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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 ``*An atomistic study of grain boundaries and surfaces in gamma U-Mo*”

, for publication in the *Journal of Nuclear Materials*. This article provides the first high temperature computational studies on body-centered cubic (bcc) Mo grain boundaries and the first computational studies whatsoever of bcc U and U-Mo alloy grain boundaries. This work is new, extensive, and we feel adds greatly to the scientific community.

The phenomenon of Mo depletion at grain boundaries is an important factor in the accelerated swelling behavior of U-Mo fuel. However, the physical origin of Mo depletion at grain boundaries is still unclear. In this work, molecular dynamics simulations have been performed to calculate the grain boundary and surface energies of bcc U, bcc Mo and alloys of U-Mo from 600 K to 1200 K to elucidate the driving force behind Mo depletion at grain boundaries. Also, a series of hybrid Monte Carlo/Molecular Dynamics simulations were performed to actively demonstrate the phenomenon of Mo depletion at grain boundaries.

It is observed that the lower grain boundary energy of bcc U, compared to bcc Mo, provides the driving force for Mo depletion at grain boundaries. This driving force diminishes with increasing temperature, but is not eliminated. This information can be utilized as inputs to higher length scale modeling methodologies and provide specification guidance to fabricators.

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

Sincerely,

Benjamin Beeler