Atomic scale simulations of self-diffusion and Xe diffusion in U_3Si_2 for reactor conditions

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Advanced fuels are being considered for deployment in light water reactors (LWRs). Advanced fuels are designed to improve performance and fuel economics during normal operation and/ or safety margins during accidents. This is achieved through improved thermophysical properties and higher uranium density compared to standard UO_2 and can also enable the use of advance materials for other reactor components (e.g. cladding). U_3Si_2 is being considered due to its high thermal conductivity as well as its high uranium density. The reduced centerline temperature of U_3Si_2 may also have the benefit of lower fission gas diffusivity and, therefore, better fission gas retention. However, there is no experimental data available for the diffusivity of fission gas in U_3Si_2 as function of temperature.
In this work, we employ atomic scale simulations to investigate the diffusivity of Xe in U_3Si_2 for the three diffusion regimes that exist under reactor operating conditions: intrinsic diffusion (high temperature), irradiation enhanced diffusion (intermediate temperature), and athermal diffusion (low temperature). The results can be implemented in fission gas release models within fuel performance codes, such as BISON. The diffusivities of U and Si point defects are also investigated as they form a key component of bubble growth and swelling models.