Multiscale Modeling of Radiation Damage in Fusion Reactor Materials

Brian D. Wirth, R.J. Kurtz (PNNL), N.M. Ghoniem (UCLA), G.R. Odette (UCSB), D. Srolovitz (Princeton), R.E. Stoller (ORNL), H.M. Zbib (WSU) and S.J. Zinkle (ORNL)

DOE OFES Budget Meeting
Science in Technology Seminar
12 March 2002

This work was performed under the auspices of the U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.
Presentation overview

• Introduction to fusion reactor materials and radiation damage processes

• Multiscale modeling approach

• Microstructure evolution in bcc alloys under low to intermediate temperature (T < ~450°C) irradiation
  - Self-interstitial cluster properties, growth and accumulation of dislocation loops
  - Formation of sub-nanometer vacancy-solute clusters

• Impact of microstructure on mechanical property & performance
  - Dislocation - defect interactions
  - Constitutive & mechanical property modeling

• Summary & future directions
Fusion materials science program

- Similar philosophy for Fusion materials & plasma science programs

<table>
<thead>
<tr>
<th>Basic Goal</th>
<th>Fusion Plasma Science</th>
<th>Fusion Materials Science</th>
</tr>
</thead>
<tbody>
<tr>
<td>Understand 4th state of matter as it relates to fusion</td>
<td>Understand 1st state of matter as it relates to fusion</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Key Issues</th>
<th>Fusion Plasma Science</th>
<th>Fusion Materials Science</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Basic properties and microscopic phenomena</td>
<td>- particle/energy confinement and transport</td>
<td>- defect properties, dislocation propagation, phonon transport</td>
</tr>
<tr>
<td>- System properties and macroscopic phenomena</td>
<td>- MHD stability</td>
<td>- microstructural stability</td>
</tr>
<tr>
<td>- Creation and sustainment</td>
<td>- plasma - wave interactions</td>
<td>- fracture and deformation</td>
</tr>
<tr>
<td>- Interactions with environment</td>
<td>- plasma-wall interactions</td>
<td>- physical metallurgy and thermodynamics</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- corrosion and compatibility; radiation effects on materials</td>
</tr>
</tbody>
</table>
Fusion materials research must rely heavily on modeling due to inaccessibility of fusion-relevant operating regime.

- Extrapolation from currently available parameter space to fusion regime is much larger for fusion materials science than for plasma physics program.
Radiation damage processes

Lack of intense neutron source emphasizes the need for co-ordinated experiment, modeling & theory to develop fundamental understanding of radiation damage.
Low T (< ~450°C) irradiated microstructures

- Dominant microstructural features in irradiated bcc (ferritic/martensitic & Vanadium-based) alloys:
  - nm dislocation loop-complexes
  - nm precipitates
  - sub-nm bubbles & voids, grow w/increasing radiation dose

<table>
<thead>
<tr>
<th>&lt;d&gt; (nm)</th>
<th>N (m⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;100&gt;</td>
<td>20</td>
</tr>
<tr>
<td>&lt;111&gt;</td>
<td>30</td>
</tr>
</tbody>
</table>

Loop decoration of dislocations & raft formation
Multiscale modeling approach

**Molecular Dynamics**
- Point defect migration properties
- V cluster and void binding
- V loop energetics and kinetics
- defect-dislocation interactions
- defect-GB interactions
- dislocation-obstacle interactions

**Damage Accumulation Models**
- Impurity segregation and precipitation
- Primary damage state

**Ab initio**
- New interatomic potentials
- vacancy-impurity and vacancy-He interaction

**Kinetic Monte Carlo**
- Defect escape probability from cascades

**Rate Theory**
- Rate of damage accumulation
- Rate of void swelling
- Rate of impurity segregation and precipitation

**Experiments**
- Mechanical Property Changes: Embrittlement, hardening, toughness

**3D Dislocation Dynamics**

**Finite Element Modeling**

**Experiments**

**Multiscale modeling approach**

**nm**

**ps**

**m**

**msec**

**years**
Computational microscope

Experimental characterization

TEM

APT

SANS

PAS

feature ‘signals’

Multiscale modeling

self-consistent ‘understanding’

TEM, SANS, Positron theory

Apply complementary experimental measurements, closely coupled to modeling and positron theory
Ab-initio calculations lead to improved V potential

- Different EAM type potentials give very different predictions for Vanadium
- None of the EAM potentials correctly predict the stable form of the interstitial
- New interatomic Vanadium potential fit to experimental data and 1st principles calculations of: cohesive energy, bulk modulus, $C_{11}$, $C_{12}$, $C_{44}$, and vacancy formation energy

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>First Principles</td>
<td>2.60</td>
<td>3.57</td>
<td>3.48</td>
<td>3.14</td>
<td>3.15</td>
<td>3.62</td>
<td>3.69</td>
</tr>
<tr>
<td>Finnis-Sinclair</td>
<td>2.63</td>
<td>3.60</td>
<td>3.66</td>
<td>3.25</td>
<td>3.21</td>
<td>3.60</td>
<td>3.64</td>
</tr>
</tbody>
</table>

$\rightarrow$ stable interstitial

- Very good agreement with 1st principles calculations
- Split [111] interstitial is most stable

Units: eV
MD simulations of primary damage production

20 keV cascade in iron at 100K

self-interstitial atom

vacancy

R. E. Stoller, ORNL

5 nm
Self-interstitial clusters: <111> loops

- Stability of <111> self-interstitial atom (SIA) clusters revealed by recent atomistic modeling (*Finnis-Sinclair and EAM-type interatomic potentials*)

MD simulations at T=560 K reveal rapid ($E^m < 0.1$ eV) 1-D migration

- Form highly kinked, proto-<111> dislocation loops directly in cascades
- Migrate in 1-dimension with high mobility
Reaction Kinetics of Interstitial Clusters and Void Lattice Formation

Clusters of self-interstitial atoms (SIA) formed in cascades have 1D/3D defect reaction kinetics.

Void lattices form under high doses of cascade-producing irradiation.

Kinetic Monte Carlo computer simulations demonstrate that irradiation producing 1D/3D SIA clusters can lead to void ordering.

- SIA clusters having 1D/3D reaction kinetics are a primary ingredient of the Production Bias Model rate theory that links atomistic defect production to microstructure evolution under irradiation.
- Modeling studies show that the 1D/3D kinetics of SIA clusters are essential for void lattice formation and stability.

Void lattice in Mo, Evans et al., 1971

Extremely mobile interstitial clusters diffuse by 1D/3D migration, with average 1D path length L

U.S. Department of Energy
Pacific Northwest National Laboratory
Dislocation loop formation in ferritic steels

• New insight: \( <100> \) junctions form through interaction of highly mobile, \( <111> \) loops:

\[
\frac{a_o}{2} [111] + \frac{a_o}{2} [1 \bar{1} \bar{1}] \rightarrow a_o [100]
\]

• Large density of \( <100> \) loops observed (TEM) at high dose

- Junction propagates or dissolves by 2-step mechanism

Energy landscape favors \( <100> \) growth
Growth mechanisms of \(<100>\) loops

- Despite being metastable with respect to \(<111>\) loops, \(<100>\) loops grow by absorption of smaller \(<111>\) loops

\[
\langle 100 \rangle + 2 \frac{1}{2} \langle 111 \rangle \rightarrow \langle 211 \rangle \rightarrow \langle 100 \rangle
\]

- Atoms shown in white, are rotating to join the \(<100>\) loop according to above reaction
Dislocation decoration & rafting

Decoration

SIA Cluster Interaction with Dislocation Demonstrating the Importance of Cluster Rotation on Dislocation Decoration
50 keV cascade aging in Fe at 563 K

- Rapid formation of sub-nanometer 3-D clusters
- Small clusters are mobile and cluster growth often involves coalescence

Vacancy cluster evolution movie

\[5 \text{ nm}\]
Validation of sub-nm vacancy-solute clusters

Positron annihilation spectroscopy

Predicted positron lifetimes

Vac/Cu \( \tau \) (ps)
- 3/6  173
- 4/6  216
- 17/5  350
- >50/x  520

Measured positron lifetimes

KMC predicts vacancy-Cu clusters

\( \tau \) (ps) - 60°C
- 178
- 355

\( \tau \) (ps) - 288°C
- 222
- 520
Summary of nanostructural evolution

• Radiation damage produces primary defects (vacancies & self-interstitials) in highly non-equilibrium, spatially correlated process

• Self-interstitial clusters in Fe-alloys formed with a/2<111> Burgers vector, undergo easy 1-dimensional glide

• At high dose (> ~0.1 dpa) in Fe-alloys, collisions between <111> loops result in the formation of dislocation loops with Burgers vector a<100>

• <111> loops which escape collision migrate to dislocations forming loop rafts which decorate dislocations

• Remaining vacancies cluster to form small 3-dimensional nanovoids
Impact on mechanical properties

- Irradiation-produced nanostructures impede dislocation motion & significantly impact mechanical properties & structure performance
  - hardening, decreased ductility, yield drops and dislocation channeling

**Load-Elongation Curves for V-4Cr-4Ti**

- Irradiated in HFBR to 0.5 dpa

---

**Dislocation channeling in V-4Cr-4Ti**

- \( T_{\text{test}} = T_{\text{irr}} = 270^\circ C \)
Edge dislocation - SFT interaction (Cu)

- Atomistic (MD) simulations of individual dislocation - obstacle interactions provide fundamental understanding of radiation hardening and flow localization phenomena.

![Dislocation Diagram]

**EAM Cu:**

- $(10^{10} \text{ Pa})$
- $c_{11} = 17.6$
- $c_{12} = 12.9$
- $c_{44} = 8.23$
- $\mu = 5.88$
- $\gamma_{\text{SFE}} = 11.40 \text{ mJ/m}^2$

- Dislocations inserted and equilibrated at 100 K, SFT inserted across the glide plane and shear stress applied to move the dislocation.
Dislocation - SFT interaction (300 MPa) near \(<111>\) projection

- SFT is a relatively strong obstacle $\phi \sim 80^\circ$
- SFT sheared but neither absorbed or destroyed
Decouple Multiscale Localization Mechanisms

- Isolate and properly integrate multiscalar parts - and determine what controls observables

Microconstitutive
dislocation-obstacle
interactions and
processes controlling
local $\sigma_{crss}(\varepsilon_{local})$

$\sigma_{crss}$
softening
hardening

$\Delta x - \varepsilon_{local}$

Micromechanics
deformation patterns
and localization-
depend on $\sigma$, $\sigma$-state
redistribution

Continuum
Mechanics
large geometry-
change deformation &
load- instability-
necking
Understanding Loss of Uniform Strain Capacity

- Assessment of engineering tensile data to demonstrate a modest true-strain softening, persistence of irradiation hardening and applicability of $J_2$ incremental plasticity theory
Micromechanics of Universal MC Shape & Shifts

Atomic scale dislocation-bond breaking processes modeled as the basis for the existence of a universal master toughness-temperature shape and magnitude of the shift due to irradiation hardening

New intrinsic property of bcc structures?
Summary & future focus

- Radiation damage is inherently multiscale phenomena - US Fusion Materials program applying multiscale modeling, closely coupled with theory & experiments to develop *fundamental understanding of radiation damage in structural alloys*

- Examples of radiation damage in bcc alloys at $T <\sim 450^\circ C$
  - nanostructural dislocation loop evolution
  - sub-nanometer vacancy cluster formation
  - effect of nanometer defect clusters on dislocation motion (hardening)
  - impact of radiation hardening on deformation & failure

- Future focus -> Investigate the impact of high He production rates on bcc alloy material evolution, properties and performance
Displacement Fields of Helium in Iron

Point defect displacement fields are well approximated by line force dipoles. Fits of atomistic He displacement fields to dipole equations enables calculation of interaction energies and forces between helium atoms and other microstructural features at higher length and time scales.

Schematic of displacement field represented by a line force defect (unequal force dipoles) and separation into dilatant center (equal force dipoles) and dipole part (equal but opposite force dipoles).

3D view of He interstitial displacement field showing a multi-lobed shape that is a characteristic of the octahedral site and the elastic anisotropy of Fe.

U.S. Department of Energy
Pacific Northwest National Laboratory
Mechanisms of Dislocation Unlocking from Cluster Atmospheres

$Z=D=40, L=50, b=1/2(-101), \text{Stress} = 200 \text{ MPa, Attractive Clusters}$