Materials Models and Simulations for Nuclear Fuels (MMSNF-8) Workshop
Albuquerque, Oct. 19-21, 2009

Models and Simulations of Nuclear Fuels: Results and Strategy

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To facilitate the discovery and design of innovative nuclear fuels, multi-scale models and simulations are used to predict irradiation effects on the thermal conductivity, oxygen diffusivity, and thermal expansion of oxide fuels. The scientific method used in this approach covers a large spectrum of time and space scales, from electronic structure to atomistic levels, through meso-scale and all the way to continuum phenomena. The multi-scale approach is illustrated using results on UO2 fuels with a focus on predictions of point defect concentrations, stoichiometry, and phase stability. The high performance computer simulations include coupled heat transport, diffusion, and thermal expansion, gas bubble formation and temperature evolution in a fuel element consisting of UO2 fuel and metallic cladding. Uncertainty evaluation reveals that ignoring the composition dependence of fuel properties in the simulations can lead to large errors (>10%) in the calculations of the centerline temperature and the thermal displacements. The second part of the talk is dedicated to a discussion of an international strategy for developing advanced, innovative nuclear fuels. After a brief review of the international status of nuclear fuels research, including results from American, European, and Japanese national laboratories and universities, a strategy for enhancing collaborations is proposed. The presentation ends with a discussion of existing and emerging international collaborations such as the Materials Models and Simulations for Nuclear Fuels workshops and the OECD/NEA Working Party on Multi-Scale Modelling of Fuels and Structural Materials for Nuclear Systems.