Comparison of point defect migration energies in uranium nitride calculated using ADP and EAM interatomic potentials

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Choosing an interatomic potential one should consider its ability to predict the properties essential for the particular problem. Many problems are related to point defects and their migration. One of the most common methods of calculating defect migration barriers is the nudged elastic band method (NEB) [1]. Sometimes it can determine a migration mechanism incorrectly. The other common method is the direct molecular dynamics calculation of the defect diffusion coefficient depending on temperature, which require much more computational resources. Comparing both methods we have determined migration mechanisms and migration barriers of different point defects in uranium monoitride (UN) predicted by two existing potentials, namely EAM [2] and ADP [3]. In addition, we have noticed that uranium self-interstitial atoms interact with nitrogen point defects in different ways in those potentials.

[1] Henkelman G, Uberuaga B P and Jónsson H 2000 *The Journal of chemical physics* **113** 9901–9904
[2] Kocevski V, Cooper M W, Claisse A J and Andersson D A 2022 *Journal of Nuclear Materials* **562** 153553
[3] Tseplyaev V and Starikov S 2016 *Journal of Nuclear Materials* **480** 7–14