The Effect of Electron-Ion Coupling on Radiation Damage Simulations of a Pyrochlore Waste Form

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Abstract

We have performed molecular dynamics simulations of cascade damage in the gadolinium pyrochlore $Gd_2Zr_2O_7$, comparing results obtained from traditional methodologies that ignore the effect of electron-ion interactions with a "two-temperature model" in which the electronic subsystem is modeled using a heat diffusion equation to determine the electronic temperature. We find that the electron-ion interaction friction coefficient γ_p is a significant parameter in determining the behavior of the system following the formation of the primary knock-on atom (here, a U^{3+} ion). The mean final U^{3+} displacement and the number of defect atoms formed is shown to decrease uniformly with increasing γ_p; however, other properties, such as the final equilibrium temperature and the oxygen-oxygen radial distribution function show a more complicated dependence on γ_p as the greater, but more uniform, heat dissipation caused by the electron-ion interaction allows atoms in the two-temperature model simulations to have greater kinetic energy and vibrate more around their equilibrium positions within the crystal lattice.