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Molecular dynamics simulations of the defect evolution in tungsten on successive collision cascades

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Molecular dynamics (MD) simulations of successive collision cascades within the same simulation domain and further defect evolution were performed using two different inter-atomic potentials (IAP) in tungsten, one EAM based and the other a 'quantum accurate' machine learning potential, SNAP. The micro-structural changes are analyzed as a function of displacements per atom (dpa) up-to irradiation dose of 3 dpa. Five simulations are carried out at primary knock-on atom (PKA) energies of 20 keV and 50 keV with 3000 PKAs each, for observing stochastic differences in the evolution of damage. The simulation output was analysed after each PKA. The annealing simulations at different temperatures of damage accumulated at different dpa are also analysed using Machine Learning and deterministic methods for defect analysis. Results for the variation of the number of defects, number of defect clusters, their size and morphology distribution are compared for the two energies and two IAPs.

It is seen that for a given IAP, the number density of defect clusters as a function of dpa does not depend on the energy of the PKA used in the simulations implying that, like dpa, it could be a good measure of material property changes in irradiated materials. In contrast, the defect sizes depend strongly on the energy of the PKA. It is also seen that the micro-structure resulting from the EAM potential was mostly composed of <111> and <100> dislocations, while that from the SNAP potential was mostly composed of small, sessile, C15 ring like structures with a smattering of smaller <111> dislocations and very few <100> dislocations. The rings formed in SNAP potential remain stable and sessile for 10 ns simulations even at 2000K, resulting in significantly different microstructure from the EAM based potential. The results from the two IAPs with regard to defect morphology are validated against the experimental results of dislocation types, density and size distributions.

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