Development of a mesoscale approach to the swelling of nuclear fuels

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Observations of lattice parameter change in UO_2, and in uranium alloys (e.g., UC, UN) can be interpreted to a large extent by the formation of interstitial loops. In these cases, the change in lattice parameter is given by $\Delta a/a = 1/3 N_L \Delta v^{loop}$, where N_L is the dislocation loop density and Δv^{loop} is the lattice volume change per loop, $\Delta v^{loop} = \pi R_0^2 b$, R_0 is the loop radius, and b - the Burgers vector. Our preliminary atomistic MD-simulations support the direct production and subsequent saturation of dislocation loops in several metals with different crystal structures. The results show that the emission of the dislocation loops lead to a periodic change of the lattice parameters. In our simulations, we used the following materials Al (fcc lattice), Fe (bcc lattice), and Zr (hcp lattice). The dislocation loops were introduced into the simulated system by indentation. The MD simulation results are compared to continuum theory and serve as a validation test of the dependence of lattice parameter change on interstitial loop characteristics. This approach is being extended to bubble nucleation and interdiffusion phenomenon and will facilitate the development of a kinetic model of radiation damage in nuclear fuels.