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MD simulations of high-dose irradiation in Tungsten: The Role of Defect Boundary & Morphology

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The molecular dynamics (MD) simulations of successive collision cascades (SCC) within a single simulation domain have recently been employed to predict radiation damage at varying dpa levels [1,2]. We carry out SCC simulations with different primary knock-on atoms (PKAs) and interatomic potentials (IPs)—namely, traditional EAM and machine learning potentials (MLIPs). Since dpa serves as the primary metric for quantifying irradiation-induced changes in key material properties irrespective of incident energy, we analyze defect properties as a function of dpa while noting their sensitivity to the PKA energy, choice of IP, and agreement with experiments. We compare defect characteristics—such as overall defect density, boundary defect density (accounting for all point defects, except that for dislocation loops only peripheral defects are counted), swelling, defect morphology and size distribution—with experimental data from Transient Grating Spectroscopy (TGS) [3] and transmission electron microscopy (TEM) at various dpa levels. Notably, the boundary defect density remains consistent across different energies and IPs and aligns well with TGS measurements, whereas the total defect count varies significantly. Differences in defect morphologies observed across potentials are discussed in the context of formation energies for various self-interstitial atom (SIA) configurations, as well as the influence of training data and parameters in MLIP development [4,5]. We also discuss the computational methods and challenges for a scalable and detailed analysis of SCC performed by extending the Csaransh [6] and SaVi [7] algorithms. Our work thus provides a comprehensive assessment of the sensitivity of defect properties to both incident energy and potential choice, showing that the boundary defect density is an important factor that exhibits energy-independent behavior and experimental agreement similar to dpa. The results highlight the immense predictive capabilities—and current limitations—of SCC in fusion materials research.

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Primary author: BHARDWAJ, Utkarsh (Bhabha Atomic Research Centre)

Co-author: WARRIER, Manoj (Bhabha Atomic Research Center)

Presenter: BHARDWAJ, Utkarsh (Bhabha Atomic Research Centre)

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