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Dear Editorial Board,

Journal of Nuclear Materials

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled `` Molecular dynamics investigation of grain boundaries and surfaces in U3Si2,” for publication in the *Journal of Nuclear Materials*. This is the first study into interfacial properties of U-Si nuclear fuel.

This manuscript leverages a recently developed MEAM interatomic potential describing the U-Si system in order to investigate the nature of interfaces in U3Si2. The interfacial energy as a function of temperature is investigated for ten symmetric tilt grain boundaries, eight unique free surfaces and voids of radius up to 35 Å. The point defect segregation energy for U and Si interstitials and vacancies is also determined for two grain boundary orientations. Finally, the entropy and free energy change for a grain boundary is calculated as a function of temperature.

The information within this manuscript can be utilized by mesoscale methodologies to study a variety of phenomena. The inclusion of realistic grain boundary, surface energies and free energy changes allows for the investigation of grain growth, void formation, void morphology and swelling in U3Si2. Realistic segregation energies can be incorporated to parametrize sink strengths utilized in phase-field defect evolution models. The ability to accurately describe each of these phenomena is critical in understanding microstructural evolution of nuclear fuel in-reactor.

There are no previous or concurrent submissions related to this work.

Sincerely,

Benjamin Beeler