Investigating the Effects of Existing Damage on Primary Damage Formation in Zirconium

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The primary driver for the change in properties of nuclear reactor materials comes as a result of the formation of atomic-scale defects as a result of neutron collisions with the material's lattice structure. Over time, interstitial and vacancy type defects build up to concentrations far exceeding thermal equilibrium which leads to nucleation of extended defect structures that alter the performance of the material. Typically, molecular dynamics is the method for calculating the primary damage response but is often done in a perfect lattice. Here we investigate the effects of existing microstructure and elevated defect levels on defect production and clustering from collision cascades using multiple interatomic potentials for zirconium at various temperatures to better understand damage accumulations after long irradiations. Results can be incorporated into higher level models, such as cluster dynamics, as a source term that varies as a function of accumulated fluence.