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Kinetic Monte Carlo calculations of defect diffusion in hcp metals: effect of defect anisotropy

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The study of point defect clustering in hexagonal-close-packed (hcp) metals is dominated by a consideration of the geometry of the hcp lattice and lattice parameters ratio (c/a). Because of this crystallographic anisotropy, defect anisotropic diffusion is expected (jump distances and jump rates depend on jump directions). This study has focused on hcp $\alpha$-Zirconium (c/a 1.594, lower than ideal 1.633 and similar to Titanium, c/a 1.587). We have created a new and original model for the understanding of the microscopic evolution (defect diffusion) in hcp metals, using a kinetic Monte Carlo simulation technique. This technique allows us to understand the evolution of damage accumulation, due to either neutron or electron irradiation, for long times (hours-months).

Using the input data obtained from Molecular Dynamics simulations on defect energetics and cascade damage, we present results obtained on irradiation of hcp $\alpha$-Zr under different conditions with the above mentioned kinetic Monte Carlo model. Using 25 keV cascades we have studied the evolution of the microstructure during irradiation under environment conditions of 600K, dose rate $10^{-6}$ dpa/s and final dose of 0.5 dpa. We have considered isotropic motion for vacancies and we have studied how the accumulation of damage is affected considering from one dimension to three dimension movement for interstitials. Results on electron irradiation of hcp $\alpha$-Zr with this kinetic Monte Carlo model have also been obtained in order to compare with experimental results. Finally, our results on $\alpha$-Zr will be extrapolated to Titanium that has very useful applications in nuclear fusion reactors.

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