A modified Embedded-Atom Method interatomic potential for U-Si

Uranium-silicide (U-Si) fuels are being pursued as a possible accident tolerant fuel (ATF). This uranium alloy fuel benefits from higher thermal conductivity and higher fissile density compared to UO2. In order to perform engineering scale nuclear fuel performance simulations, the material properties of the fuel must be known. Currently, the experimental data available for U-Si fuels is rather limited. Thus, multiscale modeling efforts are underway to address this gap in knowledge. In this study, a semi-empirical Modified Embedded Atom Method (MEAM) potential is presented for the description of the U-Si system. The potential accurately describes not only the primary phase of interest (U3Si2), but also a variety of U-Si phases across the composition spectrum. A ternary U-Si-Xe potential is also developed for the investigation of fission gas behavior in U-Si systems.