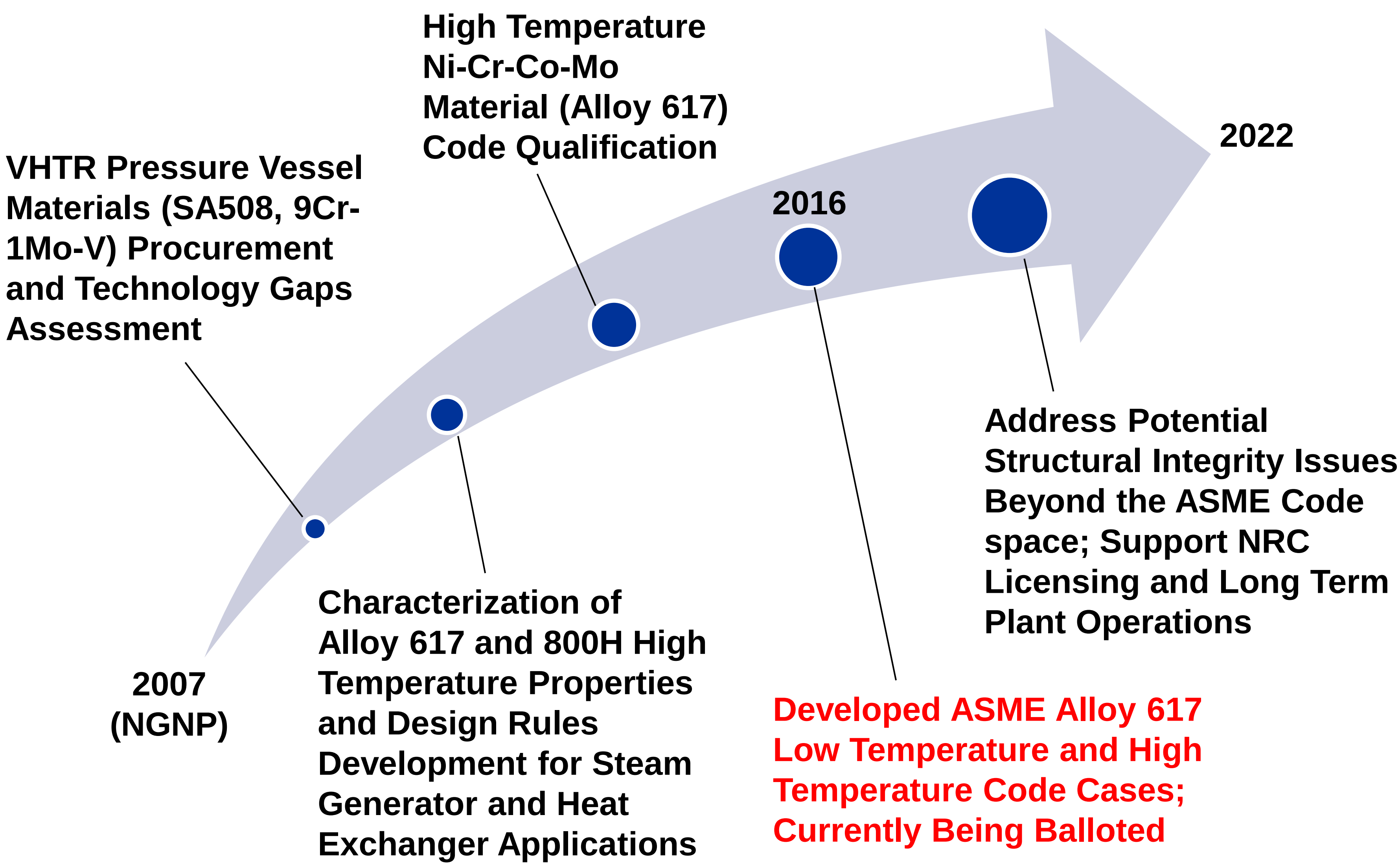
Advanced Materials R&D

High Temperature Materials
- Technical Lead: Richard Wright, INL

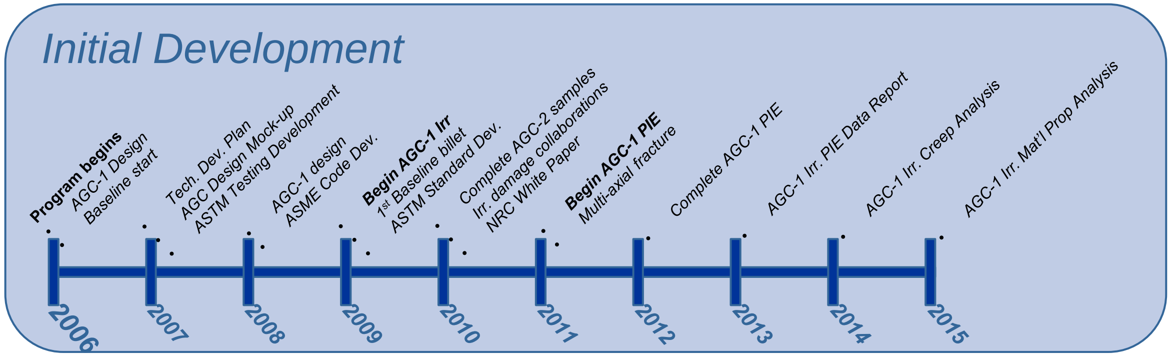
Graphite
- Technical Lead: Will Windes, INL

Fast Reactor Structural
- Technical Lead: Sam Sham, ANL

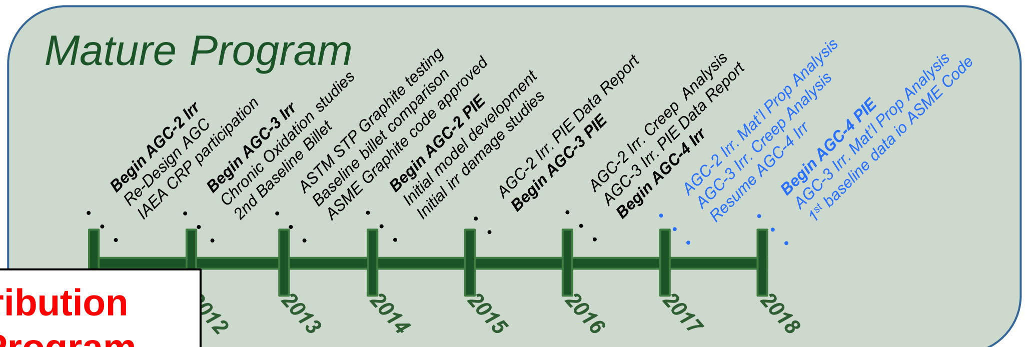
Significant Milestones of High Temperature Materials Program



Graphite Program



- **Program starts 2006**
- **Large initial investment**
- **AGC-1**
  - Prototype test train
  - Lessens learned from design & irradiation



- **Improved/Final AGC Design**
- **Initial data allows:**
  - Collaborations

A very significant contribution made by the Graphite Program on the introduction of probabilistic design methods for graphite into a nuclear construction code (ASME Section III, Division 5)

ysis:

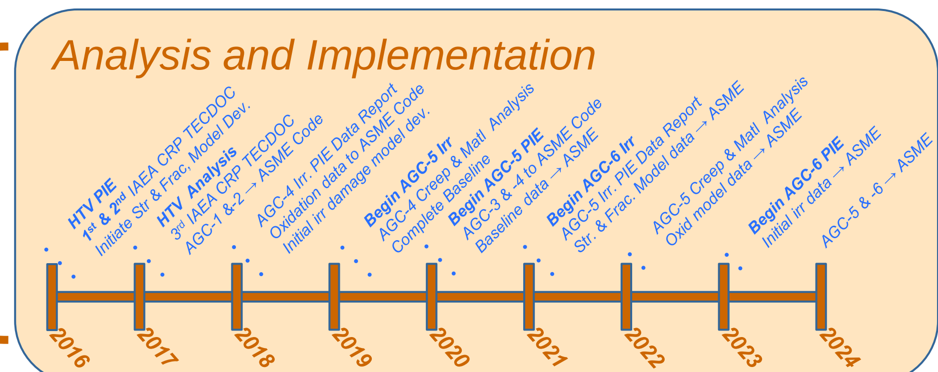
data → **ASME**

m studies

GC analysis

a → **ASME**

- Behavior Models → **ASME**
- **ASME Code complete**



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Fast Reactor Structural Program – Advanced Materials Development

2008 Established Alloy Development Priority List

- Considered a large class of structural materials for further development
- Involved 5 U.S. national Laboratories and 5 U.S. universities
- Considered experience from Fusion, Gen IV, Space Reactor, and development activities in Fossil Ener…
- Established alloy… priority list:
  - Ferritic-Martensit…
    - Grade 92 (NF6…
    - Grade 92 with th… mechanical treatment (TMT)
  - Austenitic stainless steels
    - HT-UPS
    - NF-709

2009-2012 Alloys Downselection

- Established comprehensive downselection metrics
- Considered tensile properties, creep, creep-fatigue, toughness, weldability, thermal aging, sodium compatibility, mechanical and TMT processes
- Integrated R&D activities by D…
  - Oak Ridge Nati…
  - Ar…
  - …d 9Cr, Gr92, …aterial)
  - …UPS (Fe-14Cr-16Ni), Modified HT-UPS, A709 (Fe-22Cr-25Ni), 316H (baseline material)
- Based on overall performance w/ comprehensive metrics (and accelerated test data), Optimized-Gr92 with TMT and A709 were downselected for further assessment

2013-2015 Intermediate Term Testing to Confirm Enhanced Properties

- Further optimize mechanical and TMT processes
- Procure larger heats
- Validate…
- …adiation campaign planning
- Development of roadmap for ASME nuclear code cases

2016 – 2022

Phase I:

100,000h, 650C Alloy 709 Nuclear Code Case

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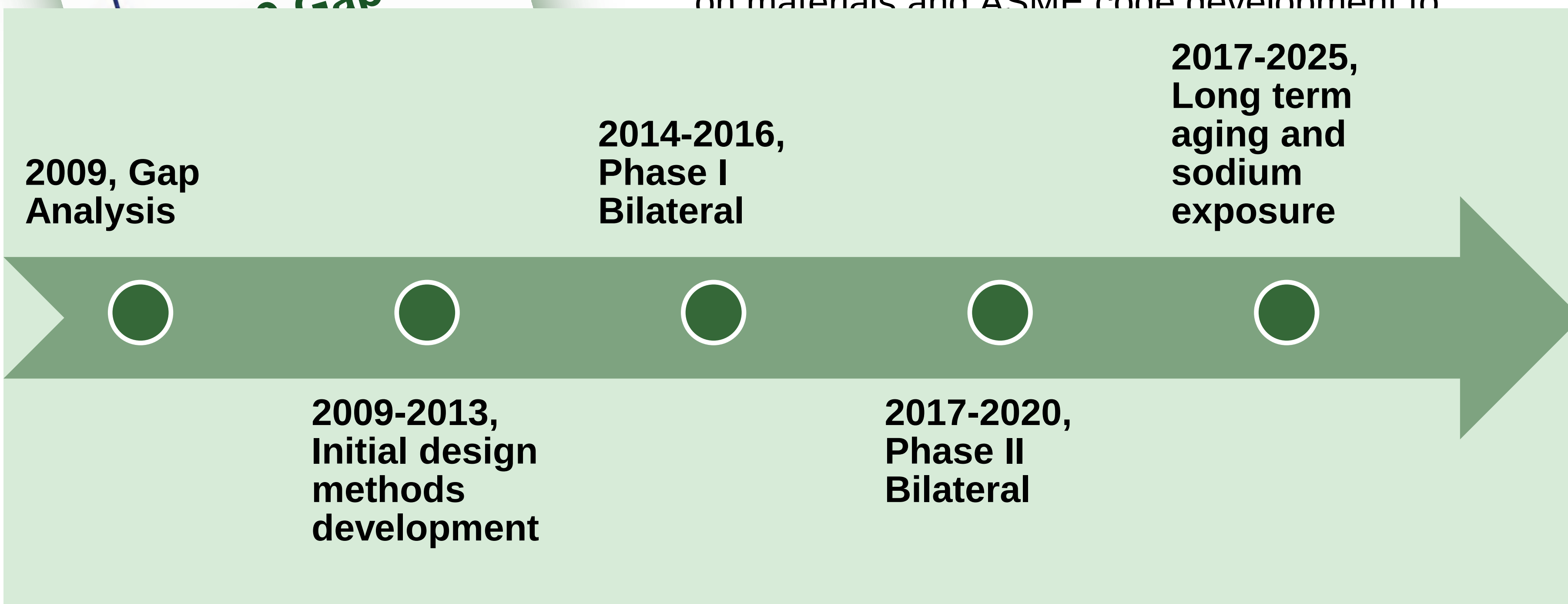
Fast Reactor Structural Program – Materials Design Technology

- Conduct research and development on advanced materials in support of code qualification and codes and standards development required to apply the materials for SFR applications
- Allowing more flexible designs and/or enhancing safety margins through design methods improvement
- Gap analysis conducted in 2009 on required actions on materials and ASME code development to



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NEUP Projects

NEUP Program research activity is an integral part of the R&D portfolio of the ART Materials Program

Active NEUP Projects
Project 12-3541, Accelerated irradiations for high dose microstructures in fast reactor alloys (University of Michigan)
Project 12-3882, Neutron irradiation damage in pure iron and Fe-Cr model alloys (University of Illinois, Urbana-Champaign)
Project 13-4791, Mechanistic models of creep-fatigue crack growth interactions for advanced high temperature reactor components (Oregon State University)
Project 13-4900, Corrosion of structural materials for advanced supercritical carbon-dioxide Brayton cycle (University of Wisconsin-Madison)
Project 13-4948, Fundamental understanding of creep-fatigue interactions in 9Cr-1MoV steel welds (Ohio State University)
Project 13-5039, Multi-resolution testing for creep-fatigue damage analysis of Alloy 617 (Arizona State University)
Project 13-5252, Long-term prediction of emissivity of structural material for high temperature reactor systems (University of Missouri)
Integrated Research Project (IRP)
Project 13-5531, High Fidelity Ion Beam Simulation of High Dose Neutron Irradiation (University of Michigan)

NEUP Projects – Cont'd

Active NEUP Projects
Project 14-6346, Integrated computational and experimental study of radiation damage effects in Grade 92 Steel and Alloy 709 (University of Tennessee-Knoxville)
Project 14-6562, Development of novel functionally graded transition joints for improving the creep strength of dissimilar metal welds in nuclear applications (Lehigh University)
Project 14-6762, Microstructural evolution of advanced ferritic/martensitic alloys under ion irradiation (University of Illinois, Urbana-Champaign)
Project 14-6803, Dissimilar joints between 800H alloy and 2¼Cr & 1Mo steel (Pennsylvania State University)
Project 15-8308, Creep and creep-fatigue crack growth mechanisms in Alloy 709 (North Carolina State University)
Project 15-8432, Multi-scale experimental study of creep-fatigue failure initiation in a 709 Stainless Steel alloy using high resolution digital image (University of Illinois, Urbana Champaign)
Project 15-8548, Assessment of Aging Degradation Mechanisms of Alloy 709 for Sodium Fast Reactors (Colorado School of Mines)
Project 15-8582, Mechanistic and Validated Creep/Fatigue Predictions for Alloy 709 from Accelerated Experiments and Simulations (North Carolina State University)
Project 15-8623, Characterization of Creep-Fatigue Crack Growth in Alloy 709 and Prediction of Service Lives in Nuclear Reactor Components (University of Idaho)

NEUP Projects – Cont'd

New NEUP Projects
NEUP Project 16-10578: Thermal Hydraulic & Structural Testing and Modeling of Compact Diffusion-Bonded Heat Exchangers for Supercritical CO2 Brayton Cycles (Georgia Institute of Technology)
PNEUP Project 16-10714: ASME Code Application of the Compact Heat Exchanger for High Temperature Nuclear Service (North Carolina State University)
NEUP Project 16-10324: Model Calibration-Based Design Methodologies for Structural Design of Supercritical CO2 Compact Heat Exchangers under Sustained Cyclic Temperature and Pressure Gradients (Oregon State University)
NEUP Project 16-10285: Tribological Damage Mechanisms from Experiments and Validated Simulations of Alloy 800H and Inconel 617 in a Simulated HTGR/VHTR Helium Environment (Purdue University)
NEUP Project 16-10732: High Temperature Tribological Performance of Ni Alloys Under Helium Environment for Very High Temperature Gas Cooled Reactors (VHTRs) (Texas A&M University)
NEUP Project 16-10210: Tribological Behavior of Structural Materials in High Temperature Helium Gas-Cooled Reactor Environments (University of Wisconsin, Madison)
FY 2017 New Calls
RC-1 Materials Compatibility for High-Temperature Liquid Cooled Reactor Systems
RC-3 SiC/SiC Composites
Integrated Research Project (IRP) RC-1: Codification of Compact Heat Exchanger Usage for Nuclear Systems
NEUP Project - \$800K over three years IRP on Compact Heat Exchangers - \$5M over three years

Creep Deformation and Fracture Modeling of Grade 91 Steel

Acknowledgments

- **Grain boundary and interior material boundary modeling**
  - Robert Dodds Jr., Emeritus M.T. Geoffrey Yeh Endowed Chair Professor
  - Kristine Cochran, consultant
- **Crystal plasticity modeling**
  - Tim Truster, University of Tennessee
- **Overall modeling framework**
  - David Parks, Massachusetts Institute of Technology

Allowable Stresses for 60-year Design Life

- Grade 91 steel is a creep-strength enhanced ferritic/martensitic steel that has been selected as a reference construction material for a number of sodium fast reactor (SFR) designs
  - AFR-100 being developed by DOE and designs from Japan, Korea and India
- Long design lifetime, typical 60 years, reduces the levelized cost of electricity and hence improves the economics of SFR plants
- Desirable to design pressure boundary and core support components that would operate for the entire design life of the plant, without replacement
- ASME Code design allowable stresses depend on design lifetime and operating temperature
- Extrapolation of creep rupture data using a factor of 3X on rupture time is permitted by ASME Code for creep strength enhanced ferritic/martensitic steels such as Grade 91
- For 60-year design life (500,000h assuming 95% plant availability), data with rupture times up to 167,000h are required
- Time-temperature engineering parameter such as Larson-Miller parameter is used by ASME Code to combine data from different temperatures and rupture times to perform extrapolation

Allowable Stresses for 60-year Design Life – Cont'd

- Whether adequate conservatism is retained when extrapolating allowable stress data is a long standing issue that has been considered by the U.S. Nuclear Regulatory Commission (NRC) and its Advisory Committee on Reactor Safeguards (ACRS) as one of the high priority issues that need to be resolved for high temperature reactor system designs.
- An R&D program to elucidate and to understand important features of creep deformation and fracture behaviors through material characterization and modeling was recommended by ANL
- Modeling involves the use of high-performance continuum mechanics simulation tools and the incorporation of mechanism-based constitutive models of deformation and microstructural evolution
- Objective is to corroborate the conservatism of the ASME time-dependent allowable stresses obtained by extrapolation, and to retire this issue before the license application of an SFR design.

Microstructures and Creep Fracture Process of Grade 91 are Complex

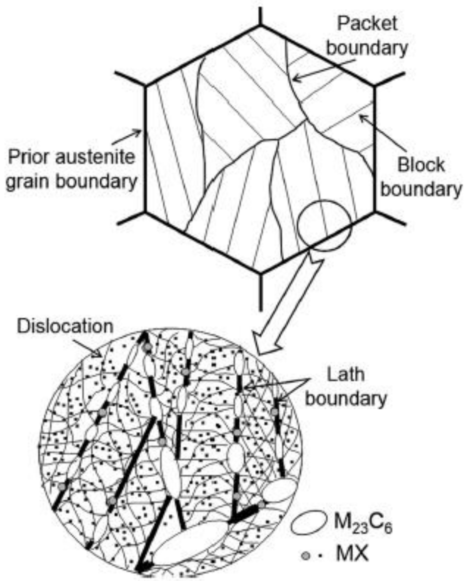


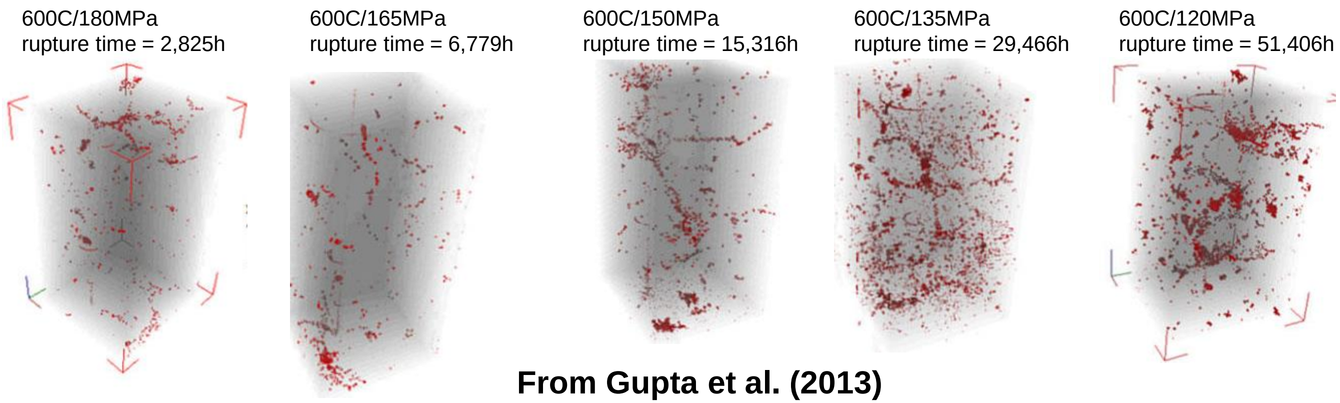
Figure taken from: Abe (2016)

Tempered Martensite Microstructure

- Prior austenite grains and GBs
- Martensite packets and blocks: grow larger with long exposure times thus increasing austenite grain size
- Laths: grow larger & fewer in number with long exposure as migration leads to absorption of their GBs
- Larger particles/precipitates concentrated on PAGBs and packet/block GBs
- Much smaller, uniformly distributed smaller particles within laths

Representative Physical Dimensions Before Loading

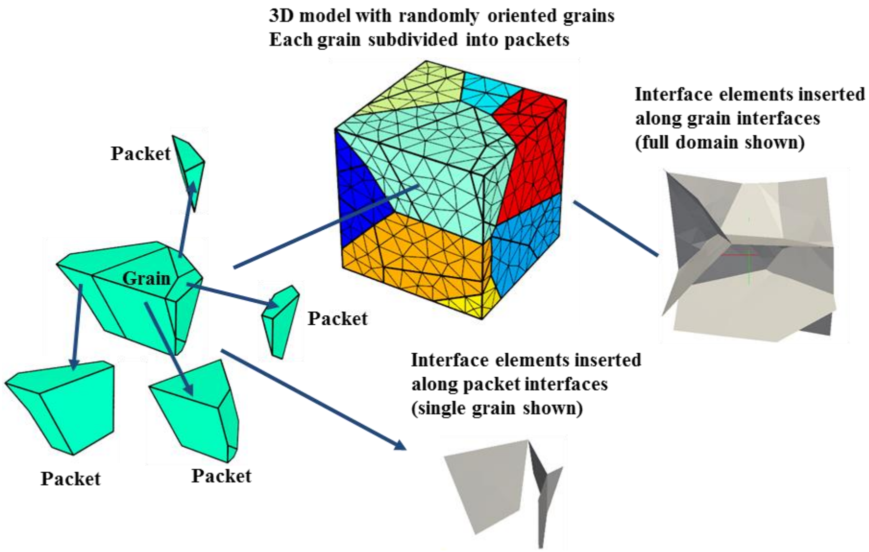
- PAGs > 20 um
- Packets/blocks 5-15 um
- Lath edge lengths 2-3 um, thickness < 0.5 um
- $M_{23}X_6$ up to several ums w/ elongated shape
- MX carbonitrides much less than a um



From Gupta et al. (2013)

- 3D visualization of reconstructed image of creep voids from synchrotron micro-tomography and serial sectioning (11%Cr)
- Showing transition of transgranular to intergranular creep rupture failure and corresponding reduction in creep ductility due to creep voids

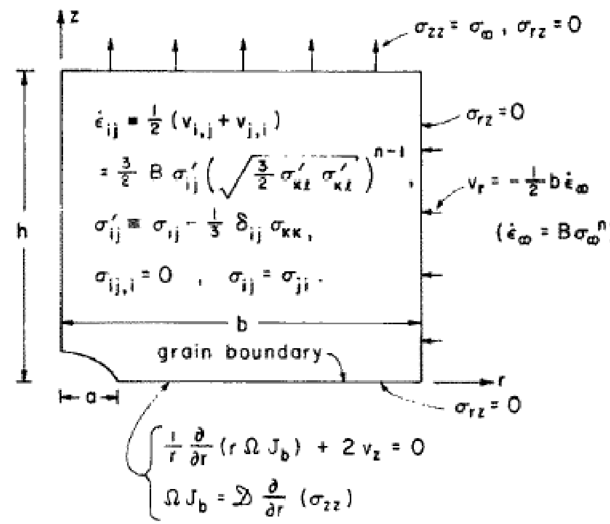
Finite Element Modeling Details - Prior Austenite Grain and Packet Boundaries



Interior Boundaries:

- PAG boundaries and packet boundaries are explicitly modeled using cohesive finite elements
- Cavity nucleation, growth and coalescence
- GB Sliding

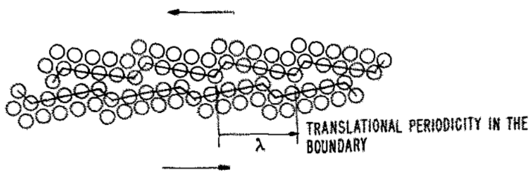
Cavity growth model: Based on results from coupled GB diffusion and creep deformation models of Rice and Needleman (1980) and Sham and Needleman (1983)



Cavity nucleation Model: Based on a synthesis of literature models. Nucleation rate is driven by a combination of normal traction to the boundary and neighboring creep rate

Finite Element Modeling Details - PAG and Block Boundaries (Cont'd)

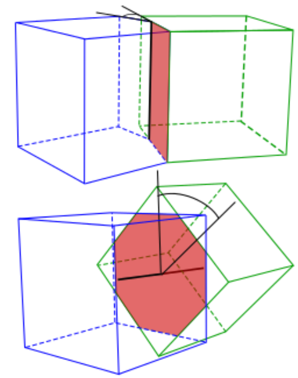
GB Sliding: Based on a model given by **Ashby (1972)** where the shear stress is proportional to the relative GB sliding:



$$\tau = \eta_b \dot{\Delta}; \quad \eta_b \equiv \frac{kT}{8bD_B\delta}$$

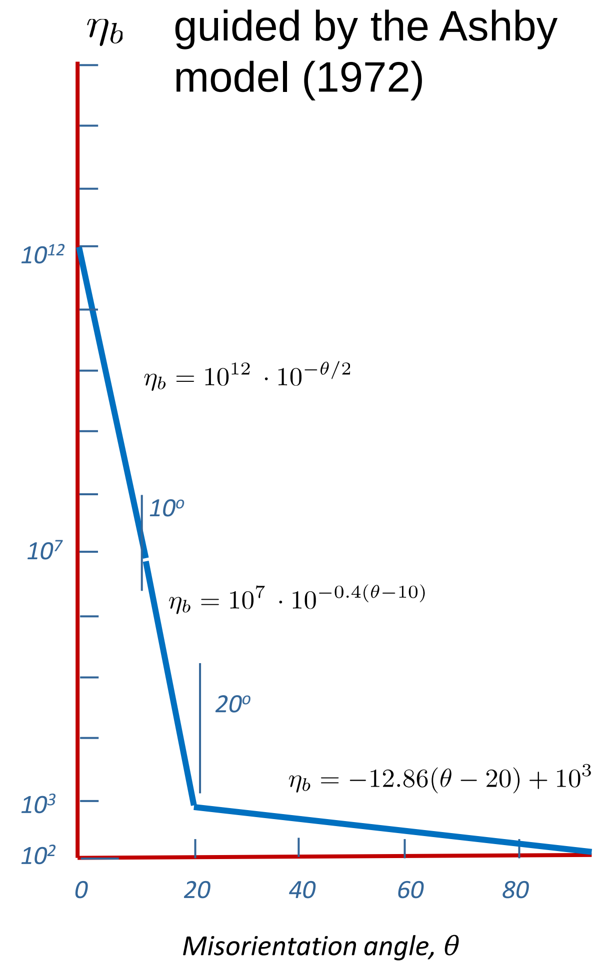
The GB sliding resistance is related to the GB misorientation angle

LAGBs have small diffusion coefficients and thus large η_b; high angle grain boundaries (HAGBs) have high diffusion coefficients and thus small η_b

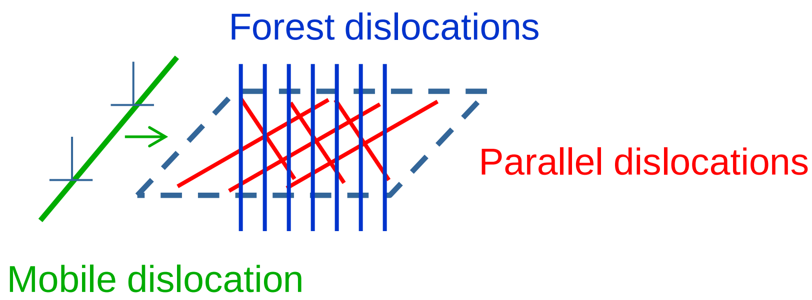


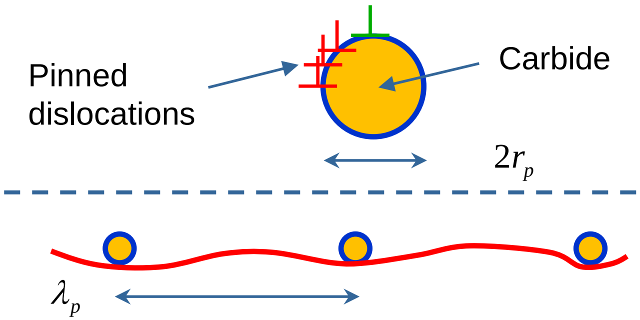
3D cell simulations demonstrated that $\eta_b > 10^{12}$ (MPa-hr-mm^{-1}) effectively eliminates GB sliding for the grain property values of Grade 91. Values of $\eta_b < 10^{3\text{ to }4}$ effectively allow free sliding.

Simple dependence of η_b on misorientation angle adopted for Grade 91, guided by the Ashby model (1972)



Finite Element Modeling Details - Crystal Plasticity Models in PAGs





Grains:

- Dislocation density based crystal plasticity
- Glide and climb dislocation mechanisms
- Statistically stored and geometrically necessary dislocations modeled
- Back stress to account for loading path reversal (e.g., creep-fatigue loading)
- Different crystallographic orientations from PAG to PAG
- Model blocks within PAGs
- Model effects of MX and $M_{23}C_6$ carbide coarsening

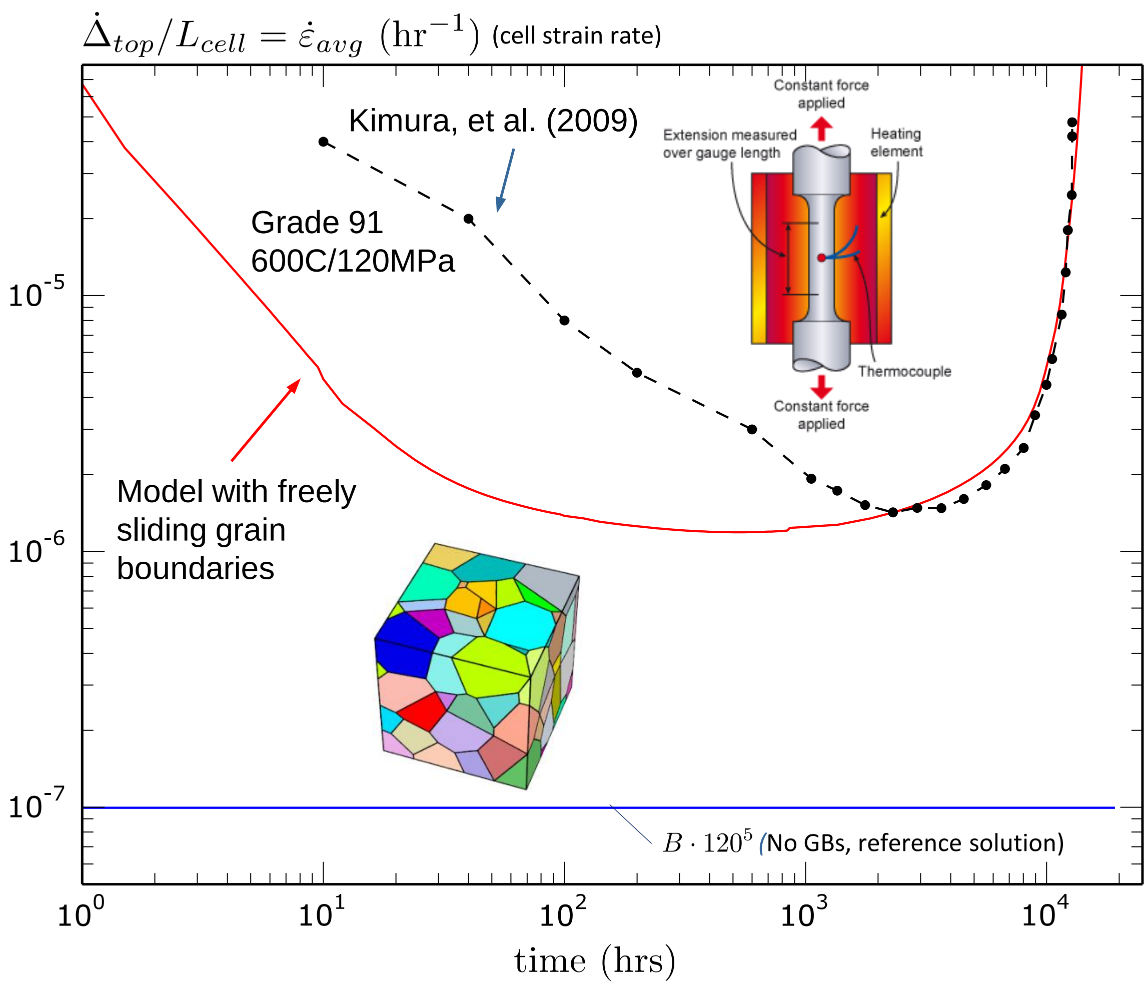
Modeling Development Work Flow

- Grain boundary and interior boundary modeling:
- Develop cohesive elements incorporating GB cavitation and sliding
- Coupled with isotropic material model (power law creep) for the grains to test development

- Crystal plasticity (CP) development and implementation to model grain deformation
- Test (CP) development without introducing GB and interior boundaries

- Integrate both components to study creep deformation and fracture

Preliminary 3D Grain Boundary Model Results (Without Crystal Plasticity)



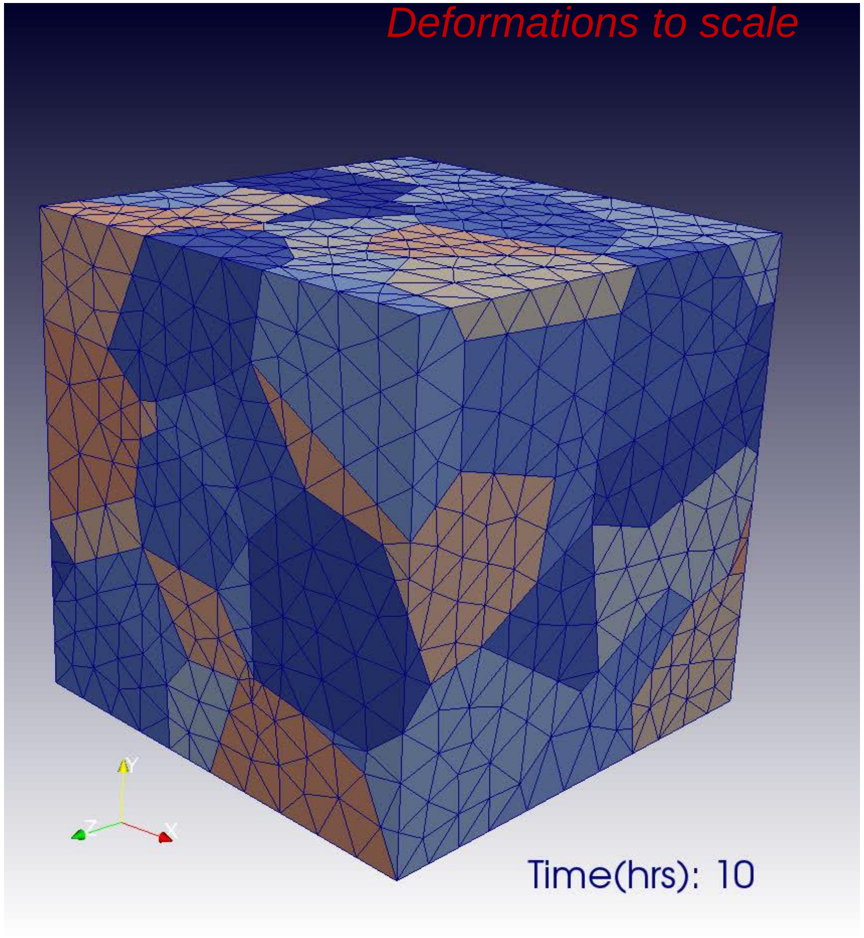
Fixed properties for these simulations

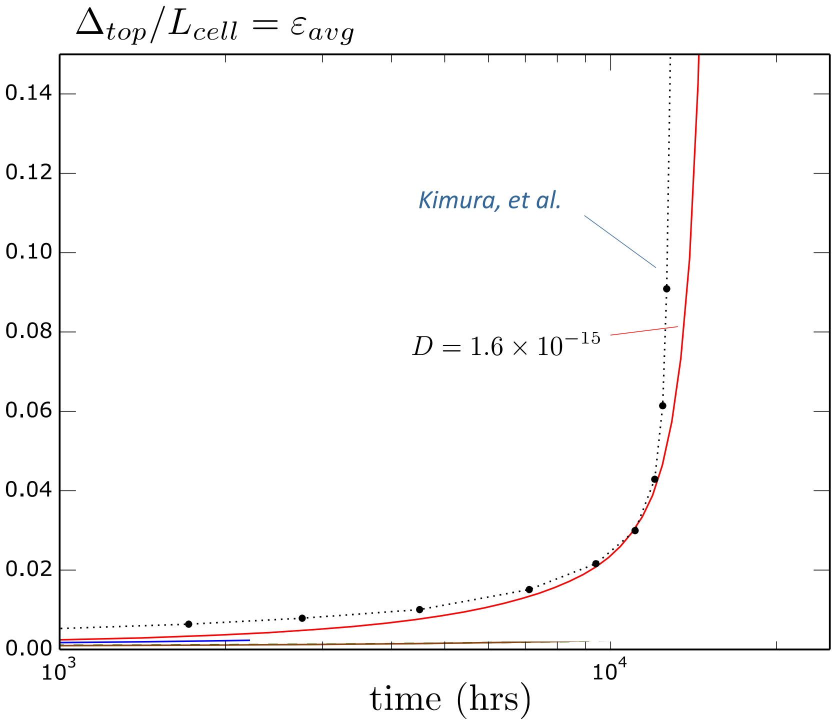
$E = 150,000$ MPa
$\nu = 0.285$
$n = 5$
$B = 4 \times 10^{-18}\ \mathrm{MPa^{-n} \cdot h^{-1}}$
$a_0 = 0.0005$ mm $(0.5\ \mu\mathrm{m})$
$b_0 = 0.005$ mm $(5\ \mu\mathrm{m})$
$a_0/b_0 = 0.1$, Porosity $= 0.01$
$D = 1.6 \times 10^{-15}$
$\eta_b = 100\ \mathrm{MPa \cdot hr \cdot mm^{-1}}$
Nucleation of new cavities: off

- Model shows a clear primary-like creep effect up to ~600 hours
- Free GB sliding
- Strain rate decreases until grain-to-grain contact conditions and shear stress on GBs reach a steady state

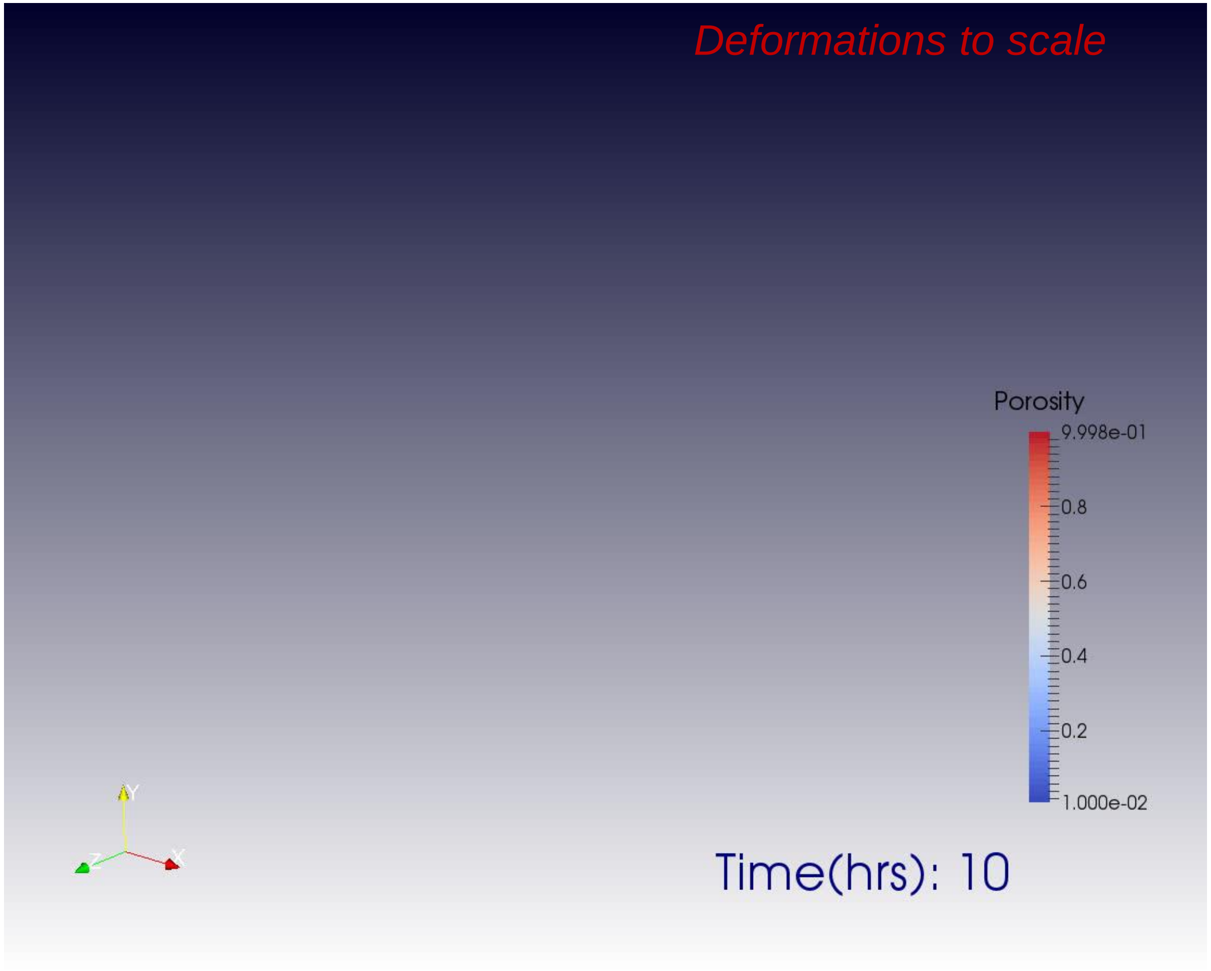
Primary creep trend caused by stress re-distribution of high stresses at triple points caused by grain boundary sliding

3D Simulation Results – Video of Deformation





3D Simulation Results – Video of GB Porosity Evolution

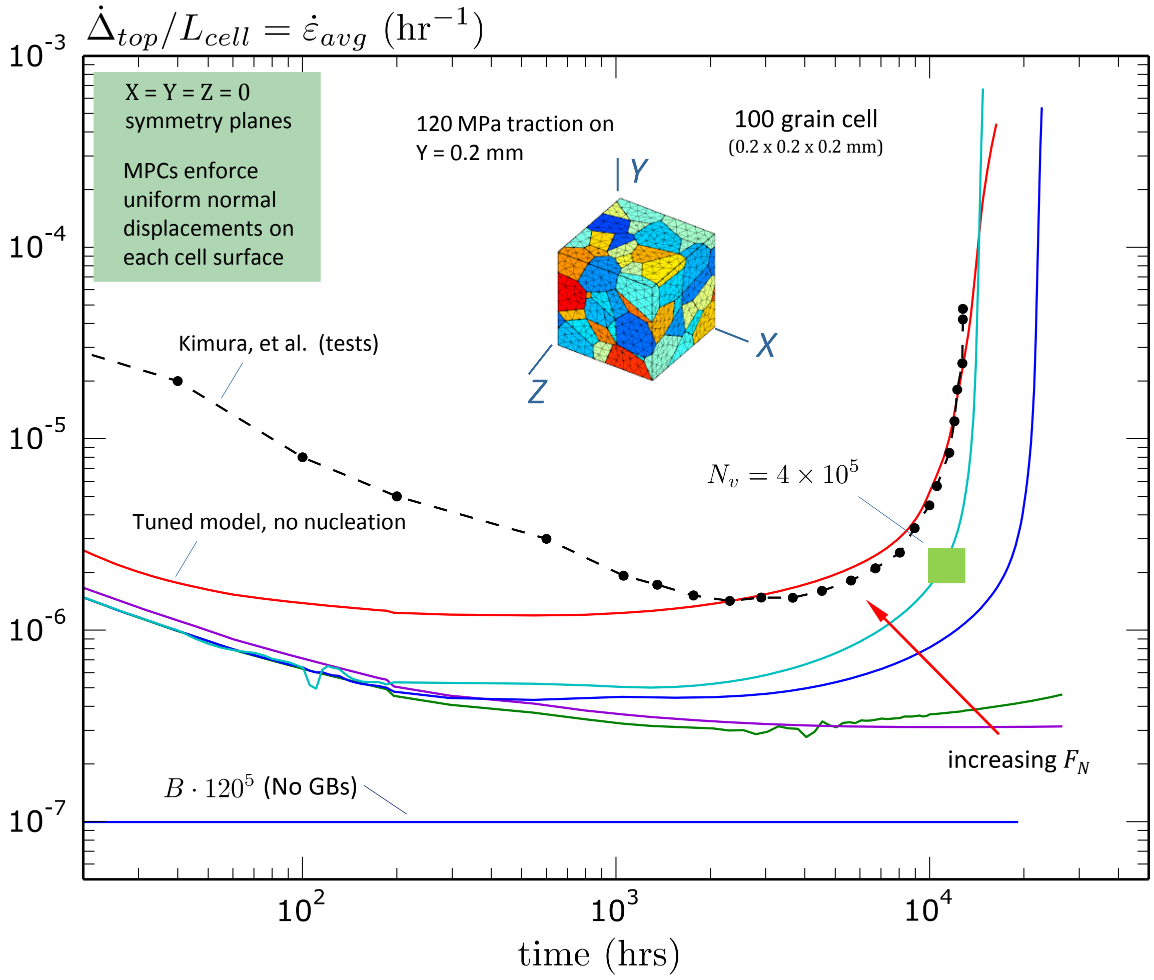


- **Only GBs become visible**
- **First shown when $(a/b_0)^2 > 0.5$**
- **Damaged GBs mostly normal to loading direction (Y)**

time (hrs)	**Cell strain**	**# failed GBs**
4960	0.010	0
6960	0.015	3
8460	0.020	12
10460	0.030	39
12460	0.050	67
13460	0.080	90
14210	0.120	106

467 GBs in model

Parametric Study on Continuous Cavity Nucleation



<u>Fixed properties for these simulations</u>

$E = 150,000$ MPa

$\nu = 0.285$

$n = 5$

$B = 4 \times 10^{-18}$ MPa$^{-n} \cdot$ h^{-1}

$D = 1.6 \times 10^{-15}$ MPa$^{-1} \cdot$ h$^{-1} \cdot$ mm^3

$\eta_b = 100$ MPa $\cdot$ hr $\cdot$ mm^{-1}

$a_0 = 250$ nm

$b_0 = 60\ \mu$m

$(a_0/b_0)^2 = 0.000017$

$N_v(t=0) = 5000$ cavitites/mm^3

- Tensile traction increased to 120 MPa on top (+Y) surfaces over 0.5 hrs. Held constant.

$$\dot{N} = F_N \left(\frac{T_n}{\Sigma}\right)^{\beta} \dot{\varepsilon}_e^C$$

$\beta \equiv 0$; F_N varies

$N_I = 1/\pi/b_0/b_0 = 88$

F_N/N_I: 0, 1131, 11310, 22619

Detailed results next slides

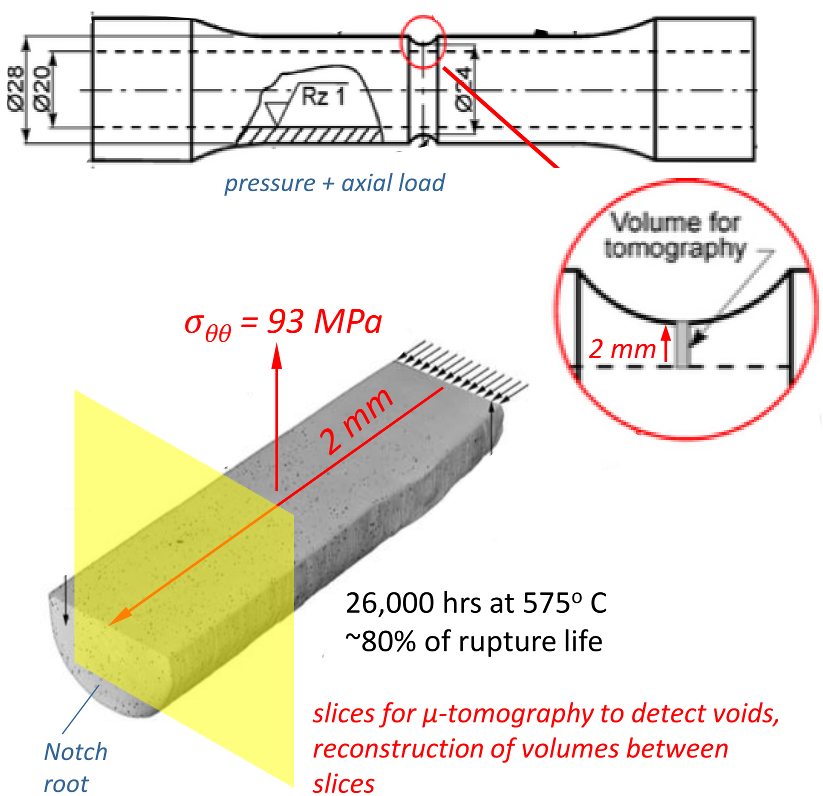
Cavity Density Measurements

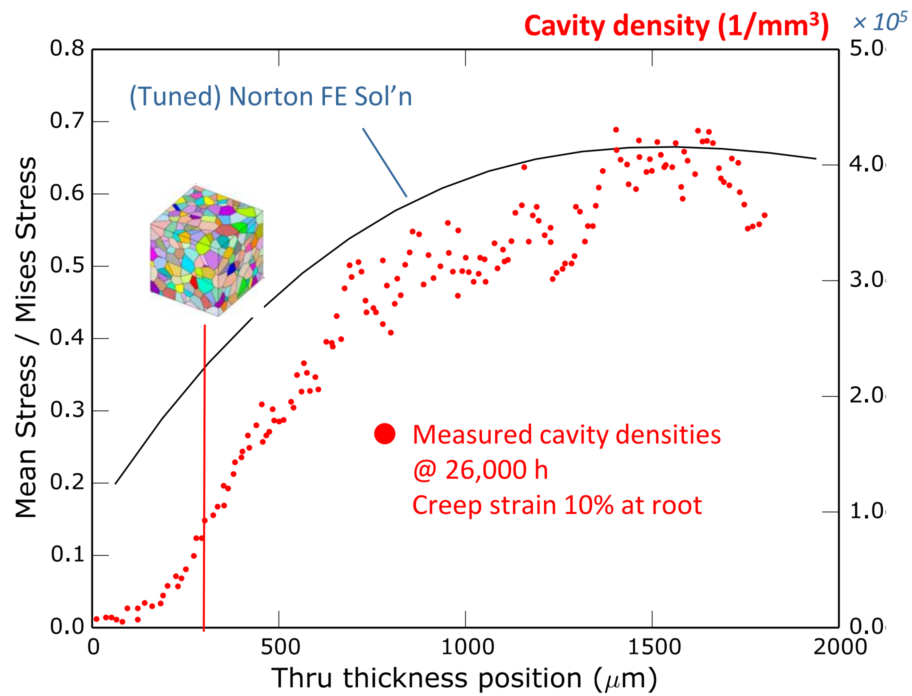
Contents lists available at ScienceDirect
Materials Science and Engineering A
journal homepage: www.elsevier.com/locate/msea

~Gr91 w/ 1% W

Microtomographic investigation of damage in E911 steel after long term creep

F. Sket[a,c,*], K. Dzieciol[b], A. Borbély[b], A.R. Kaysser-Pyzalla[c], K. Maile[d], R. Scheck[d]





- Measurements reveal clear evidence of cavity nucleation as function of increasing stress/strain levels from inside surface-to-notch root
- Cavity size distributions also measured
- **Same order of magnitude of cavity density at location with same triaxiality as uniaxial creep rupture test (at lower temperature and shorter time)**

Summary

- The interaction of cavity nucleation, growth and coalescence process with grain boundary sliding, and the effect of grain boundary orientation dependence have been extensively studied using the cell model
- Implementation of the crystal plasticity model and optimization of model parameters are ongoing
- The integration of the crystal plasticity model and grain boundary modeling has begun

THANK YOU