Accelerated Development of Advanced Steels for Nuclear Applications

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Joint EC-IAEA Topical Meeting
Barcelona, Spain
- Key Problems of Irradiated Structural Materials
- Designing New Radiation-Resistant Materials
  - Relationship between processing and microstructure
  - Nano-structured Advanced Steels
- Multiscale Modeling as an Aid to Materials Development
  - Ab initio, MD, DD, and Continuum Methods
Next Generation Nuclear Plant (NGNP) - GEN-IV Utilizes High-Temp Materials for 2022 Operation

**AREVA - ANTARES Layout**

Coolant = helium at 5-9 Mpa
Core outlet temperature = 900-950 °C.
IHX & Core Barrel Materials: In-617, Steel, 800H.

Westinghouse Layout
Development of Fusion Energy Requires High-Temperature Structural Materials

HAPL – Inertial Fusion

- Heat Flux: FW ~1 MW/m²; Divertor ~5 – 15 MW/m²
- Neutron Flux: ~ 3 – 5 MW/m²
- Particle Flux: Divertor ~10^{21}-10^{22} m^{-2}s^{-1} 

ITER- Magnetic Fusion

Environment

- Heat Flux: FW ~1 MW/m²; Divertor ~5 – 15 MW/m²
- Neutron Flux: ~ 3 – 5 MW/m²
- Particle Flux: Divertor ~10^{21}-10^{22} m^{-2}s^{-1} 

Mechanical Loads: Pressure ~ 2-5 MPa
Structural Materials in Nuclear Energy Face Unprecedented Operating Environments

- Thermal
- γ-Ray
- X-Rays
- Neutron
- Ions
- Particles
- b.u.

- Convection
- Radiation
- Chemical Activity
- Oxidation/Reduction
- Corrosion
- Stress-Corrosion Cracking

1. Energy Interaction with Media
2. Energy Transfer through Media
3. Energy Exchange between Media

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Heat Flux (MW/m²)

Duration (s)

ICF 1st Wall X-Rays
W, SiC
W, SiC
Be, C, Fe, W
C, SiO₂, SiC
Re, Ir, W, Mo, HfC
Al₂O₃, SiC

ICF 1st Wall ions
Sun surface
Reentry Vehicles
Rocket Nozzles
Solar Collector
Fusion Divertor
Fission (fast breeder)
Fusion 1st Wall
Fission Reactor (LWR)

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Metals
Refractory
Constraints on the Development of Advanced Structural Steels

- Radiation Effects Constraints
- Compositional Constraints
  - Low-activation
  - Allowable phases, phase stability and microstructure.
- Operational Constraints;
  - Startup/ shut-down at low temperature
  - Thermodynamic efficiency at high-temperature.
Radiation Damage Problems of Structural Materials in Nuclear Energy

- Radiation hardening & embrittlement (<0.4 $T_M$; > 0.1 dpa)

- Phase instabilities & radiation-induced precipitation (<0.3-0.6 $T_M$; > 10 dpa)

- Irradiation creep (<0.45 $T_M$; > 10 dpa)

- Volumetric swelling from void formation (<0.3-0.6 $T_M$; > 10 dpa)

- High temperature helium-embrittlement (<0.5 $T_M$; > 10 dpa)

Can we break the shackles that limit conventional structural materials to ~300°C temperature window?

Additional considerations such as He embrittlement and chemical compatibility may impose further restrictions on operating window.
Radiation Effects Lead to a Narrow Design Window

Short timescale (e.g. $10^{-12} - 10^{-9} \text{ s}$):
- Atomic Displacements;
- Fast Transport;
- Lattice Defects (Vacancies and Interstitials).

Long timescale (e.g. $10^{-3} - 10^6 \text{ s}$):
- Microstructure Evolution (Voids, Bubbles, Dislocations, Phases);
- Dimensional Instabilities (Swelling and Creep);
- Shear Bands (Localized plasticity);
- Helium Embrittlement.

Compositional Constraints imposed by low activation

- Optimize alloy composition for re-cycling in several hundred years, and for minimum decay heat in accidents
- Eliminate elements that induce high radioactivity at shutdown, and those with long-term half-lives.

Figure 1. Specific activity response of the three material candidates.

Figure 2. Contact $\gamma$ dose rate response of the three material candidates.
Composition & Processing Constraints for Optimum Microstructure

- **First Generation Steels** (1960’s) introduced carbide formers V, Nb and some W: 2¼ Cr- 1 Mo, HT-9 → $10^5$ hrs/ 600 °C/ 60 MPa
  - Considered for fast reactors
- **Second Generation Steels** (1970-1985): T-91 (Fe-9Cr-1Mo-0.2V-0.08Nb-0.05N-0.4Mn-0.4Si-0.1C)
- Duplex microstructure (delta-ferrite/ martensite) → $10^5$ hrs/ 600 °C/ 100 MPa.
- **Third Generation Steels**: NF-616 (or grade 92) → $10^5$ hrs/ 620 °C/ 140 MPa.
  - Generation 3a Steels (fusion grades): F82H (Japan), Eurofer (Europe), and ORNL 9Cr-2WVTa (US) ……Low activation
  - Generation 3b Steels (ODS steels): Oxide Dispersion Strengthened Steels
- **Fourth Generation Steels** (NFAs): NF-12, SAVE → $10^5$ hrs/ 650 °C/ 120 MPa
- **Fifth Generation Steels** Nano-structured Steels → $10^5$ hrs/ 700 °C/ 120 MPa.
Historical development of improved high-temperature steels has exhibited slow and steady progress – Thermal Efficiency Improved 5 points in 70 years.

Based on


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<th>Type of power plant</th>
<th>Efficiency</th>
<th>Availability</th>
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<td>Hard coal</td>
<td>47%</td>
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<tr>
<td>Electric motor</td>
<td>95%</td>
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</table>
Utilization of Multiscale to Design Radiation-Resistant Steels

**Constraints**
- Low Activation
- Low DBTT
- Low Swelling
- Creep Resistance
- Weldability

**Consequences**
- Limit elements with long decay chains
- Narrow range of Cr content, reduce C%
- High Sink Strength (many interfaces)
- Slow coarsening kinetics
- Grain boundary vacancy sources
- Prevent recovery
- Reduce helium

**Composition/Microstructure**
- Cr, W, V, C
- Y, Ti, O
- M$_{23}$C$_6$ Carbides
- Pyrochlore Oxides: (e.g. Y$_2$Ti$_2$O$_7$ - cubic)
- Martensitic phase

**Designed Steels**
- Gen-I
- Gen-II
- Gen-III
- Gen-IV
- Gen-V
- Nano-structured super ODS steels
Effect of Neutron Irradiation on the Ductile to Brittle Transition Temperature in Ferritic/martensitic Steels

Better high-temperature stainless steels are needed

347 stainless steel at 650°C

- Key issues are Creep and Corrosion
- Significant gains in recent years for improved creep resistance via nano carbide/nitride
- Cr-oxide used for corrosion resistance can be compromised by H₂O, C, or S species
- Al-oxide offers better corrosion resistance but additions of Al degrade creep resistance
Development of New Alumina-Forming, Creep Resistant Austenitic Stainless Steel

Temperature for 100,000h rupture life (°C)

- Designed for 600-800°C structural use under aggressive oxidizing conditions
  - superior oxidation resistance to conventional chromia-forming alloys
- Comparable cost to current heat-resistant austenitic stainless steels

800°C in air, 72h

Alumina-Forming Austenitic (AFA) Alloy Family

100,000 h Creep Rupture Temperature [°C]

LMP \{=(T [°C]+273)(C+\log t_{rupture [h]}), C=20\}

AFA Alloy Grades

**AFA**\(^{\text{HP}}\): Fe-(25-30)Ni-(14-15)Cr-(3.5-4.5)Al-(1-3)Nb + Hf/Y \sim 850-900°C Al\(_2\)O\(_3\) limit

**AFA**: Fe-(20-25)Ni-(14-15)Cr-(2.5-3.5)Al-(1-3)Nb base \sim 750-800°C Al\(_2\)O\(_3\) limit

**AFA**\(^{\text{LN}}\): Fe-12Ni-14Cr-2.5Al-0.6Nb 
\sim 650°C Al\(_2\)O\(_3\) limit

- Superior corrosion resistance without loss of creep resistance
- Properties approaching Ni-base alloys at stainless steel cost
- Key is Nb: promotes Al\(_2\)O\(_3\) and strengthens via nano NbC
Processing & Character of Oxide Dispersion Strengthened Steels

After Kimura, Kyoto University
Nano-structured Yttrium-Titania Pyrochlore Precipitates Improve High-Temperature Strength

After Kimura, Kyoto University

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Graphs showing the tensile stress and strain for different materials under irradiation. The graphs indicate improved high-temperature strength after irradiation with nano-structured Yttrium-Titania Pyrochlore precipitates.
Recent research suggests high-strength steels that retain high-toughness are achievable

- Generally obtained by producing high density of nanoscale precipitates and elimination of coarse particles that serve as stress concentrator points

![Graph showing fracture toughness vs. ultimate tensile strength](image)

- 1st and 2nd generation steels (HT9, 2 1/4Cr-1Mo, etc.)
- Ultra high strength steels (nanocomposited ODS, Aermet, etc.)
The Case for Multiscale Modeling as a Complement to Empirical Approaches for Accelerated Development of Future Structural Steels
Multi-scale Modeling Strategy

- Continuum Mechanics
- Statistical Mechanics
- Dislocation Dynamics
- Monte Carlo
- Classical MD
- Quantum Mechanics

Space

- m
- mm
- μm
- nm

Time

- fs
- ps
- ns
- μs
- ms
- s
- ks

σ = 165 Mpa
Advances in Computational Materials Science
Enabled Fundamental Understanding of Plasticity & Fracture

- Force on dislocations
  \[ f = f_s + f_{\text{img}} + f_{PK} \]
  \[ f_{PK} = \sigma \cdot b \times t \]

- Equation of motion for dislocation segments
  \[ K \frac{dQ}{dt} = F \]
  \[ F = \sum_{j=1}^{N} f_j \quad f_j = \int_{\Gamma_j} Cf \mid ds \mid \]
  \[ K = \sum_{j=1}^{N} k_j \quad k_j = \int_{\Gamma_j} C^T BC \mid ds \mid \]

N.M. Ghoniem, S.-H. Tong, L.Z. Sun, 

Velocity of dislocations
DD Simulations of Plasticity

Experimental Validation of Plasticity Models & Size Effects

Motivation:
- Model the plastic deformation of micron and submicron-size single crystals to study size effects.

Objectives:
- Study the crystal-size dependence of the stress versus strain response based on statistical analysis for nickle-micropillars oriented for single slip using 3D parametric dislocation dynamics coupled with the boundary element method.
Simulated Stress-Strain & Pillar Deformation

Solid lines (high load sensitivity): \( \dot{\sigma} = E (\dot{\varepsilon} - \dot{\varepsilon}^p) \)  
Dashed lines: low load sensitivity \( \dot{\sigma} = \begin{cases} E (\dot{\varepsilon} - \dot{\varepsilon}^p), & \text{for } \dot{\varepsilon}^p \leq \dot{\varepsilon} \\ 0, & \text{for } \dot{\varepsilon}^p > \dot{\varepsilon} \end{cases} \)

Engineering Stress (MPa) vs. Engineering Strain (%)

Experimental and Simulation Results

Flow Strength (MPa) vs. Pillar Diameter (nm)

- Computer simulation results
- Frick et. al (2008)
- Dimiduk et. al (2005)

Slope = -0.69

\[ \beta = 21 & \theta = D/25 \]

Bulk strength

Slope = -0.64
Dislocation-Precipitate Interaction for Alloy Design

- Alloy design (ex. Precipitation strengthening)
  - Dislocation-precipitate interactions
  - Elastic interaction and coherency strain
    - Solved by Takahashi and Ghoniem
  - Dislocation core effects
    - Essential to make accurate investigations of the dislocation-precipitate interactions

• Dislocation-precipitate interaction problem

Formulation

Dislocation Problem  
Solved by PDD

Correction Problem (Precipitate Problem)  
Solved by BEM

Superposition Principle
Effect of Elastic Shear Modulus Mismatch

Critical shear stress, CSS ($\tau/\tau_0$)

$d=5\text{nm}$
$d=7.5\text{nm}$
$d=10\text{nm}$

Orowan looping

(L=50nm)
Advances Have been Made to Couple Ab Initio and Continuum Methods for Alloy Design

- The lattice resistance to slip is modeled with Ab initio Density Function Theory (DFT).
- Peierls-Nabarro continuum model is coupled with DFT calculations to determine the core structure of dislocations.
- Image forces, coherency strains, and changes in lattice resistance between matrix and precipitates are modeled in 3-D geometry.
Ab Initio – PDD simulations of \( \text{Y}_2\text{O}_3 \) Interaction with Dislocations

- The \( \gamma \)-surface energy of Fe-O interface is much larger than that of Fe-Y.
- The \( \gamma \)-surface energy of \( \text{Y}_2\text{O}_3 \) has a strong dependence on the slip system.
Simulation conditions (3D-DD)

- The position of slip plane is changed upward and downward (y/D).
- See the influence of the coherency strain.

Y$_2$O$_3$ particle
Diameter (D) = 5nm
Interaction between a dislocation and Y$_2$O$_3$ precipitate in iron (y/D=0.3)

This part is repulsive with ppt. (Influence of coherency strain)

The dislocation start to go around the ppt.

This part is ATTRACTIVE with ppt. The character of the dislocation is changed from the initial.

It is easy for dislocations to complete the Orowan Mechanism.
Critical Resolved Shear Stress

The strength increases as the position of slip plane is shifted downward.

The strength rapidly decreases as the position of slip plane is shifted upward.

Maximum strength does not appear at the center.

These trends must result from the combination of Orowan mechanism and the influence of coherency strain.
➤ Design of radiation-resistant materials is evolving from empirical rules to a science-based approach;

➤ Multiscale Modeling is being integrated with empirical data for accelerated alloy development;

➤ The problem of strength-ductility optimization of advanced steels is a great computational challenge: several advances have been made

➤ The general problem of optimum steel design is still open for many advances.