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Role of compression metallization in UO₂ fission-product energy cascade track: multiscale electron-phonon analyses

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10 Abstract

11 While the electronic stoppage of charged fission fragments is relatively well understood, the 12 subsequent energy cascade is not. Recent efforts to investigate this cascade and predict the resulting 13 damage have used a two-temperature model (TTM) of the electronic and phononic systems coupled 14 with a classical molecular dynamics (MD) simulation of the crystal lattice. In order to accurately 15 predict the track radius produced by a fission fragment in UO₂, this model (TTM+MD) requires that 16 UO₂, an insulator, have metallic properties, e.g., a substantial electron thermal conductivity and heat 17 capacity. However, it has been predicted that UO₂ becomes metallic under large pressures, and we perform ab initio (DFT-HSE) simulations to support this prediction. We show that the average U-U 18 19 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, 20 phonon, and electron-phonon coupling properties of UO₂ for variations in the pressure. In particular, 21 22 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 23 24 simulations provide a set of the track radii predictions which bracket and include the experimentally 25 observed radii. The accuracy of the ab initio parameterized TTM+MD simulations depends on the 26 pressure and degree of electron-phonon non-equilibrium assumed during the *ab initio* calculations. 27 We suggest improvements to the current TTM+MD methodology in light of these results. Still, we 28 show that the pressure-induced transition of UO_2 from insulator to metal and subsequent energy 29 transfer from the electronic to phononic systems can accurately explain radiation damage during swift, 30 heavy ion stoppage in UO_2 . We make some additional observations regarding the accumulation and 31 recombination of damage along the ion track and make comparison to the common SRIM model of 32 ion stoppage and damage accumulation.

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37	lectronic stopping, irradiation	

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