Corresponding Author

Benjamin Beeler
North Carolina State University
2500 Stinson Dr, Raleigh, NC 27607
919.515.3737
bwbeeler@ncsu.edu

Dear Editorial Board,
Journal of Nuclear Materials

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled "Atomistic Investigation of Plastic Deformation and Dislocation Motion in Uranium Mononitride", for publication in the journal Applied Sciences.

This work employs molecular dynamics (MD) simulations to investigate the deformation behavior and dislocation motion in UN. The Kocevski potential predicted the principal slip system as $\frac{1}{2}\langle 110\rangle\{110\}$, aligning with experimental data, while the Tseplyaev potential predicted slip on $\frac{1}{2}\langle 110\rangle\{111\}$. The study demonstrates that MD simulations of stress-strain curves in single crystals with free surfaces yield accurate estimates of the nanoindentation hardness of UN. This methodology is particularly advantageous at elevated temperatures, where oxidation hinders direct measurements of UN's nanoindentation hardness. Both edge and screw dislocations are found to move via the kink-pair nucleation mechanism before displaying a linear variation of their velocity with stress. Based on these results, complete dislocation mobility functions were fitted. The threshold Schmid stress was estimated between 179 and 197 MPa, corresponding to an upper-limit uniaxial yield stress of 548–603 MPa for polycrystalline UN. These values show the expected orders of magnitude and can be used as inputs for plasticity or dislocation dynamics models. Finally, we observed that, at intermediate stresses, the subsonic steady-state motion of the edge dislocation in UN can be interrupted by jumps that have a maximum velocity equal to the average sound velocity.

To the best of our knowledge, this study is the first computational investigation of the stress-strain behavior and dislocation properties in UN, and the first that attempts to fit complete mobility functions for dislocations in a nuclear fuel. We believe this work provides a baseline for the computational study of dislocations in nuclear fuels that can be expanded and built upon by, e.g., conducting the analysis at higher temperatures which are more relevant for the operational conditions of nuclear reactors.

We believe our research offers valuable insights into the behavior of the UN and adds greatly to the scientific community.

Sincerely,

Benjamin Beeler