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Multiscale computer modeling of nuclear fuel properties at radiation and thermal impacts

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Description and prediction of behavior of nuclear engineering materials under operating conditions is one of the challenging goals in actual materials science. To solve this problem, when the restricted experimental information is only available (e.g. for the new kinds of nuclear fuel), the most perspective method seems to be theoretical description based on multiscale approach. In this case the various subtasks are jointly solved on different various time and spatial scales using theoretical physics and computer modeling. The cooperation of different techniques (such as quantum calculations, atomistic simulation, dislocation dynamics, phase field modeling, kinetic equations and continuum mechanics) allows predicting behavior of the nuclear materials in the absence of experimental data in the analyzed range of temperature, fission rate and other external conditions.

In this work, we developed multiscale computer models for various types of nuclear fuel: UN, U-Mo, UO2. The work includes several stages of model development: development of a set of novel interatomic potentials; study of primary irradiation damage (collision cascades and radiation track); calculation of basic properties of matter (diffusion coefficients, dislocation and grain boundaries properties, phase transitions); mesoscale model for evolution of phase-structural composition and change of mechanical/thermodynamics properties under operating conditions.

Country/Int. Organization

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