Atomistic modeling of mixed oxide fuel properties and radiation effects

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The fuel element under irradiation is submitted to a wide variety of coupled phenomena involving among others temperature, mechanical load, radiation damage, chemical interaction between the material and the fission products. The PLEIADES fuel performance platform co-developed by CEA can predict the behavior of standard or innovative fuel elements under operating conditions. It is nevertheless still a challenge for R&D to refine the constitutive laws used in fuel performance codes by a more physically based description of the fuel materials, and improve the capability to predict the fuel behavior.

We will present applications of atomistic calculations aiming at determining material properties and radiation effects of mixed oxide fuels that are useful to fuel performance codes, either directly or in a multiscale modeling scheme. In particular, in MOX fuels, the influence of the plutonium content on thermal properties, such as the heat capacity, is not well established. Similarly, the effect on bulk and defect properties in MOX of a few percent of minor actinides, such as americium resulting from irradiation and from the fabrication process out of used fuel, is also not known and is investigated in our study.