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Role of compression metallization in UO_2 fission-product energy cascade track: multiscale electron-phonon analyses

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Abstract

While the electronic stoppage of charged fission fragments is relatively well understood, the subsequent energy cascade is not. Recent efforts to investigate this cascade and predict the resulting damage have used a two-temperature model (TTM) of the electronic and phononic systems coupled with a classical molecular dynamics (MD) simulation of the crystal lattice. In order to accurately predict the track radius produced by a fission fragment in UO_2, this model (TTM+MD) requires that UO_2, an insulator, have metallic properties, e.g., a substantial electron thermal conductivity and heat capacity. However, it has been predicted that UO_2 becomes metallic under large pressures, and we perform *ab initio* (DFT-HSE) simulations to support this prediction. We show that the average U-U bond length decreases within and near the ion track during TTM+MD simulations, supporting the use of volume contraction to model the pressurized UO_2 cell. Additionally, we evaluate the electron, phonon, and electron-phonon coupling properties of UO_2 for variations in the pressure. In particular, we calculate the electronic heat capacity and thermal conductivity, and the electron-phonon energy coupling for use in subsequent TTM+MD simulations. The *ab initio* parameterized TTM+MD simulations provide a set of the track radii predictions which bracket and include the experimentally observed radii. The accuracy of the *ab initio* parameterized TTM+MD simulations depends on the pressure and degree of electron-phonon non-equilibrium assumed during the *ab initio* calculations. We suggest improvements to the current TTM+MD methodology in light of these results. Still, we show that the pressure-induced transition of UO_2 from insulator to metal and subsequent energy transfer from the electronic to phononic systems can accurately explain radiation damage during swift, heavy ion stoppage in UO_2. We make some additional observations regarding the accumulation and recombination of damage along the ion track and make comparison to the common SRIM model of ion stoppage and damage accumulation.

Keywords : Compression metallization, ab-initio, classical molecular dynamics, two temperature model, swift heavy ion, fission product, electronic stopping, irradiation