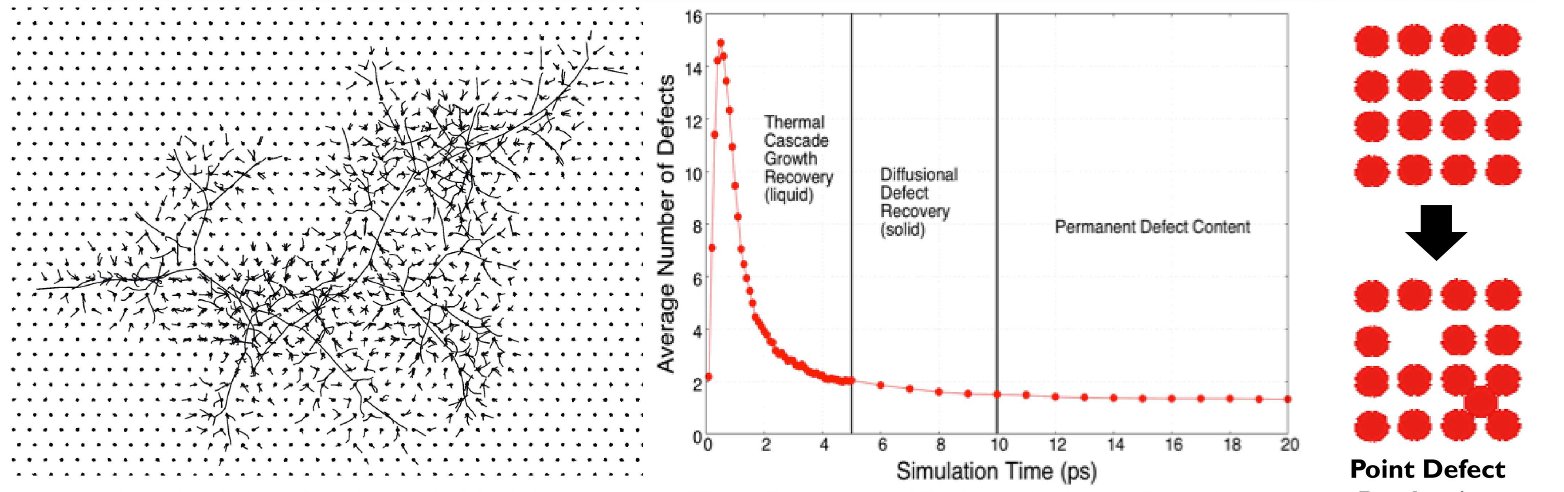
SAND2019-12055C

Sandia National Laboratories

Accelerated Atomistic Simulation of Radiation Events in Metals

Elton Chen[1,2], Chaitanya Deo[2], Rémi Dingreville[1]*
*rdingre@sandia.gov
[1] Center for Integrated Nanotechnologies, Department of Nanostructured Physics, Sandia National Laboratories
[2] G.W. Woodruff School of Mechanical Engineering, NRE Program, Georgia Institute of Technology

In Brief



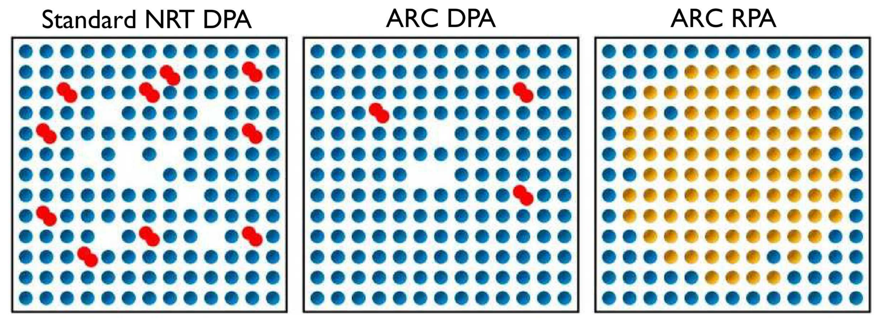
Standard Collision Cascade Model — Time Evolution of Defects during a Cascade — Point Defect Production

Problem: Atomistic modeling of irradiation damages through displacement cascades is deceptively nontrivial. Due to the high energy, high velocity nature of the atom collisions, individual cascade simulations can become very computational expensive and ill-suited for size and dose upscaling.

Approach: Expanding upon the foundation of the Frenkel Pair Accumulation (FPA)[1] technique, we have developed a new accelerated method of simulation radiation damage accumulation. By integrating the state-of-the-art Athermal Recovery Corrected (ARC) damage model[2], this method is more adapt at modeling high energy irradiation of dense materials and metals.

Results: The new method is able to replicate radiation damage up to ~50 keV. Final defect characteristics are comparable to full cascades; and cluster formation is successfully captured. Two novel applications shown are shown for reference.

Reduced-Order Atomistic Cascade (ROAC)

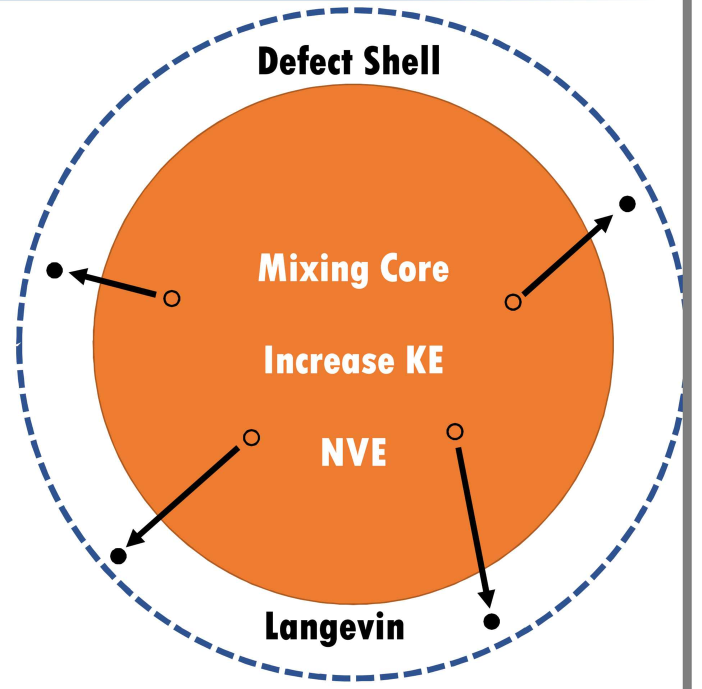


Athermal Recovery Corrected (ARC) Damage Model

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

$$\xi_{\mathrm{dpa}}(T_\mathrm{d}) = \frac{1-c_{\mathrm{dpa}}}{(2E_\mathrm{d}/0.8)^{b_{\mathrm{dpa}}}}T_\mathrm{d}^{b_{\mathrm{dpa}}} + c_{\mathrm{dpa}}$$

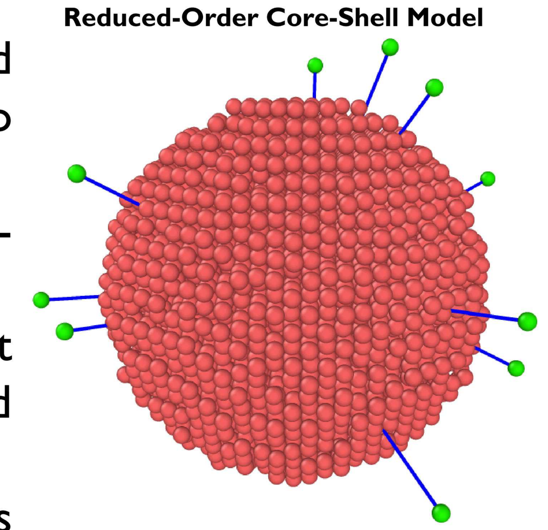
$$\xi_{\mathrm{rpa}}(T_\mathrm{d}) = \left(\frac{b_{\mathrm{dpa}}^{c_{\mathrm{rpa}}}}{(2E_\mathrm{d}/0.8)^{c_{\mathrm{rpa}}}} + 1\right)\frac{T_\mathrm{d}^{c_{\mathrm{rpa}}}}{b_{\mathrm{rpa}}^{c_{\mathrm{rpa}}} + T_\mathrm{d}^{c_{\mathrm{rpa}}}}$$



Reduced-Order Core-Shell Model

The newly developed Athermal Recovery Corrected (ARC) damage model[2] is adopted in order to incorporate the effects of thermal spike.

- Cascade is approximated as a spherical core-shell.
- Displacement Per Atom (DPA), point defect production, is modeled by the atoms displaced into the cool defect shell.
- Replace Per Atom (RPA), atomic mixing, is modeled by the melting of the hot mixing core.



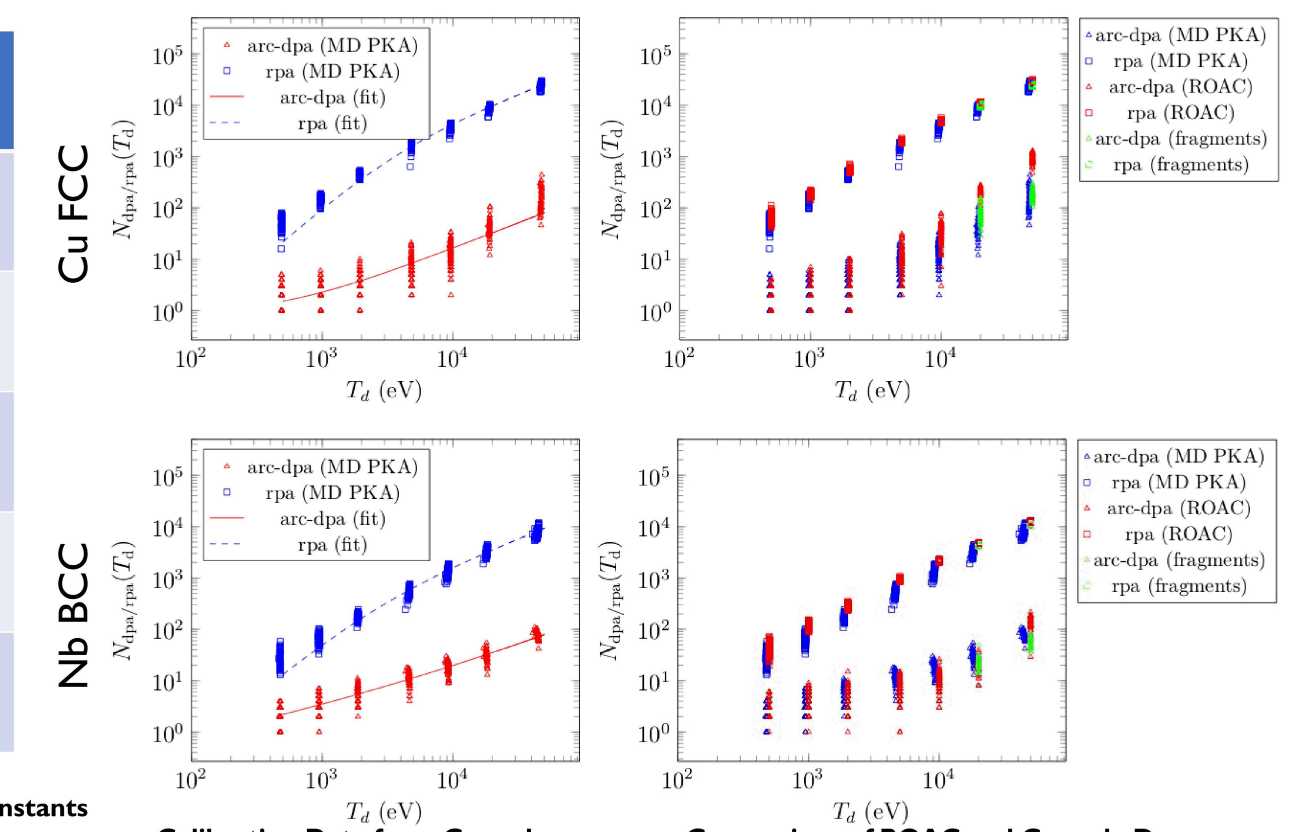
MD Implementation

Damage Fitting / Reproduction

- 100 full collision cascades are simulated at each 500 eV, 1 keV, 2 keV, 5 keV, 10 keV, 20 keV and 50 keV to generate the initial calibration data for ROAC.
- ARC DPA function is fitted to the point defect damage.
- ARC RPA function is fitted to the on-lattice atom mixing damage.
- Material constants are calculated for both FCC Cu and BCC Nb.
- ROAC is verified to successfully replicate cascades across the spectrum.

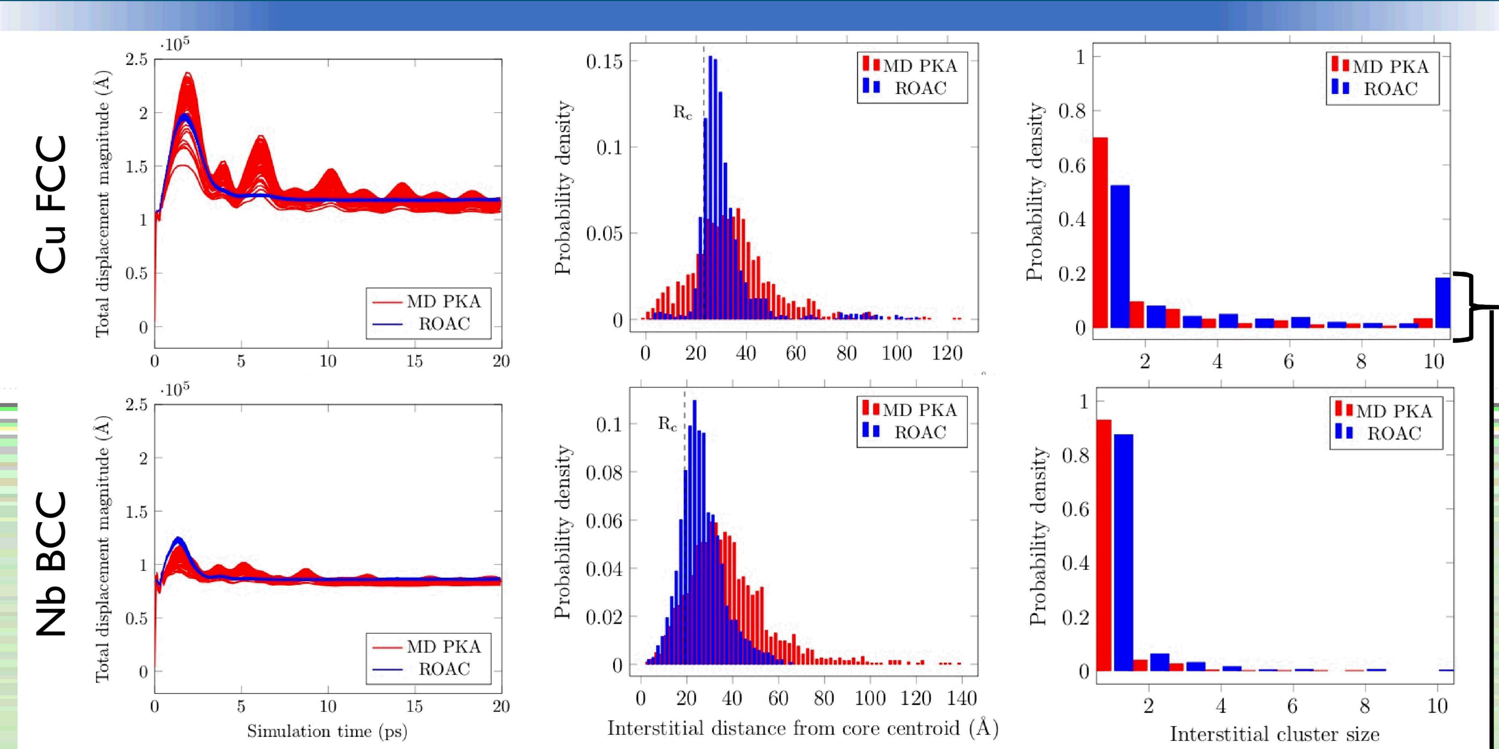
	Cu FCC	Nb BCC
E_d	50.0	56.0
b_{dpa}	-1.070	-0.485
c_{dpa}	0.200	0.172
b_{rpa}	3359	2627
c_{rpa}	1.27	1.11

Fitted Material Constants

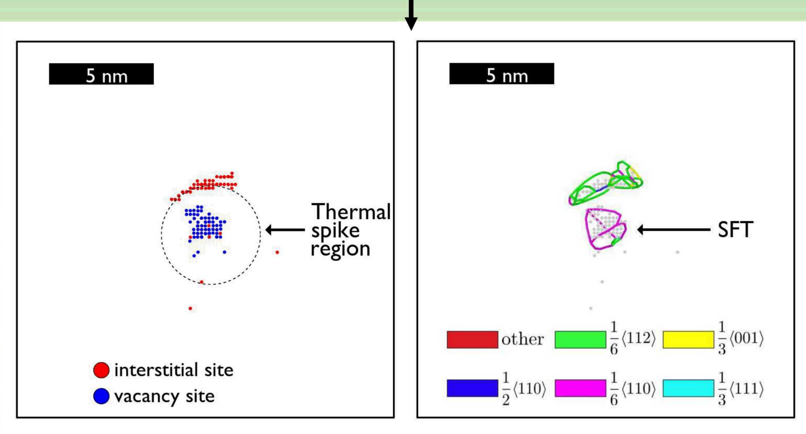


Calibration Data from Cascade — Comparison of ROAC and Cascade Damage

Defect Characteristics

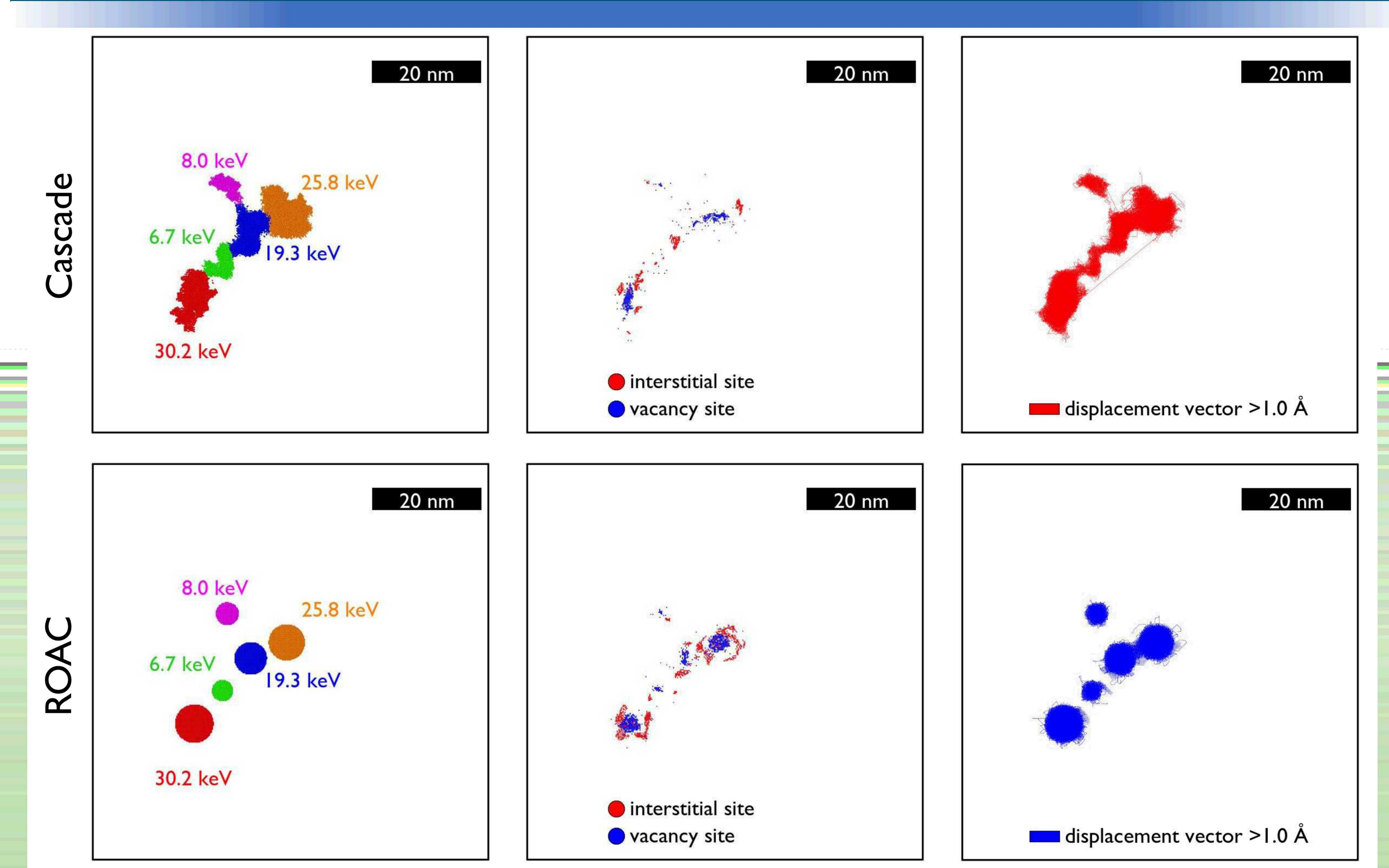


- ROAC defect structures are more dense and less varied due to the spherical core-shell.
- Compact core-shell geometry also enhances the thermal shock and production of defect clusters and Stacking Fault Tetrahedra (SFT) in Cu, a common trait in FCC metals[3].



ROAC Production of Defect Clusters & SFT

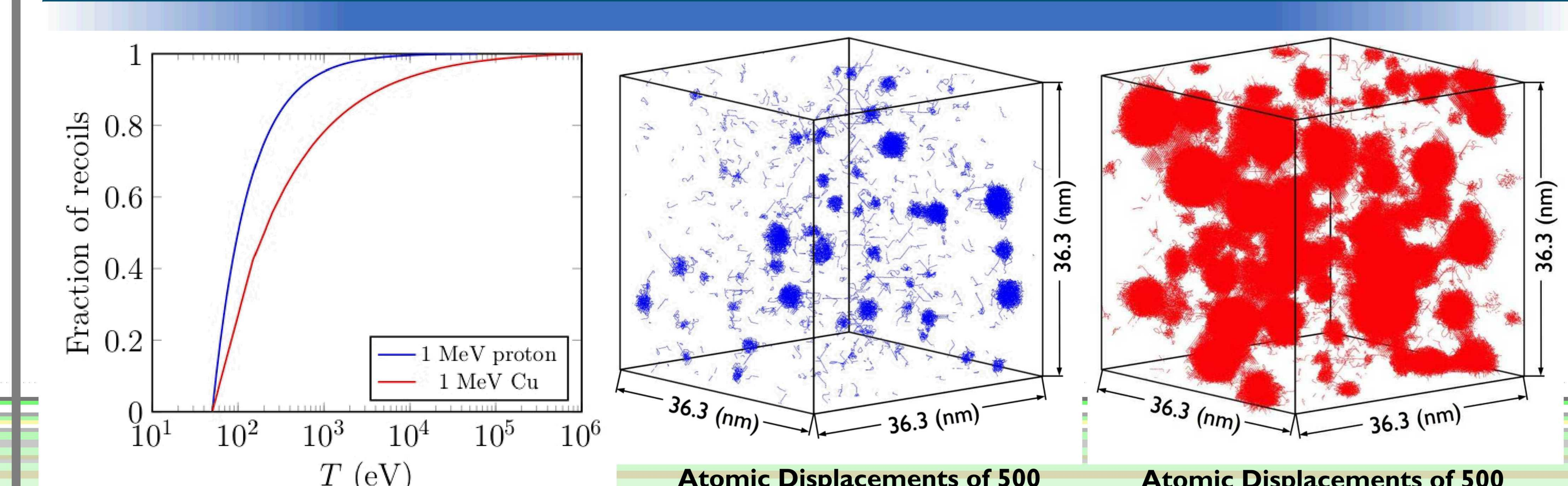
Application: Cascade Fragmentation



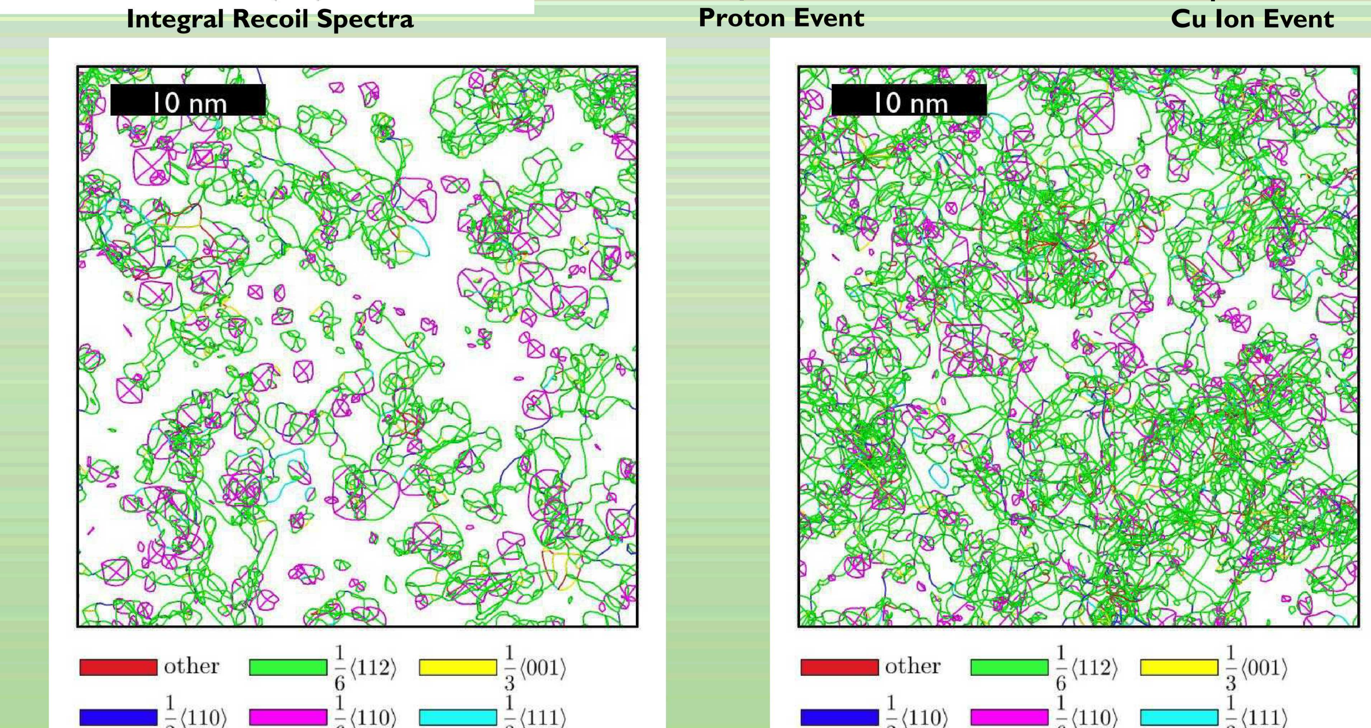
100 keV Fragmentation — Point Defect — Atomic Mixing

- High energy cascade (~100 keV) can be broken up to into smaller fragments.
- ROAC reduces computational cost by instantaneously develop a full cascade.
- Final damage characteristics can be tune by cascade fragmentation criteria.

Application: Ion Bombardment



Integral Recoil Spectra — Atomic Displacements of 500 Proton Event — Atomic Displacements of 500 Cu Ion Event



0.0279 DPA - 1 MeV Proton — 0.0279 DPA - 1 MeV Cu Ion

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology &Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND No. ____________

[1] Chartier, A., et al. "Early stages of irradiation induced dislocations in urania." *Applied Physics Letters* 109.18 (2016): 181902.
[2] Nordlund, Kai, et al. "Improving atomic displacement and replacement calculations with physically realistic damage models." *Nature communications* 9.1 (2018): 1084.
[3] Calder, A. F., et al. "On the origin of large interstitial clusters in displacement cascades." *Philosophical Magazine* 90.7-8 (2010): 863-884.