# Defect Clustering and Xenon Migration in $UO_2$

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## Abstract

Existing nuclear fuel performance codes depend on empirical correlations of microstructural features, such as defects, voids, gas bubbles and grains. Hence, they cannot reliably predict the fuel behavior under extreme conditions of operation of the next generation of nuclear reactors. Replacing current fuel performance models with fundamental science-based models and methods requires the use of multiscale modeling to accurately determine microstructural effects on properties. In an effort to reliably model microstructural evolution in $UO_2$, we have used molecular dynamics simulations to study defect creation by 1 keV U recoils in$UO_2$. Dynamic annealing was highly effective and fewer than 10% of displaced atoms survived as Frenkel pairs. The cation interstitials were well separated from cation vacancies. By comparing five different potentials, we find that the extent of defect clustering bears a relation to the melting temperature and oxygen ion mobility given by the interatomic potential. We will also discuss fission track damage, the mobility of Xe near grain boundaries for various concentrations of Schottky defects in polycrystalline $UO_2$ at elevated temperature, and coupling atomistic simulations to phase field models.