Determination of Dose Effects on Defect Accumulation under Irradiation in Nanoporous Gold and Niobium via Atomistic Simulations

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This study explores the radiation resistance of Nb nanofoams and nanowires. Nanostructured metals present a high density of interfaces and surfaces as sinks for radiation produced point defects and thus may offer a means to developing radiation tolerant materials. Current work in the modeling of radiation damage in nanofoams and nanowires typically looks at defect accumulation of a single primary knock on atom and its impact on the structure. For this work, dose effects have been investigated by varying the number and energies of primary knock on atoms, including the consideration of damage accumulation due to radiation events with a spectrum of energies. Molecular dynamics simulations are coupled with machine learning tools to develop a statistical characterization of the nanofoam structure and the defect clusters formed as a consequence of irradiation. The study investigates the impact of structure properties such as ligament length and diameter on defect accumulation mechanisms and defect properties, such as formation and binding energies as well as the relationship between energies of the primary knock on atoms and changes in structural and mechanical properties. Results suggest that the presence of interfaces and surfaces in nanofoams affects the formation and migration of defect clusters leading to a more radiation resistant metallic structure.

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