Large scale simulations of nuclear materials

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Management of nuclear waste requires in-depth understanding of various processes that determine the properties and behavior of radionuclide-bearing materials. Most of these processes happen at atomic scale and their kinetic aspect can be simulated by atomistic modeling techniques. Using large supercomputing resources available at Forschungszentrum Jülich we perform large scale simulations of kinetic processes occuring in nuclear materials. We present results of simulations of radiation damage cascades in novel waste forms such as monazite and pyrochlore ceramics. In particular we discuss the newly derived primary knock-on atom (PKA) dislocation probabilities and threshold displacement energies. The obtained energies are substantially different from the generic values assumed by software, such as SRIM, used for simulation of irradiation experiments. We will discuss the impact of the new threshold displacement energy values on simulation results performed with SRIM code and on understanding the results of irradiation experiments performed on the monazite- and pyrochlore-type ceramics. Because irradiated graphite represents significant amount of nuclear waste we also perform large scale simulations of this material. We will discuss the results of our studies of graphite surface chemistry, namely interaction of ideal and defective surfaces with water and simple molecules. We will also show the results of our simulations of diffusion processes of different species in graphite, including self-diffusion of carbon atoms (^{14}C). The comparison of the simulation results to the available experimental data will be broadly discussed. Last but not least, we will provide important information on energetics of defect formation in the considered materials, discuss the applied novel computational approaches and the applicability of large scale simulations to the research on nuclear waste.