Predicting Radiation-Induced Microstructural Change via Implementation and Validation of Multiscale Cluster Dynamics in MOOSE

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Overview

- Create a MOOSE-based application, “Geminio”, to predict & understand radiation-induced microstructural change.
- Extend MOOSE into a new field – long-term radiation damage.
- MIT is interested in contributing the completed work as a MOOSE module so that it may be coupled to multiscale simulations.
Objectives

**Current Implementation**

- **Timeline**
  - $10^6$ s: Microstructure evolution, Rate theory
  - $10^6$ s: Defects/Solute diffusion, Kinetic Monte Carlo
  - $10^{-6}$ s: Cascade annealing, Molecular dynamics
  - $10^{-15}$ s: Cascade, Binary collision approximation
  - $10^{-18}$ s: Collision

- **Study methods**
  - Microstructure evolution
  - Defects/Solute diffusion
  - Cascade annealing
  - Cascade
  - Collision

**Current Implementation**

- **Binary collision**
  - Lammmps
  - Cascade annealing
  - Defects production spectrum

- **Molecular dynamics**
  - SRIM/TRIM
  - Dose rate
  - PKA energy spectrum

- **Rate theory**
  - MOOSE
  - Evolution of defects size distribution
  - Spatial dependent
  - Computation acceleration
    - Grouping
    - Fokker-Planck

**Benefits:** Predict radiation damage on long timescale (to 100’s of DPA), guide radiation-resistant material design, explain experiments
Accomplishments

• Cluster Dynamics has been implemented in MOOSE
• Spatial dependence (for ion irradiation) is working
• Results can be linked to properties such as void swelling
• This tool would be applicable to study other phenomena described by rate theory such as precipitation

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<thead>
<tr>
<th>Task</th>
<th>Y1</th>
<th>Y2</th>
<th>Y3</th>
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<tbody>
<tr>
<td>Build kMC and CD model scaffolds</td>
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<tr>
<td>Design standardized CD dataset format</td>
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<td>✓</td>
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<td>Compile data for Si, model &amp; real materials</td>
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<td>Preconditioning &amp; HPC efficiency optimization</td>
<td>✓</td>
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<td>Validation experiments &amp; test cases</td>
<td>✓</td>
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<td>✓</td>
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<tr>
<td>Documentation, generalization, UI, module release</td>
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Accomplishments – Explaining Tungsten Self-Ion irradiation Experiments

Discussion:
- A good agreement has been achieved with experiment
- The break of power-law originates from the mobility of SIA clusters even at very low temperature (30K)
- Provides alternative explanation for TEM-observed cluster sizes

- Publication under re-review in Journal of Nuclear Materials
Next Step – Spatial Dependence

- Swelling behavior in Fe

Experiment condition:
- 450 C
- 3.5 MeV Fe\(^{++}\) self-ion irradiation
- Peak dose rate: 4.6\(\times\)10\(^{-3}\) dpa/s

Future Focus – Direct Link to Rapid Radiation Measurements

Transient grating spectroscopy

MD simulated signal

Follow-on funding to be sought from NSF, DOE-BES

Status, Variances, Changes

- Heavy use of Fission supercomputer at INL HPC
  - No other resources used or needed
  - Will use Short lab’s transient grating spectroscopy (TGS) system, SEM/FIB & TEM for experiments

- No variances, no changes in scope or budget

- On schedule, on budget