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Determination of the Threshold Displacement Energy in

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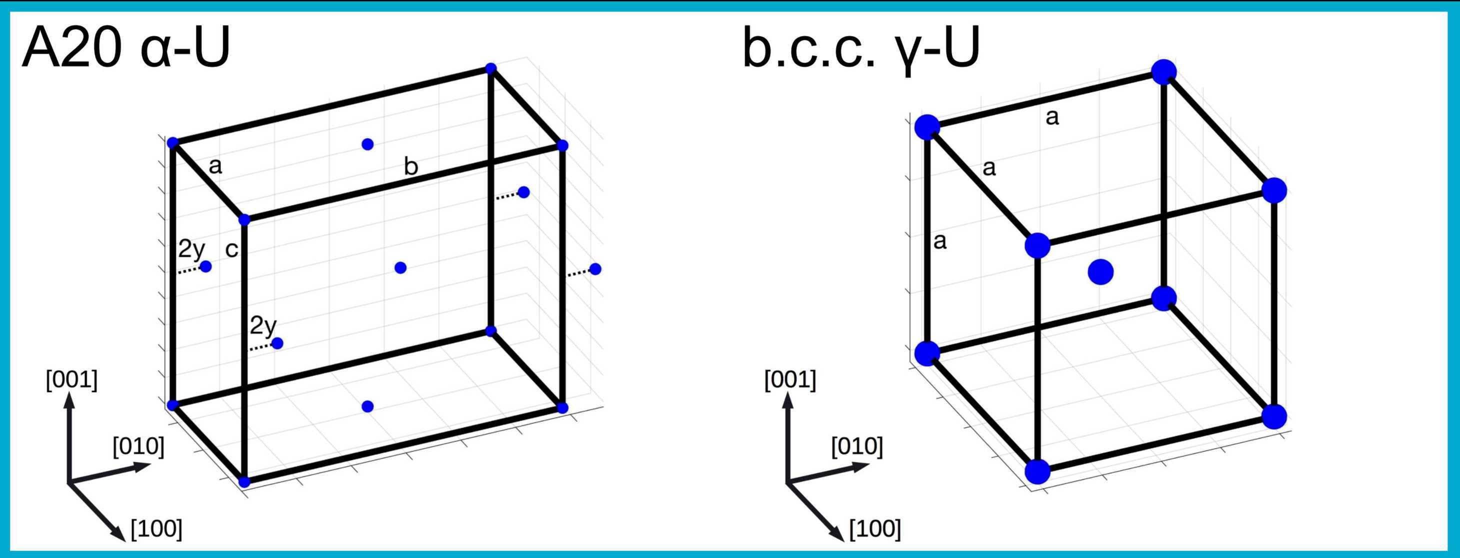
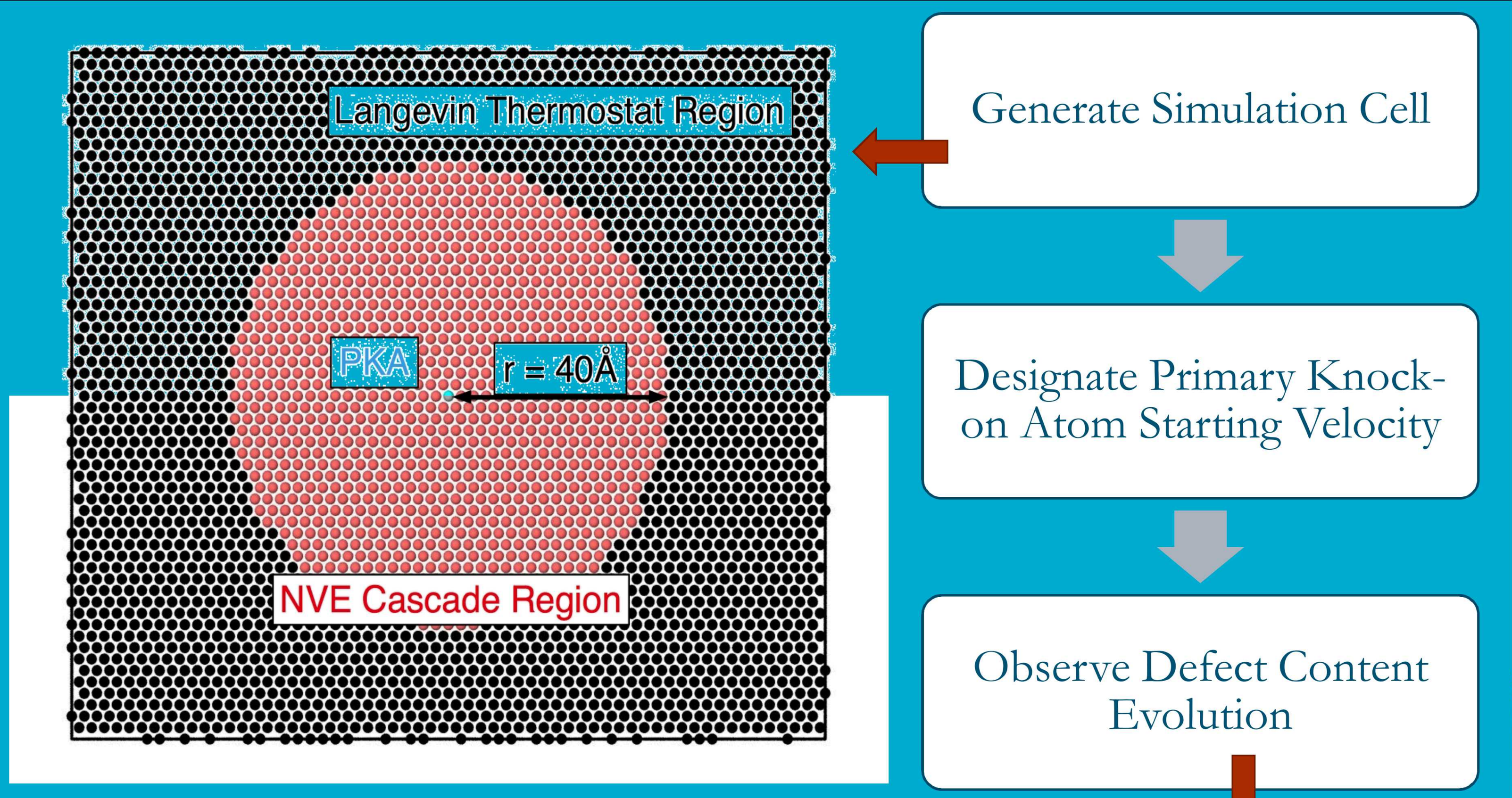
Metallic Uranium Phases



Due to the *f* electron shell, metallic uranium exist in multiple phases under different temperature and pressure conditions. The three most commonly observed solid phases are the orthorhombic α−U , the tetragonal β−U and the cubic γ−U. The ground state α−U exists in a rare strukturbericht A20 structure. At approximately 935K, α − U transforms into b.c.t β−U; at 1045K β−U transforms into b.c.c γ−U, and persists until melting at 1406K. In practice, the β phase is typically ignored due to its relatively small stable region. In order to accurately evaluate the radiation resistances of α and γ Uranium, the differences in thermal and structural conditions must be considered.

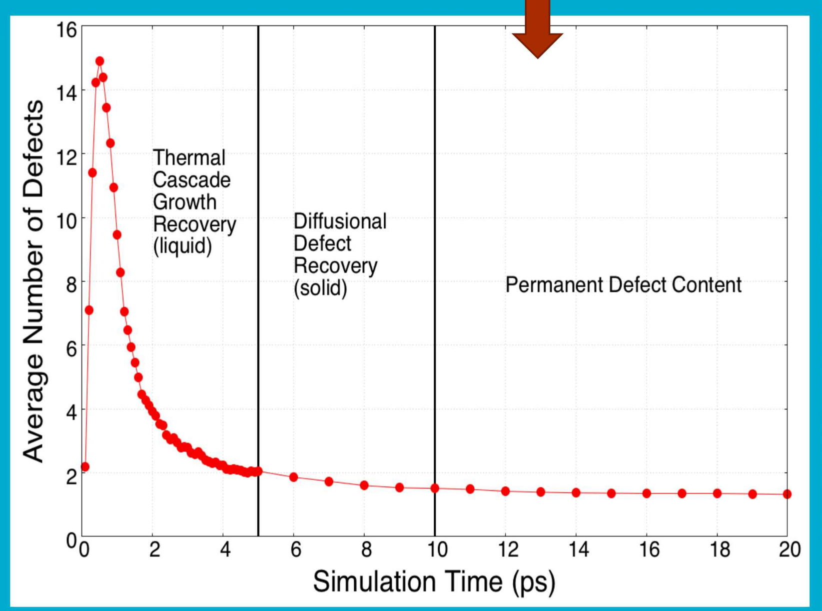
Methodology



Threshold Displacement Energy (TDE) is evaluated statistically by repeating isolated cascades. Simulation cells are surrounded with a Langevin buffer region to prevent self-interaction.

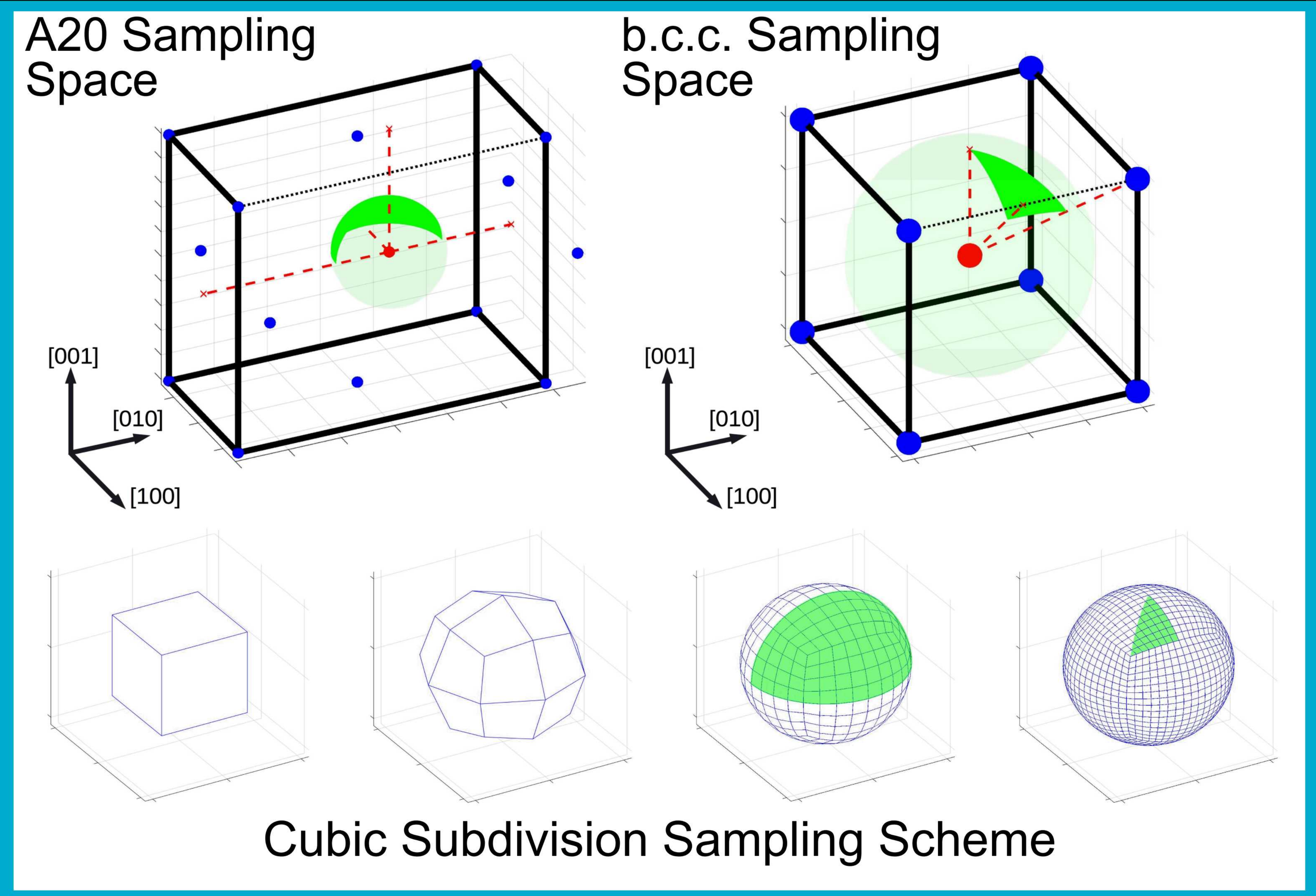
A cascade is initiated by giving the Primary Knock-on Atom a significant recoil velocity. Defect contents are generated in three stages:

1. Liquid-like thermal spike
2. Solid defect diffusion
3. Permanent defect content



Stage 1 and Stage 2 are affected the thermodynamic conditions. At Stage 1 thermal spike grows larger with increasing temperature, due to lattice loosening. At Stage 2 defect diffusions more frequently annihilate interstitial vacancy pairs at higher temperatures.

Recoil Particle Orientation Sampling

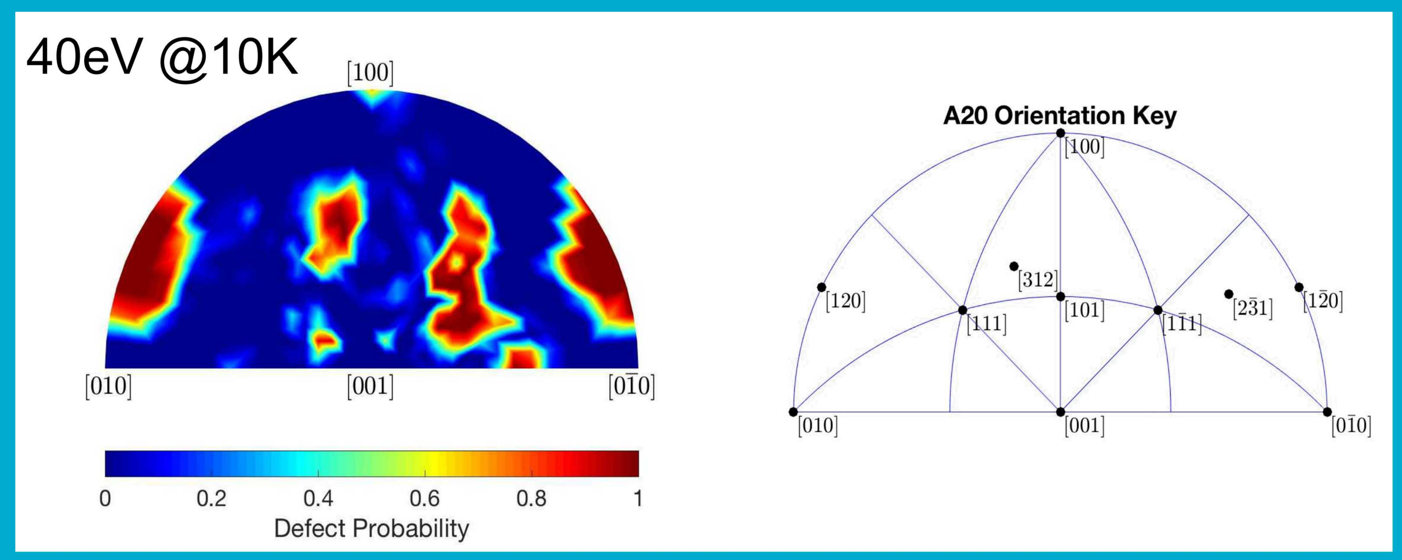


To account for the differences in phase structures, Primary Knock-on Atom recoil directions are uniformly sampled from the minimum symmetrical orientation space of each respective lattice. Sampling scheme is derived from the cubic subdivision spherical approximation. Symmetry operations available to the unit cube match those of the A20 and b.c.c. structures, ensuring an uniform and complete orientation sampling. For α−U and γ−U, 417 and 153 recoil directions are sampled respectively.

Total Statistical Sampling

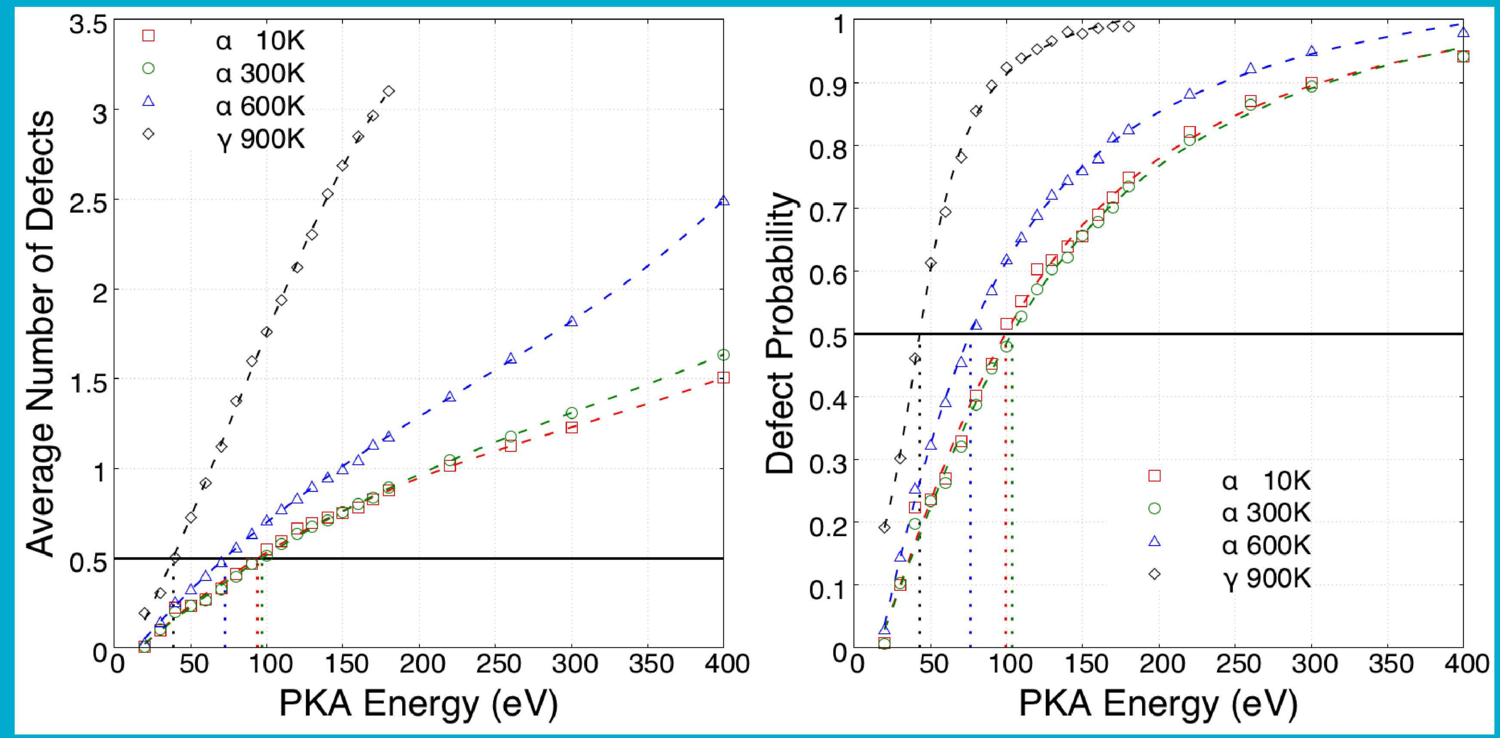
For cascades in γ−U, recoil particles are assigned velocities equivalent to 17 different recoil energies ranging from 20eV to 180eV. For cascades in α −U, the recoil particles to are assigned 21 different recoil energies, expending the range up to 400eV. With each recoil energy and orientation combination, 20 random seeds are used to generate statistical variances. Overall 175,140 individual cascades are simulated for α−U at 10K, 300K, 600K, and 52,020 individual cascades are simulated for γ−U at 900K.

Results



Through combination uniform recoil direction sampling and random seeding, a directional defect probability can be generated at each given recoil energy. Examination of the defect probability distributions reveals several recoil tunneling directions favoring defect production. The large difference in defect probability distribution at low recoil energies further emphasizes the necessity to properly account for the lattice structure when calculating TDE.

Generalized Threshold Displacement Energy

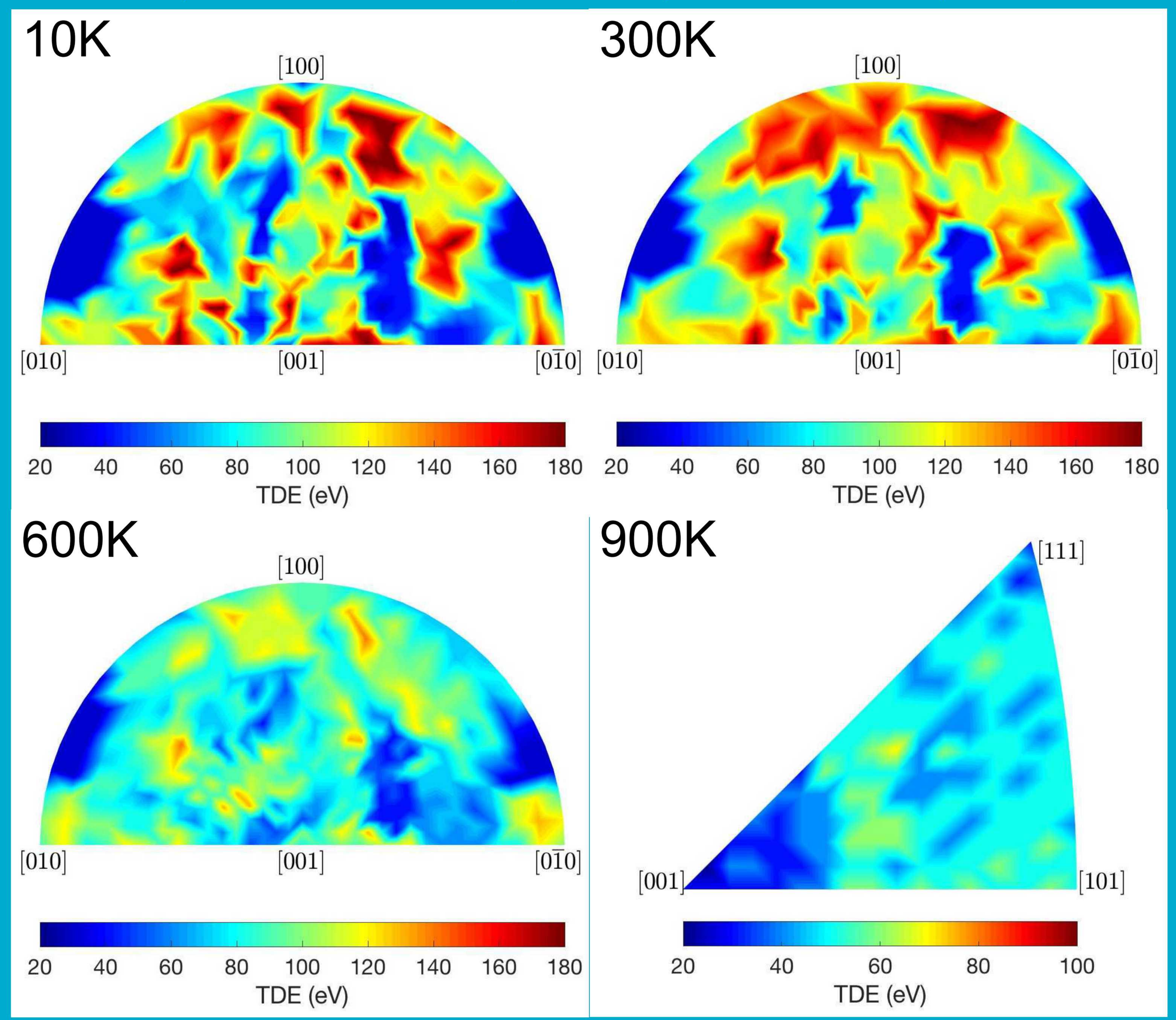


By averaging over all recoil directions, defect probabilities and average defect number can be reduced to functions of recoil energies. At each temperature, Threshold Displacement Energies are then calculated by checking defect probability 50% or average defect ½.

	E_d (eV) Average Defect	E_d (eV) Defect Probability
α @10K	99.2659	93.9178
α @300K	103.498	96.699
α @600K	76.0916	72.4146
γ @900K	42.9929	38.5157

Directional Threshold Displacement Energy

TDE can be similarly calculated at defect probability 50% at each sampled recoil direction.



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