

**A KINETIC MONTE CARLO MODEL FOR HELIUM DIFFUSION AND CLUSTERING IN FUSION ENVIRONMENTS** -- B. D. Wirth (University of California, Berkeley) and E. M. Bringa (Lawrence Livermore National Laboratory)

**ABSTRACT**

Structural materials in fusion reactors will operate in harsh radiation conditions including high displacement rates from 14 MeV neutrons with accompanying high levels of hydrogen and helium production and will experience severe property degradation. Predicting their in-service performance requires a detailed understanding of the mechanisms of defect accumulation and microstructure evolution. Here, we describe a kinetic Monte Carlo (KMC) model to simulate the migration and clustering of transmutant helium gas atoms and ultimately determine the role of He in mediating the long term aging of primary defects (vacancies, self-interstitial atoms and their clusters) produced in displacement cascades.

The KMC model is based on modifications to a code that has been successfully used to study copper-vacancy clustering in Fe-Cu alloys. Since He can occupy either interstitial or substitutional sites within the bcc Fe lattice, this model involves the addition of an octahedral site sub-lattice [(0.5,0,0) and (0.5,0.5,0) sites] and is sufficient to describe He migration. As an interstitial, He diffuses between octahedral sites through unstable tetrahedral site saddle points and as a substitutional atom, He migrates via a vacancy exchange mechanism. For substitutional He jumping into a nearest neighbor vacancy, the He atom migrates along trajectories very close to the  $\langle 111 \rangle$  direction, with an activation energy of 0.12 eV. Notably, our atomistic molecular statics simulations reveal that the He atom can jump into a second nearest neighbor vacancy position along a trajectory close to the  $\langle 100 \rangle$  directions, with an activation energy of 0.66 eV.

The KMC results illustrate the mechanisms responsible for the formation of vacancy-He clusters, the rather large three-dimensional mobility of small vacancy-He clusters and the role of cluster coalescence events in assisting He cluster nucleation. Future work will clarify the mobility of vacancy-He cluster complexes and extend the simulation durations to predict He bubble nucleation.

**Reference**

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