Integration of Modeling, Theory and Experiments for Fusion Reactor Materials

Roger E. Stoller
Oak Ridge National Laboratory

ReNew: Harnessing Fusion Power Workshop
Los Angeles, CA
March 2 - 4, 2009
Role of Modeling and Experiments in the US Fusion Reactor Materials Program

• not a new initiative
  – integrated program effort has been a priority for many years, e.g. “A Whitepaper Proposing An Integrated Program of Theoretical, Experimental, and Database Research for the Development of Advanced Fusion Materials,” R. E. Stoller, G. R. Odette, and H. L. Heinisch, 1999

• focus on example of helium effects
• comment on recent applications
• role going forward
Schematic diagram: relevant phenomena and computational methods

Phenomena

- Collisional phase
- Annealing phase
- Defect/solute diffusion
- Microstructure evolution
- Quenching
- Single displacement cascade
- Multiple cascades, cascade overlap
- Defect and solute migration and clustering
- Void swelling, hardening, embrittlement, creep, stress corrosion cracking, ...

Methods

- Molecular dynamics
- Kinetic Monte Carlo
- Finite element
- Reaction rate theory
- 3D dislocation dynamics

APFIM, PAS, SANS, TEM

10^{-14} s, 10^{-11} s, 10^{-8} s, 10^1 s, 10^4 s, >10^6 s

TEM, volume and mechanical property measurements

Engineering design
Why is an integrated approach essential to understanding radiation damage in structural materials?

• Although irradiation experiments cannot be replaced by modeling alone, a purely experimental approach to understanding the effects of irradiation is also not practicable
  ▪ costs for design and execution of reactor irradiations
  ▪ costs of post-irradiation examination of radioactive materials
  ▪ declining facilities for both irradiation and examination
  ▪ **combinatorial problem:**
    – broad range of materials, phenomena, and irradiation conditions, coolants, temperature, loading conditions, dose rate, dose

• Recent advances in computational materials science (hardware and methods) and experimental techniques (LEAP, FIB, high brightness neutron and photon scattering sources) expand the range of possible direct comparisons between simulations and experiments
Why is He/dpa ratio an important parameter for fusion materials R&D?

- He generation can alter the path of microstructural evolution in irradiated materials (particularly for >100 appm He)
  - Cavity formation (matrix and grain boundaries)
  - Precipitate and dislocation loop formation

He bubbles on grain boundaries can cause severe embrittlement at high temperatures

Swelling in stainless steel is maximized at fusion-relevant He/dpa values

Management of transmutant He (e.g. trapping at engineered 2nd phases) is a key issue for fusion materials
Swelling can eliminate materials from consideration

Current fusion candidate alloys not immune to He effects:
HFIR irradiation at 400°C to 51 dpa, E. Wakai, et al. JNM (2000)

F82H (36 appm He)
10B-doped F82H (330 appm He)
Example from current work on He effects

- involves several institutions: UCSB, UCB, PNNL, ORNL
- experiments involve DOE-JAEA irradiation experiments in HFIR
- range of experimental and computational methods
  - ab initio-based development of interatomic potential for He-Fe, molecular dynamics, mean field reaction rate theory, KMC
  - next generation FM ODS steels with high density of nanometer-sized oxide clusters, APFIM, SANS, FIB-prepared TEM specimens from neutron irradiation, thermal helium desorption spectrometry of He-implanted iron specimens
**THDS Experiments**

**Instrument**
- UHV (ultra-high vacuum) sample and measurement chambers, with P~$10^{-10}$ Torr (at room temperature)
- quadrupole mass spectrometer
- tungsten crucible sample holder
- radiative heating with tungsten filament

**Specimens**
- High purity (~99.99%) single-crystalline iron implanted with 5, 10 keV He to $10^{14}$ and $10^{15}$ He/cm$^2$

**SRIM/TRIM predictions**
- He peak production ~25 nm
- V-I peak production ~12 nm
- 20 vac/He

![Graph showing damage and He concentration vs. depth](Image)
Rate-theory based modeling: initial results of cluster dynamics modeling

Data fit improved by parameter optimization, comparisons with atomistic simulations
Behavior of different He-Fe potentials

- New He-Fe potential developed, fit to *ab initio* (VASP) data on He defects in iron
  - Both forces and energies fit
  - Large defects such as $\text{He}_3\text{V}$ calculated with up to 128 atoms
- Must predict tetrahedral site as most stable site for He
  - Difficult with pair or EAM functional forms, so 3-body form used
- Old Wilson pair potential creates SIA (and vacancies) more easily than new three-body potential
- Juslin-Nordlund pair potential does not create He-vacancy clusters.
Impact of boundaries in He-Rich Environments

- Reduced activation ferritic-Martensitic steels are candidate first-wall/blanket structural materials for fusion power systems.

- A unique aspect of the DT fusion environment is substantial production of gaseous transmutants such as He and H. (~1500 appm He/150 dpa)

- Accumulation of He can have major consequences for the integrity of fusion structures such as:
  - Loss of high-temperature creep strength.
  - Increased swelling and irradiation creep at intermediate temperatures.
  - Potential for loss of ductility and fracture toughness at low temperatures.

- Trapping at a high-density of tailored interfaces is a key strategy for management of He.

He is essentially insoluble and forms bubbles in the matrix at dislocations and particles or at grain boundaries.
Characterize He Migration Energy along dislocations and in grain boundaries using atomistic simulations

Calculated Defect Migration Energies, eV

<table>
<thead>
<tr>
<th>Defect Type</th>
<th>Perfect Crystal</th>
<th>Screw Dislocation</th>
<th>Edge Dislocation</th>
<th>Σ3 / Σ11 GBs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interstitial He atom</td>
<td>0.08</td>
<td>0.40</td>
<td>0.40</td>
<td>0.46 / 0.47</td>
</tr>
<tr>
<td>Vacancy</td>
<td>0.78</td>
<td>0.43</td>
<td>-</td>
<td>0.48 / 0.74</td>
</tr>
<tr>
<td>Divacancy</td>
<td>0.89</td>
<td>0.82</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>He-Divacancy</td>
<td>1.13</td>
<td>1.11*</td>
<td>-</td>
<td>0.90 / 0.92</td>
</tr>
</tbody>
</table>

*Potentially unstable

- From saddle point energies determined using the Dimer method.
- Corroborated in several cases by “long time” MD simulations.
**In Situ He Injection Experiments**

- Use $(n,\alpha)$ reactions (Ni, B, Li ..) in mixed spectrum reactors to produce controlled He/dpa for fusion relevant conditions.
- Avoids confounding properties and irradiation effects in doping.
- Applicable to any material - e.g., SiC and a variety of specimens.
- Layer thickness and composition varies He/dpa ratio with dose
- Obtain several $\mu$m of uniform He implantation

Provide direct test of He-trapping mechanism that may reduce He effects
TEM data from FIBed specimens
Test He trapping efficiency at 9 dpa, 380 appm He at 500°C

- Both dislocation bubbles & larger voids
- Grain boundary decorated by small bubbles

- Small bubbles on 85% of oxide clusters and dislocations
- GB clear of He bubbles
Summary

Substantial progress in understanding and predicting the response of materials to fusion reactor conditions has been achieved through:

- development of relevant experimental databases, large-scale and special-purpose experiments
- continuing advances in theory and computational modeling
  - increasing scale of \textit{ab initio} calculations and large scale atomistic simulations identify new mechanisms and provide underlying support to multiscale modeling framework
  - more detailed mesoscale models enabled, improved parameter definition
  - “real” multiscale development and linking still needed where it makes sense
- enabled by close coupling of different types of experiments with a range of theory/modeling/simulation methods
Implications for Research Thrusts

The 1999 whitepaper called for an expanded effort in computational materials science that was well integrated with the experimental program which should:

– focus on the key issues in fusion materials (defined in whitepaper - see backup slide),
– include experiments designed for model validation and obtaining parameters required by the models,
– be as collaborative as possible and be leveraged by other activities,
– produce tangible useful results (e.g. more reliable predictions of properties), and finally
– provide the scientific basis for improved design and methods of structural integrity assessment.
Experimental component must include

- Focused studies of key phenomena and mechanisms, including those required for model development and validation, e.g. special experiments to understand how helium diffuses and is trapped under irradiation.
- Controlled experiments on carefully conditioned samples, specially designed to reveal the effects of material and irradiation variables, both singly and in synergistic combinations.
- Integral experiments to develop a database for alloy selection and optimization, and ultimately, engineering design.
Goal of such an effort

- provide an understanding of the behavior of candidate material systems in the fusion environment and identify limiting properties and approaches to improve performance,
- undertake the development of alloys and ceramics *(read as structural and special purpose materials)* with superior properties for service in the fusion environment through the control of composition and microstructure,
- provide the materials technology required for production, fabrication, and power system design.
List of materials issues from whitepaper

• Radiation effects Issues in structural alloys
  – Modeling radiation damage
  – Helium effects
  – Radiation induced elevations of the yield stress.
  – Static post-yield constitutive properties and deformation patterns.
  – Swelling and irradiation creep
  – Thermal creep, creep rupture and creep crack growth
  – Fast fracture and the ductile-to-brittle transition temperature (DBTT)
  – Fatigue, creep fatigue and fatigue crack growth
  – Environmentally-assisted cracking

• Silicon carbide composites
  – fiber and coating stability and the consequences to bridging mechanics,
  – hermeticity and sealing coatings
  – swelling and creep (at high helium levels)
  – radiation-induced reductions in thermal conductivity,
  – joining; and
  – the integrity of complex, thermal-mechanically loaded brittle structures.

• Other significant materials issues
  – ceramic composites and the stability and functionality of their engineered constituents
  – insulator and barrier coatings
  – corrosion and system level corrosion product transport
  – the kinetics and consequences of impurity pick-up
  – processing, fabrication and joining
  – ceramic coatings

• Issues related to development or use of alternate materials