Defect Structures Induced by High-energy Displacement Cascades in $\gamma$ Uranium

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Background

Metallic Uranium Fuel

- Metallic uranium and its alloys (e.g. U-Mo, U-Zr)
  - Candidates for next-generation fast-neutron reactors
- Advantages (Compared to Ceramic Fuels)
  - Higher thermal conductivity → lower operating temperature
  - Better neutron properties
  - Easy fabrication and processing
  - Metallurgical bonding with cladding
- Major Challenge
  - Radiation Tolerance

Background

Properties of γ Uranium

- **Stable Phases of Metallic Uranium (Akella et al., 1997)**
  - At ambient pressure
  - $T<935\text{K}$, $\alpha$ (face-center orthorhombic)
  - $935\text{K}<T<1045\text{K}$, $\beta$ (body-center tetragonal)
  - $T>1045\text{K}$, $\gamma$ (body-center cubic)
- **γ-U is the HT stable phase**
  - Stable phases of U-Mo and U-Zr alloy fuels
- **Thermal Conductivity**
  - $\lambda\approx 43.4\text{Wm}^{-1}\text{K}^{-1}(\beta, 1000\text{K}; \text{Takahashi et al., 1988})$
  - compared to $\lambda_{\text{urania}} = 3.2\text{Wm}^{-1}\text{K}^{-1}(1051\text{K}; \text{Ronchi et al., 1999})$
Methodology

Atomic Potentials

- **MEAM Potential** (Beeler et al., 2012)
  - f-electron behavior
  - Expand to U-Zr alloys
  - Stable as T>800K
  - Atomic interactions during cascades
- **EAM Potential** (Belashchenko et al., 2008)
  - Stable at low temperature
  - Analyses of defect structures
- **ZBL Potential**
  - Ballistic Collisions

### Parameters and Values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_c$ (eV)</td>
<td>5.27</td>
<td>Cohesive energy of α/γ/fcc</td>
</tr>
<tr>
<td>$R_e$ (Å)</td>
<td>4.36</td>
<td>Lattice constant of γ</td>
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<tr>
<td>$\alpha$</td>
<td>5.1</td>
<td>Bulk modulus of γ</td>
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<tr>
<td>$A$</td>
<td>1.04</td>
<td>Relative stability of α and γ</td>
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<tr>
<td>$\beta^{(0)}$</td>
<td>6.0</td>
<td>Relative stability of fcc and γ</td>
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<tr>
<td>$\beta^{(1)}$</td>
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<td>Shear elastic constants of α</td>
</tr>
<tr>
<td>$\beta^{(2)}$</td>
<td>7.0</td>
<td>Shear elastic constants of α and γ</td>
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<td>$\beta^{(3)}$</td>
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<td>$t^{(1)}$</td>
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<td>Vacancy formation energy in γ</td>
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<td>$t^{(2)}$</td>
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<td>Shear elastic constants of α and γ</td>
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<td>$t^{(3)}$</td>
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<td>Atomic volume of α</td>
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<td>$\delta$</td>
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<td>Thermal expansion of γ</td>
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<td>$C_{min}$</td>
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<td>Cohesive energy of α/γ/fcc</td>
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<tr>
<td>$C_{max}$</td>
<td>1.9</td>
<td>Cohesive energy of α/γ/fcc</td>
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</tbody>
</table>
Methodology

Displacement Cascades

- 1keV~50keV PKAs
- Averaged direction <135>
- $T=1045K$ (stable $\gamma$ phase)
- $50^3$, $80^3$ and $100^3$ unit cells
- 500ps NpT equilibrium
- NVE/NVT cascade evolution
- full relaxation (up to 1ns)
Results

Energy Influence on the Cascades

1keV PKA
50×50×50 supercell
cascade region ~3.5nm
several picoseconds

50keV PKA
100×100×100 supercell
cascade region ~15nm
several hundreded picoseconds
Results

Melt Zone

• Core of the cascade region
  • 50keV PKA
  • $r=10.8\text{nm}$

• Radial Distribution Function
  • Liquid phase as $t<100\text{ps}$
  • Solidification during relaxation

• Low density during melting stage
Results

Typical Defect Configurations

- Octahedral SIAs
  - Minor Form of SIAs
  - Dispersive Distribution

- Separate Vacancies
  - Favored for LE PKA

- Separate Dumbbells
  - \(<100>, \langle110\rangle, \langle111\rangle\)
  - Major Form of SIAs
  - Dispersive Distribution

- One Large Void
  - Major Form of Vacancies
  - Center of Cascade Region

A Typical Defect Configuration
- 50keV PKA, 1045K Displacement Cascade
- 1000ps Relaxation

Crowdions
- Very Rare
Results

PKA Direction Effect

- 4 different PKA directions
  - <100>, <110>, <111>, <135>
- Direction effect is marginal
  - 1keV is high enough to eliminate direction effect
- <135>: averaged direction
  - Used in cascades with higher energy PKAs
Results

Survival Defects vs PKA Energy

- Survival defect population vs PKA energy
  - Non-linear; power function
- Compared to NRT displacement model
  - Survival portion decreases as PKA energy rises
Results

SIA-Type Defect Structures

- 4 types of SIA defects are commonly observed
- Crowdions are rarely formed
- Almost all the SIAs are separate
- Small clusters are found only in 50keV cascades
Results

Vacancy-Type Defect Structures

- Most vacancies exist as voids
- Void size rises with PKA energy
- Facet Shape with \{110\} faces
Conclusions

- 1~50keV PKAs were introduced for HE cascade simulations
- Direction effect is marginal as $E_{PKA} > 1$keV
- SIA-type structures
  - $<100>$, $<110>$, $<111>$ dumbbells and octahedral SIA
  - Separate; no prominent clustering except for 50keV
- Vacancy-type structures
  - Facet shape with $\{110\}$ faces
Future Focuses

- Finish more 50keV cascades for better statistics
- Further investigation of SIA clusters formed in 50keV cascades
- Temperature effects
- Expand to alloy systems (U-Zr, U-Mo)
- Include fission gas (Xe)
Thanks!
Questions?