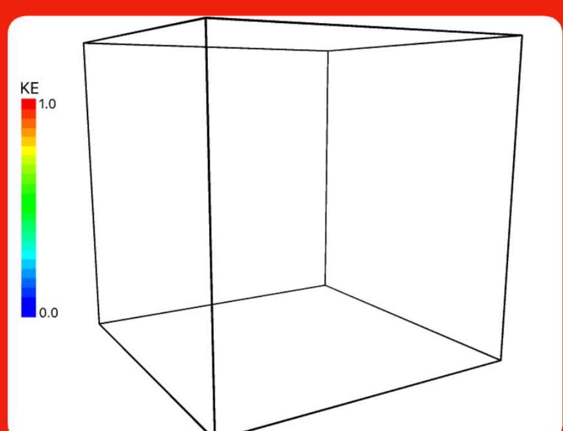
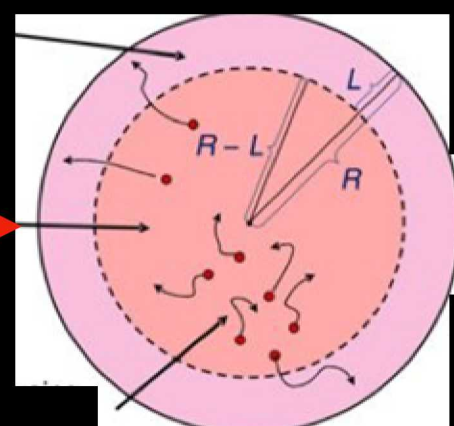
This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2019-9457C

Reduced-Order Atomistic Method for Simulating High Dose Irradiation in Metals





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Sandia National Laboratories

SAND2019-XXXX PE

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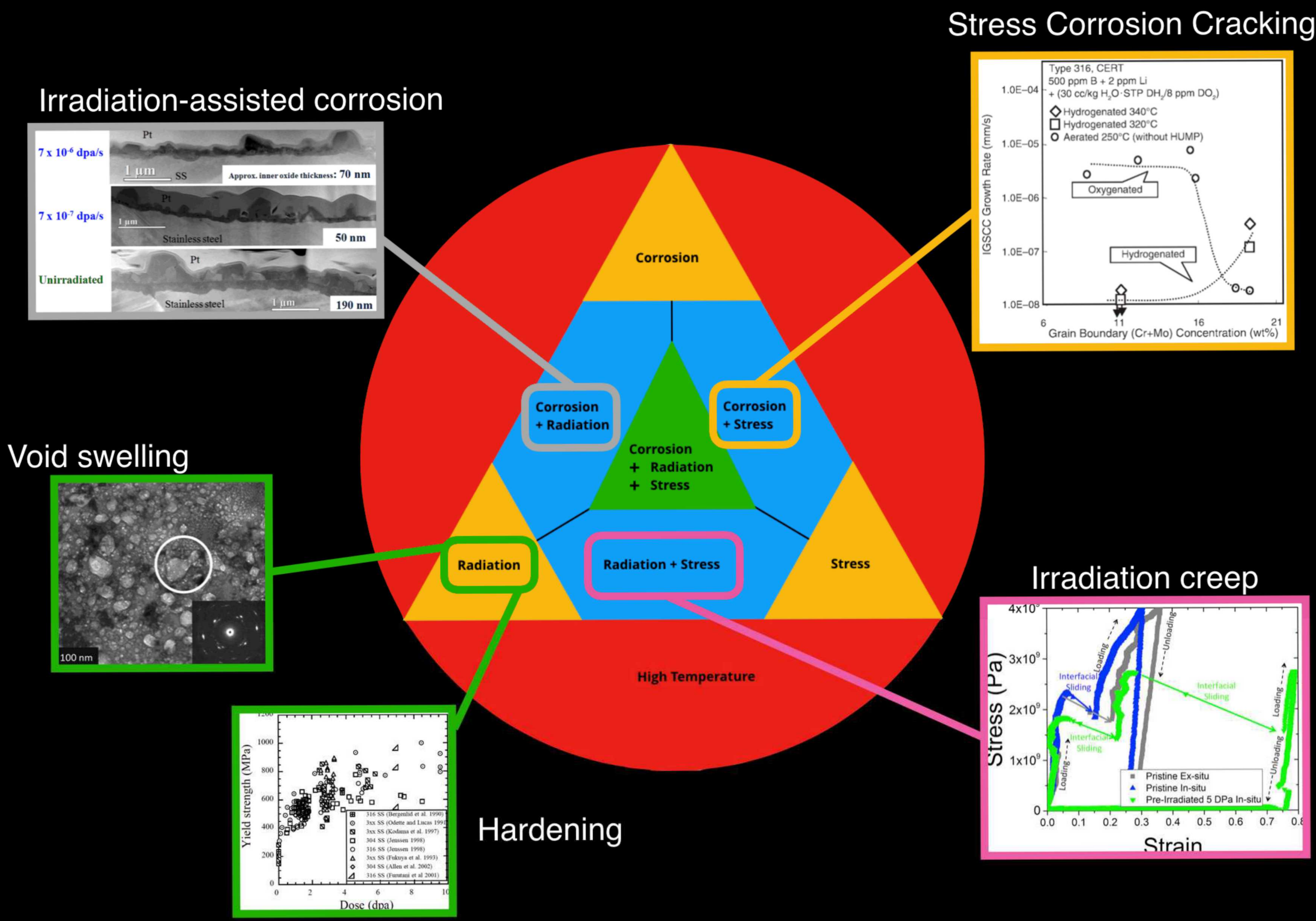
Materials Aging & Degradation in Extreme Environments



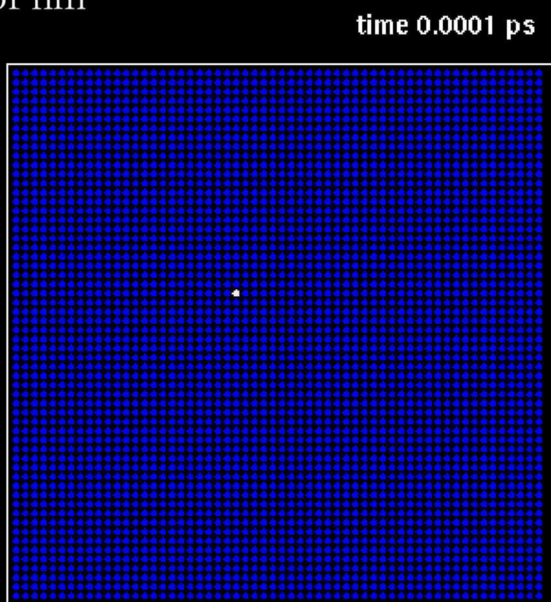
"The only source of knowledge is experience."

— Albert Einstein (1879-1955) —

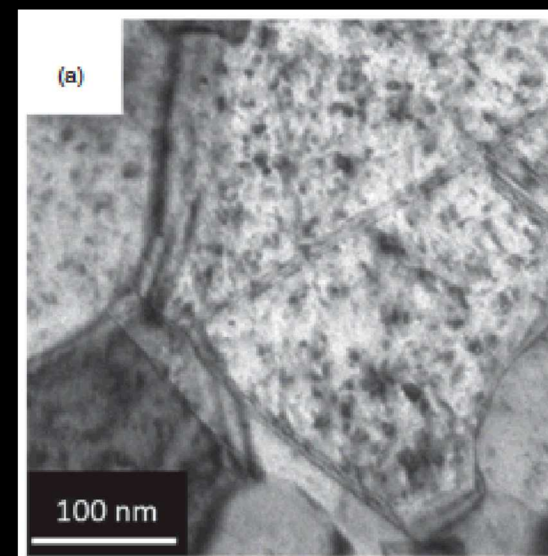
Radiation damage and aging

Picoseconds — Microseconds - Days — Seconds - Years

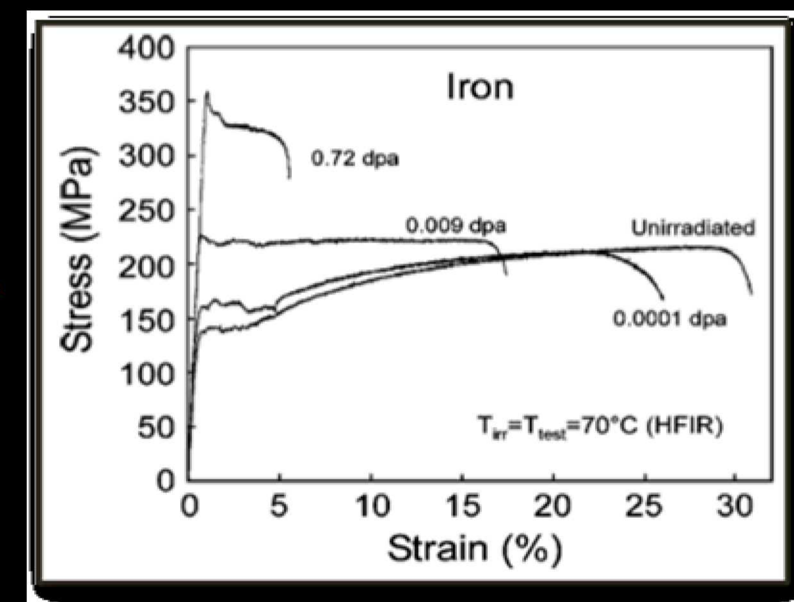
Tens of nm — Hundreds of nm - Hundreds of μm — cm - m



Nordlund (2008)



Muntifering et al. (2015) *Mater Res Lett.*



Eldrup (2002) *J. Nucl. Mater.*

"Special" Physics

- keV-energy collision between nuclei
- Energy loss to electronic excitation
- Transition to high P-T
- Long term relaxation

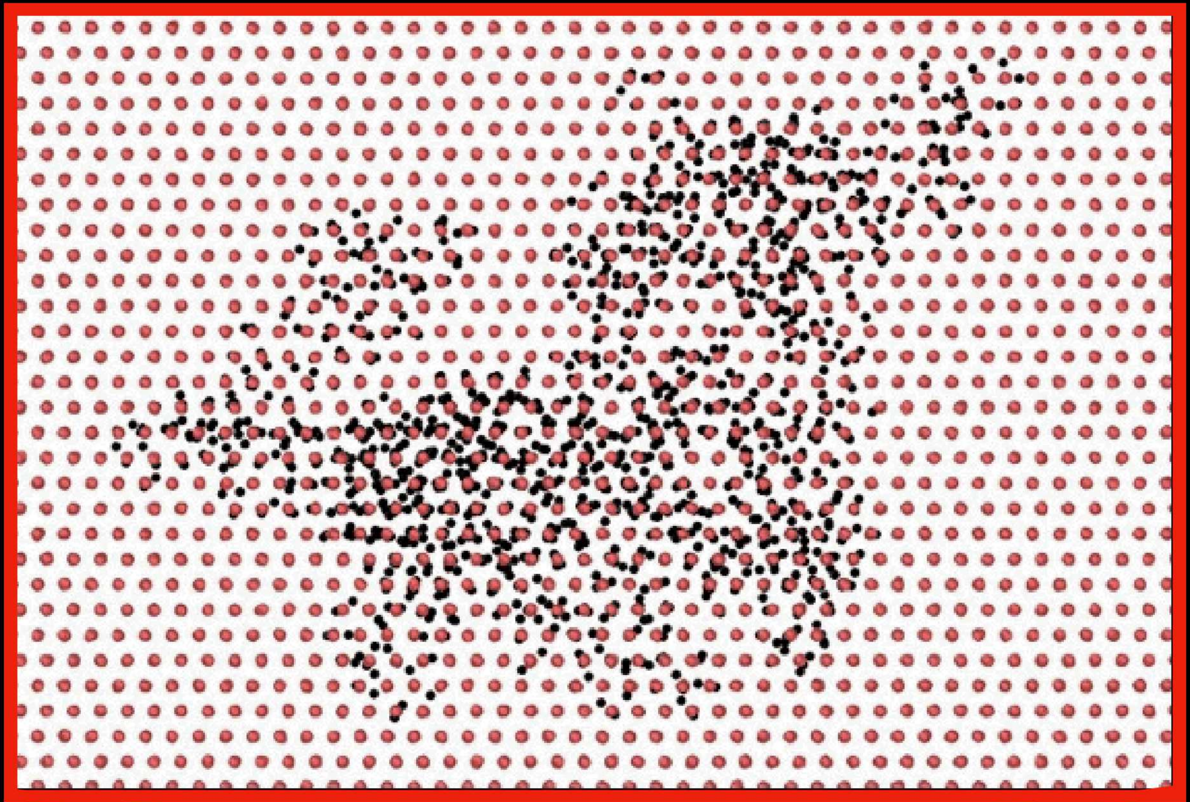
Radiation Damage

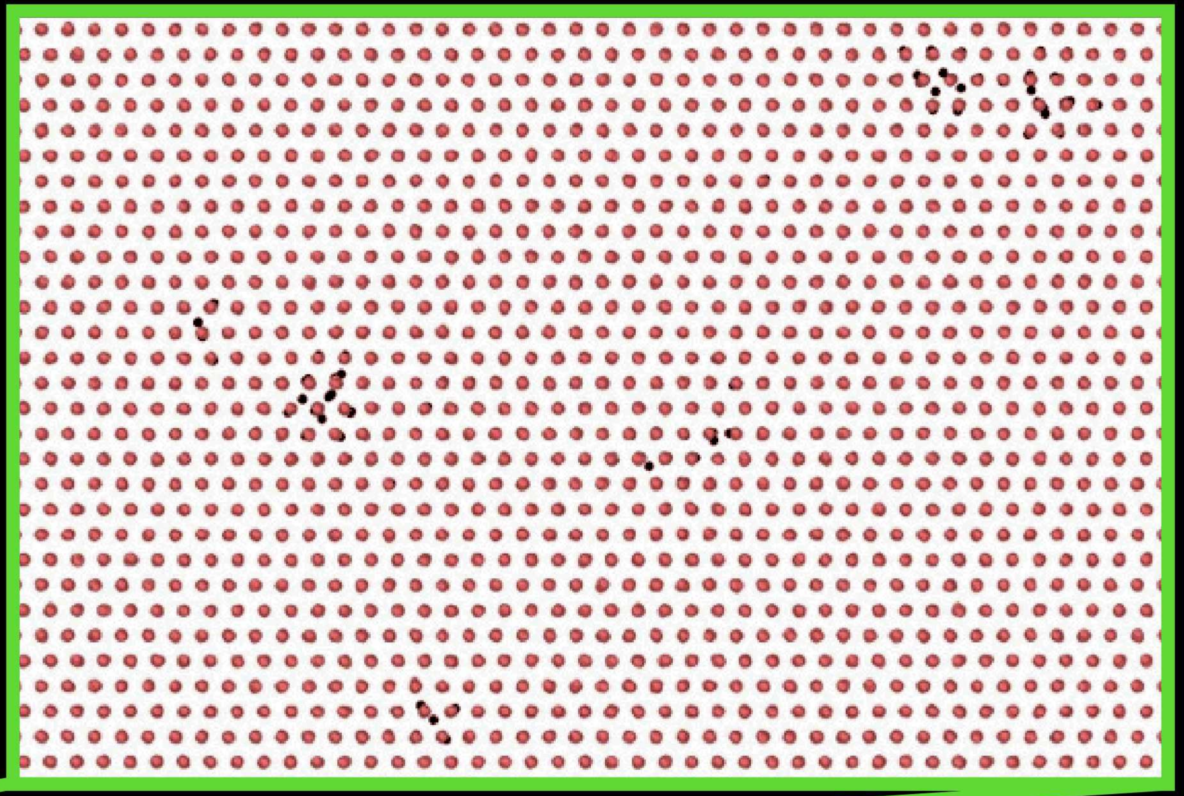
- Defect production: Frenkel pairs, Cascade
- Transmutation
- Segregation
- Amorphization
- Sputtering

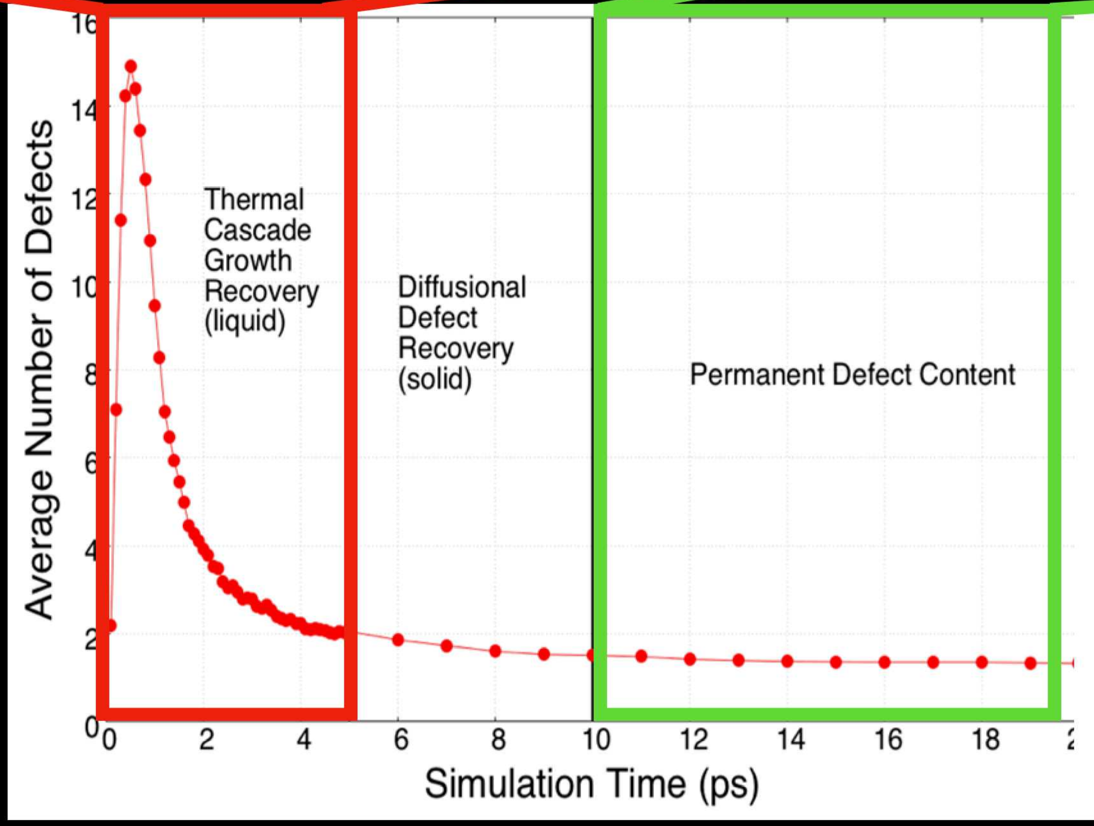
Radiation Effects

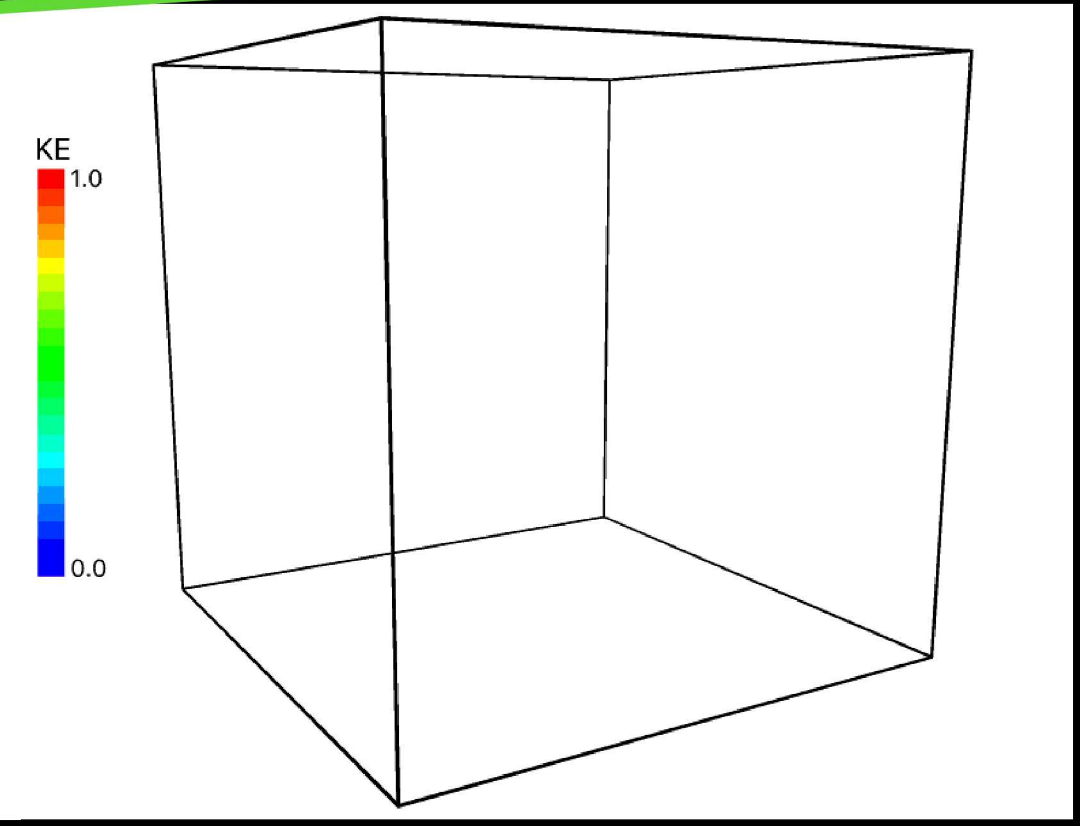
- Hardening
- Swelling
- Embrittlement

Model Damage Production at the Atomic Scale Using Molecular Dynamics: Ballistic Effects



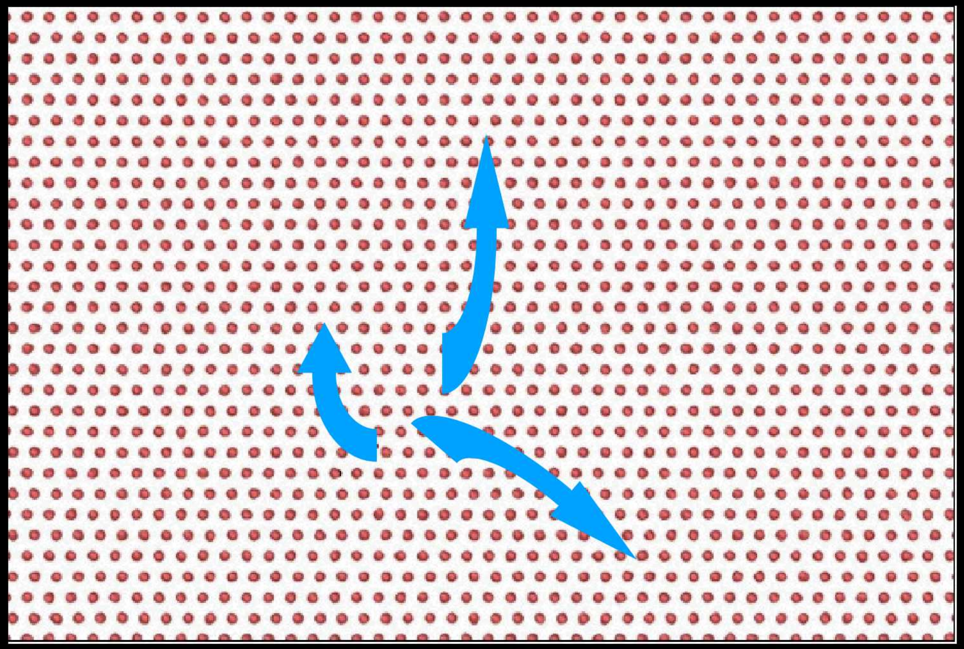




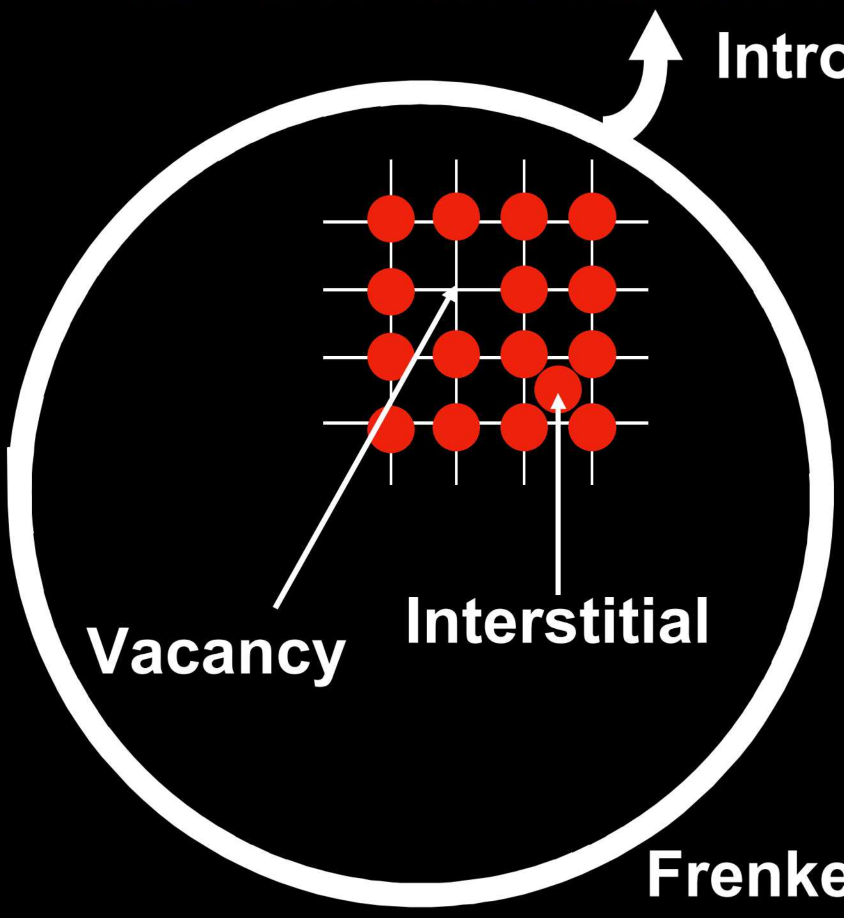


Model Damage Production at the Atomic Scale Using Molecular Dynamics: Simple Way

Electron irradiation



Introduction N FPs every 2ps

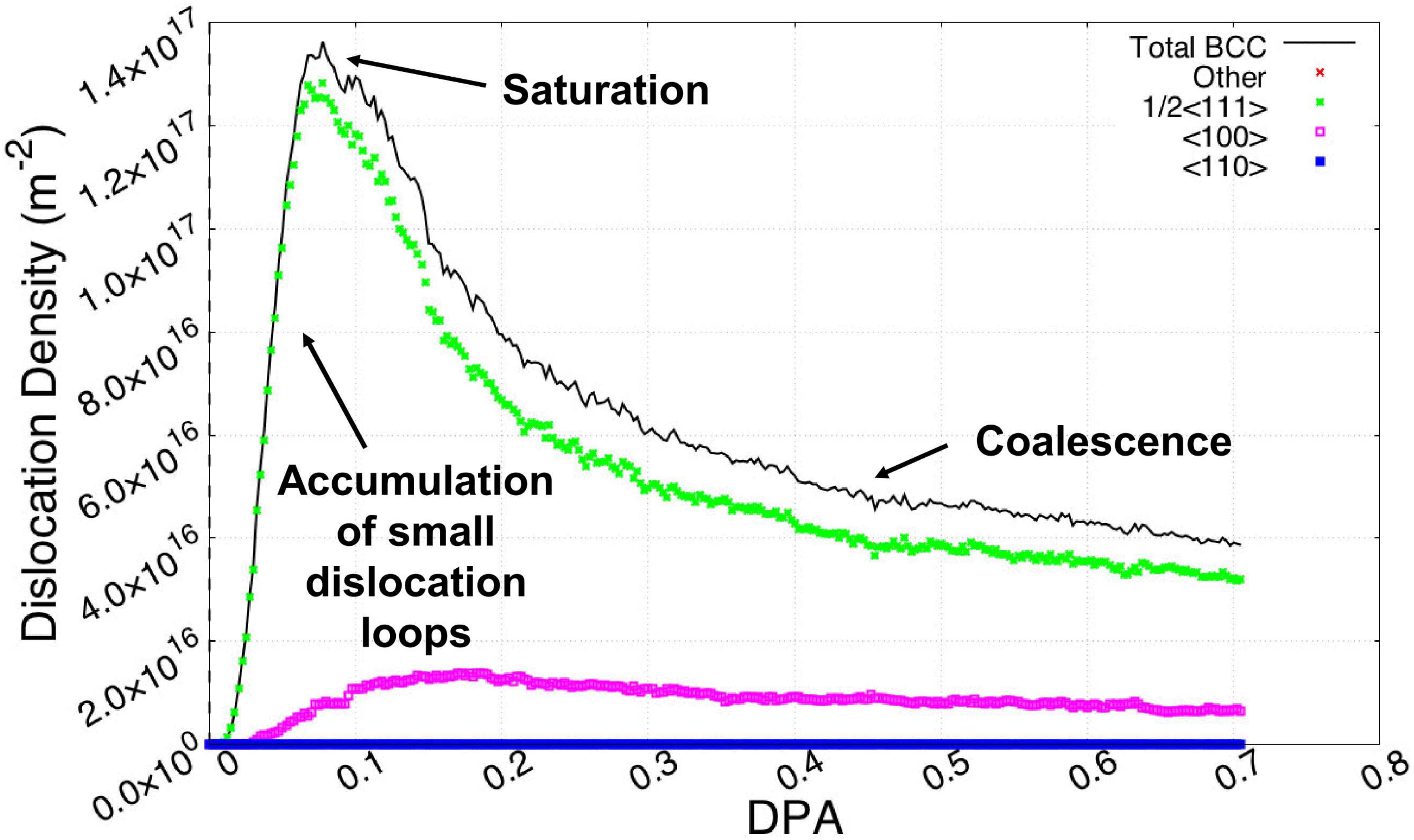


Frenkel pair

- Maximum allowed displacement (SRIM)
  - Example: First collision range for Zr/Nb targets
    - Zr → Zr: 104 A
    - Nb → Zr: 77 A
    - Nb → Nb: 103 A
    - Zr → Nb: 78 A
- Effective dose rate: 8×10^{-4} dpa/ps
  - Unrealistic dose rate!
- 300 K, constant P, T

Defect Accumulation Mechanisms:

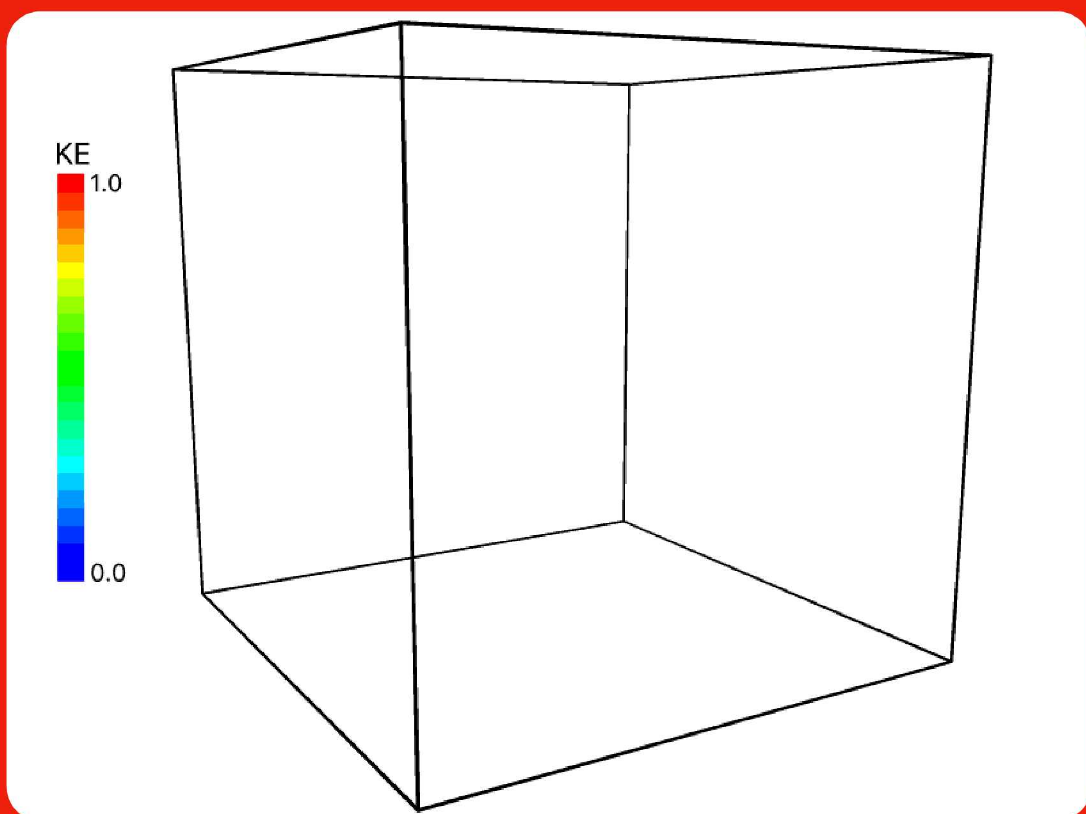
Example of Defect Accumulation in Nb



1/2<111> <100>

Beyond Frenkel Pair Accumulation: Modeling Light/Heavy Ion Irradiation

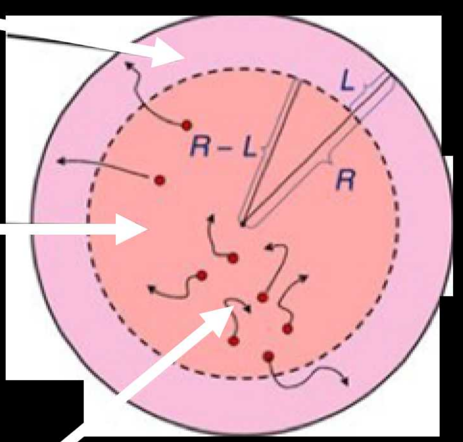
$$N_{\mathrm{dpa/rpa}}(T_d) = \begin{cases} 0 & \mathrm{for} \quad \mathrm{T_d} < \mathrm{E_d} \\ 1 & \mathrm{for} \quad \mathrm{E_d} < \mathrm{T_d} < \frac{2\mathrm{E_d}}{0.8} \\ \frac{0.8 T_d}{2 E_d}\xi_{\mathrm{dpa/rpa}} & \mathrm{for} \quad \frac{2\mathrm{E_d}}{0.8} < \mathrm{T_d} < \infty \end{cases}$$



Reduced-order representation

Periphery with atoms pushed outwards (interstitials)

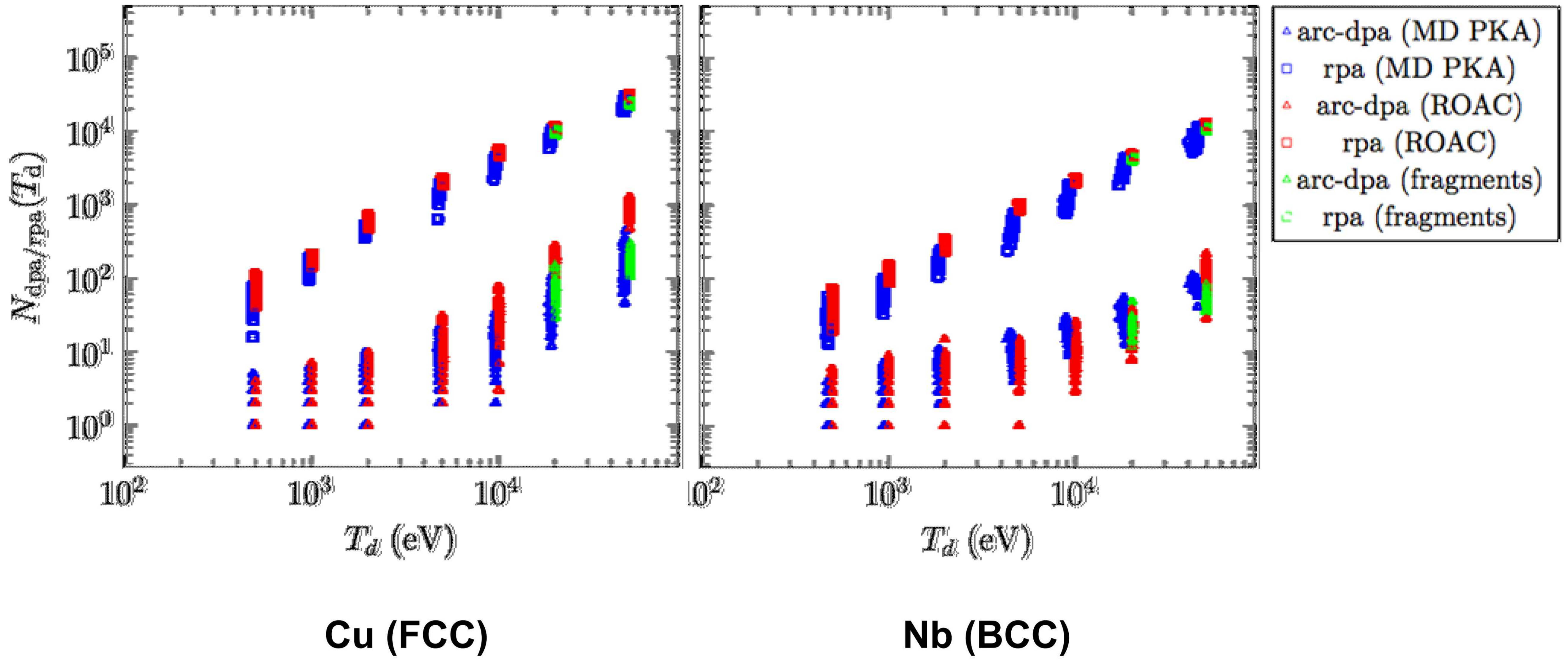
Hot cascade core



Atoms movements causing replacements within the core

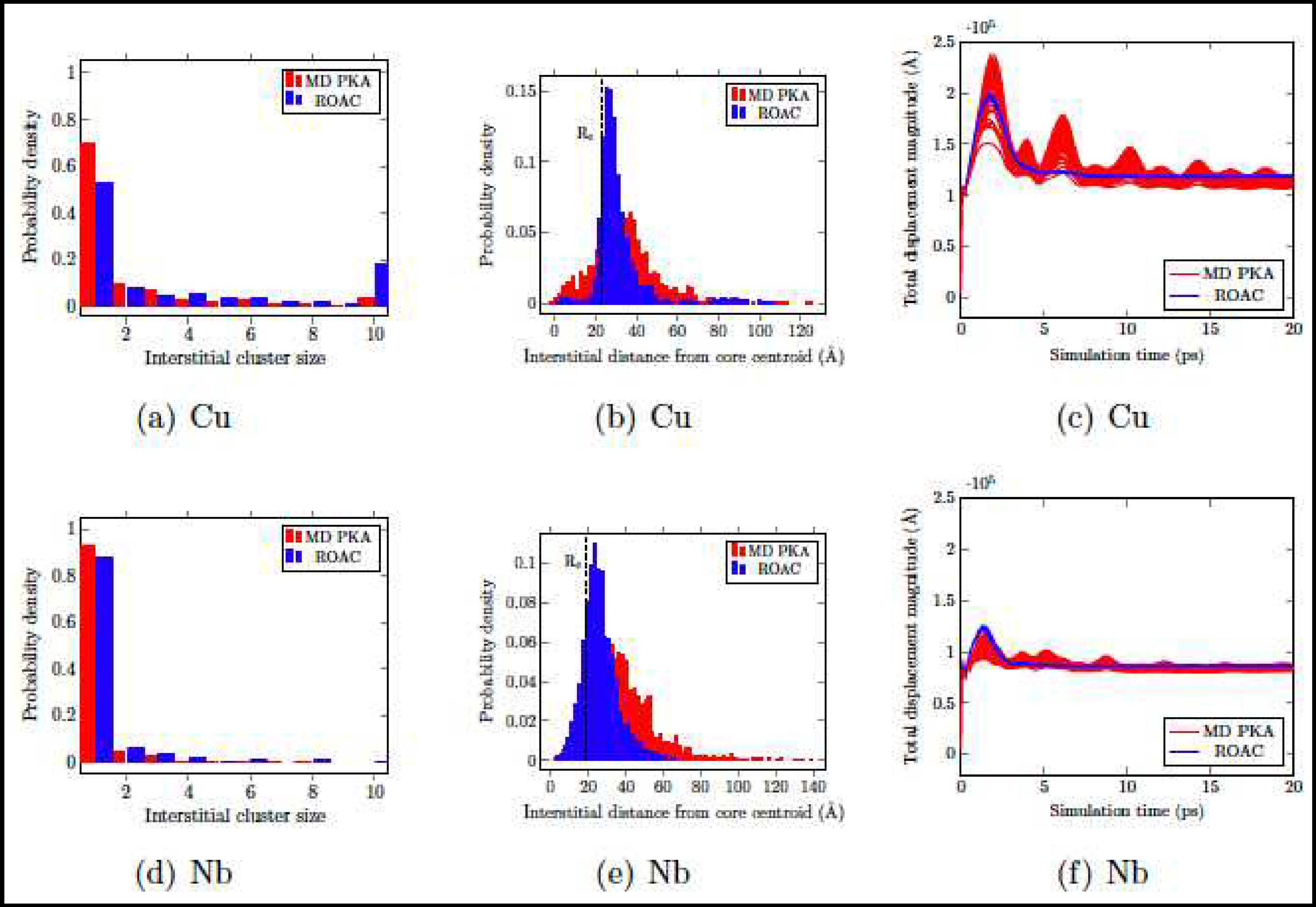
Predictability of the Reduced-Order Atomistic Cascade Model:

Defect Production



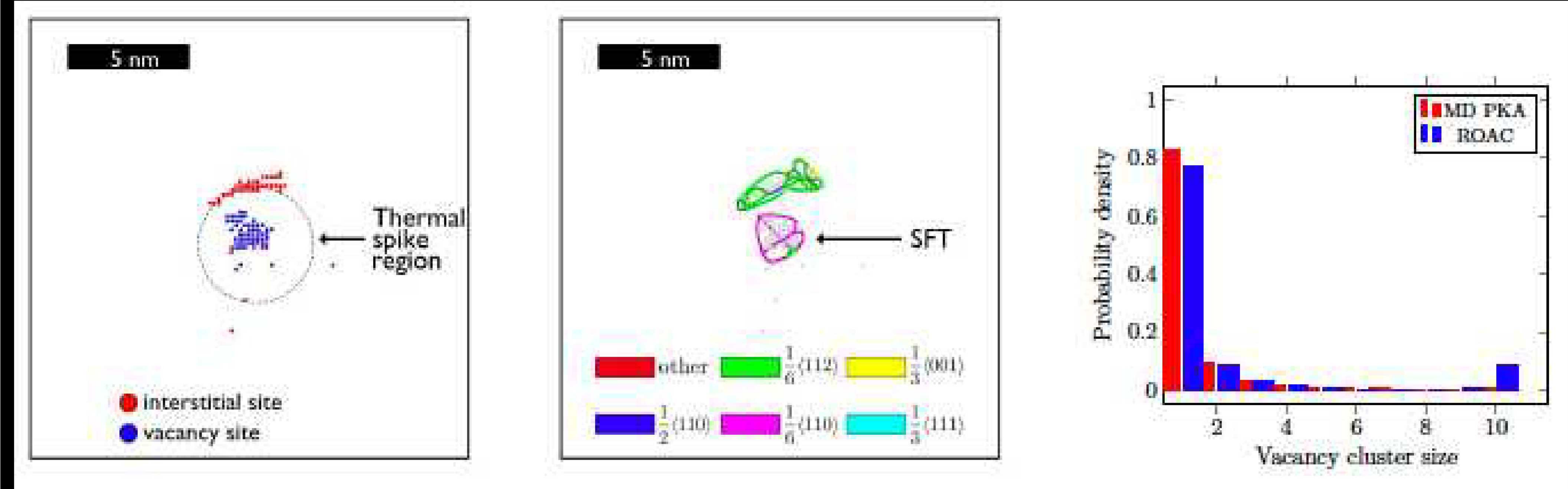
Predictability of the Reduced-Order Atomistic Cascade Model:

Defect Statistics



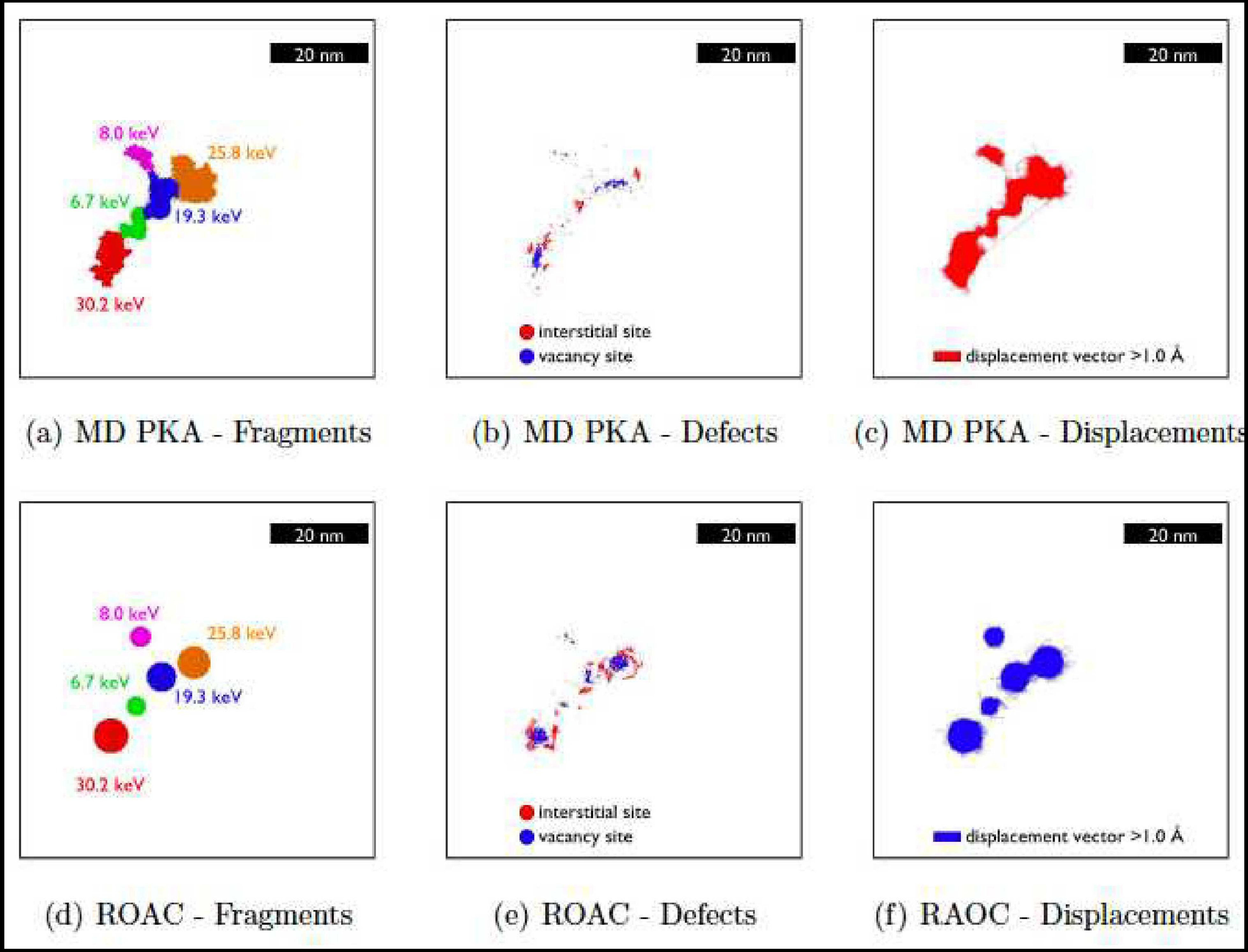
Predictability of the Reduced-Order Atomistic Cascade Model:

Defect Morphology



(a) Wigner-Seitz analysis (b) Dislocation analysis (c) 10 keV recoil in Cu

APPLICATION: CASCADE FRAGMENTATION

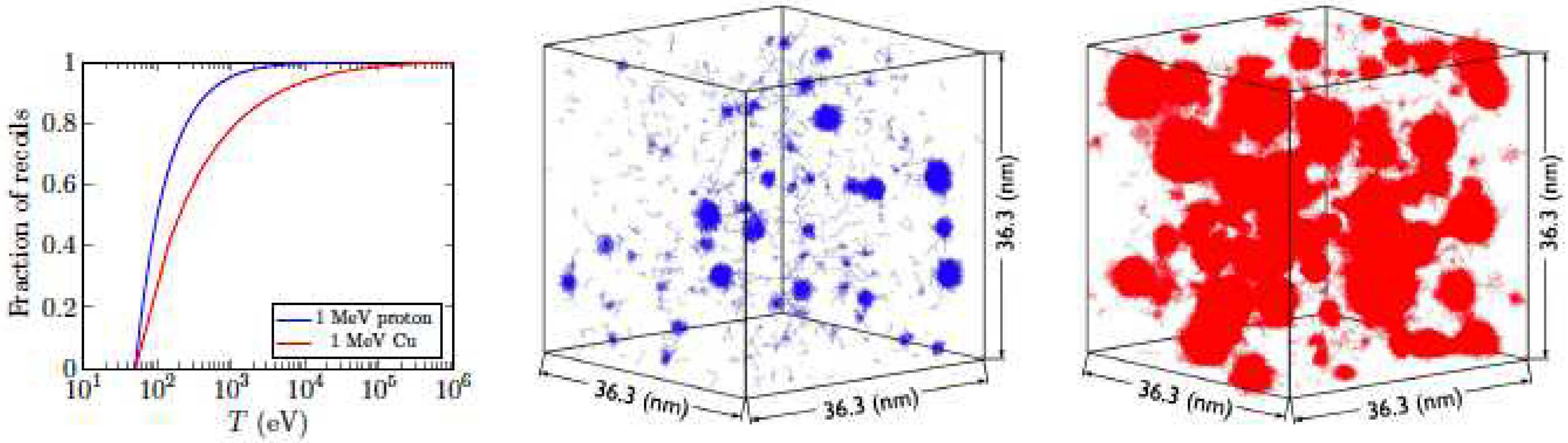


(a) MD PKA - Fragments (b) MD PKA - Defects (c) MD PKA - Displacements

(d) ROAC - Fragments (e) ROAC - Defects (f) RAOC - Displacements

High PKA cascades (100 keV here) are decomposed into subcascades.
Subcascades are spatially inserted to reproduce large cascade breakup.
Tremendous computational saving with reduced-order atomistic cascade model

APPLICATION: HIGH DOSE ION BOMBARDMENT



(a) Integral Primary Recoil Spectrum (b) 1 MeV proton source (c) 1 MeV Cu ion source

Cascades are sampled from the recoil spectra and randomly inserted into computation d

Similar in philosophy to FPA method

Application: High Dose Ion Bombardment at Phase Boundaries

Cu (FCC)

Nb (BCC)

TAKE HOME MESSAGE:

- **Simulations of the accumulation of radiation-induced defects using a Reduced-Order Atomistic Cascade Model**
  - Cascade approximated as core-shell structure
    - Atomic mixing (core)
    - Athermal recovery corrected damage (shell)
  - Verification and validation against full PKA cascade simulations yield good predictions and approximation of cascade characteristics
- **Most promising opportunities are to investigate damage accumulation and dose effects**
  - Fragmentation
  - Phase boundaries
  - Effect of radiation damage on mechanical properties