An atomic insight of the primary irradiation damages in nuclear fuel UO_2 with molecular dynamics simulations

L. Van Brutzel, A. Chartier

CEA-Saclay, DEN-DANS/DPC/SCP/LM2T, 91191 Gif-sur-Yvette, France
laurent.vanbrutzel@cea.fr

Nuclear fuel, uranium dioxide (UO_2), undergoes during is lifetime different type of irradiation which produce atomic point defects. The accumulation and diffusion of these defects create after some time major structural damage in the UO_2 matrix. Understanding at the atomic scale the creation of the primary damage is then of great interest. Experiments are difficult and expensive to set up at such length scale and under irradiated environment. Simulation could be then a good alternative to provide valuable insight of the material microscopic behaviours during irradiation. Molecular dynamics (MD) because of its intrinsic length and time scales is particularly suitable to study point defects creation under irradiation events. We will present herein a review of several MD simulations of collision cascades, thermal spikes in UO_2 single- and poly-crystals which have been carried out on massive parallel computers.

First, collision cascades with initial energies range from 5 to 80 keV have been carried out in single-crystals UO_2 to model the effects of a recoil nucleus. No amorphization appears at the end of the cascades. Only few Frenkel pairs are created and their number is lower than the number predicted by NRT law due to numerous recombinations. Clustering of vacancies has been found in the core cascades for high energy cascades. Study of cascade overlap sequence shows saturation on the number of point defects created as the irradiation dose increases.

Influence of grain boundaries on the production of point defects has also been studied. Collision cascades up to 80 keV have been initiated near different symmetrical tilt grain boundaries. In all the cases numerous point defects are created along or near the interfaces. However, for the grain boundaries with Schottky defects along the interface (misorientation angles superior to 15°) cascades seem stopped by the interface. Damage created by in poly-crystal UO_2 in which orientations and shapes of grains are randomly distributed has been also studied. Changes are found in the defect population creation during the first picoseconds of the cascade and in the microstructure at the grain boundaries.

Simulations of thermal spike in single- and poly-crystals UO_2 have been as well carried out in order to model fission tracks. The results show different primary damage type than for collision cascades. In the case of the single-crystal, for small linear energy transfer (4 kev/nm) no defects are created. The UO_2 matrix is perfectly reconstructed. For higher linear energy transfer (16 - 66 keV/nm) dislocation loops are found around the fission tracks. In the case of the poly-crystals, fusion and recrystallization of grains occurs.

Finally, the stability and the formation of xenon clusters in several extended defects such as grain boundaries and nanocavities in single-crystal UO_2 have been calculated. Static calculations show that xenon atoms are more likely to aggregate than staying homogeneously distributed. For xenon density higher then 0.12 mol/cm^3 in bubbles, the xenon crystallizes into fcc structure and small dislocation loops appear in the UO_2 matrix.