Grain boundary structures and influence on segregation properties in uranium dioxide

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Uranium dioxide (UO_2) is the standard nuclear fuel in pressurized water reactors. Fission gases such as xenon (Xe) migrate to grain boundaries and cause swelling of the fuel. The structure of grain boundaries in UO_2 and the propensity of Xe to segregate to boundaries of different structure is explored in this work using empirical potentials and density functional theory. The specific boundaries studied were symmetric Σ 5 tilt, Σ 5 twist, and an amorphous boundary. Surprisingly, we found the energy of segregation to be very sensitive to the local atomic environment of the solute atom in the host and that there is a substantial difference in the overall segregation propensity to the three boundaries selected. Possible implications of this study on Xe diffusion and in predicting macroscopic fuel behavior are discussed.