We thank the reviewers for their time and their constructive feedback. All comments have been addressed below, and, where appropriate, addressed in the manuscript.

Reviewer 1

1. Several statements in the manuscript closely resemble those in reference [10]. What is the key distinction between this study and reference [10]? Highlighting the differences would enhance the clarity of the paper.

Reference [10] evaluates two existing UN potentials, focusing on their effectiveness in predicting the thermophysical and mechanical properties of UN, with an emphasis on static (or near-static) properties. Notably, Reference [10] identified the strengths and weaknesses of each potential, highlighting areas where they performed well and where they were less reliable. It also showed preliminary indications that these potentials might be suitable for studying dynamic phenomena by predicting mechanical properties and defect formation energies with varying degrees of accuracy. Building on these findings, the present study investigates the dynamic aspects of deformation behavior and dislocation motion in UN, which provide more rigorous tests for the accuracy of force-field models. Additionally, this work strategically avoids the weaknesses identified in Reference [10] (e.g., not relying on 0 K energy minimizations with the Tseplyaev potential and avoiding structures that invoke U-U repulsion with the Kocevski potential) ensuring a more robust analysis of the dynamic properties.

The last two paragraphs of the introduction section have been expanded to address this idea.

2. Do the mechanical properties of UN influence its behavior under high temperatures and high radiation intensity? If so, this should be discussed in more detail.

The first paragraph of the introduction section has been updated to discuss how the mechanical properties of UN influence its behavior under irradiation.

3. In the abstract, please explain the symbols used when referring to the slip system, as readers may not be familiar with them.

The phrase “with angle brackets referring to the slip direction and curly brackets referring to the slip plane” has been added to the abstract.

4. Many abbreviations are not defined when first introduced in the text. Please ensure that all abbreviations are explained at their first mention.

The manuscript has been reviewed and all abbreviations have been explained at their first mention.

5. When discussing transition stress, clarify why Regime III is not considered in this study.

The paragraph on Regime III (starting at Line 261) has been updated to clarify why it is not considered for UN.

6. Why are only Tseplyaev and Kocevski's potentials considered? A justification for this choice would improve the manuscript.

To the best of our knowledge, there are 4 potentials of UN in the literature. Based on our initial tests as detailed in our prior work (<https://doi.org/10.1016/j.jnucmat.2024.155247>), we found that the Tseplyaev and Kocevski potentials are the most accurate and are potentially the only candidates to simulate the dynamical behavior of dislocations in UN. The other potentials struggled to get the most basic thermophysical properties of UN like the thermal expansion coefficient.

7. What is the main objective of Figure 2? The selection of parameter values needs to be explained.

The main objective of Figure 2 is to show the stress-strain curve predicted by each potential, which is indicative of the deformation mechanism predicted by that potential.

Apart from the supercell dimensions, the only other parameter chosen to generate Figure 2 is the strain rate. In Line 100, we already pointed out that “due to computational limitations, MD simulations of uniaxial tension are limited to nanometer-sized supercells and strain rates of at least 107 s−1”.

8. Why is the data in Figure 5 presented on a linear scale? If it is the same dataset, a semi-log scale alone might be sufficient.

Regime I is best presented on a log scale. Regime II (i.e., the linear part of the plot) is best presented on a linear scale to show that it is actually linear.

9. A wider range of temperatures for UN should be examined, as in practical applications, nuclear fuel must tolerate high temperatures, intense radiation, and long operational lifetimes, including effects such as moderator and the Doppler effect.

We agree with the reviewer that higher temperatures should be investigated and have already acknowledged this in the discussion section (Line 559) that “one limitation of our model is that it is based on simulations at a single temperature (300 K)”. However, this study represents the first step toward quantifying the dislocation properties of UN and is the first to attempt such quantification for nuclear fuel. Future research should build upon this work to address higher temperatures.

Reviewer 2

1. There are so many keywords, including five that represent the current work.

The keywords have been reduced to five: uranium nitride, molecular dynamics, plastic deformation, Peierls stress, and dislocation mobility.

2. “Many Shockley partials with a Burgers vector 1/6 (122) along the same planes”. Can you further explain?

The sentence has been changed to “We also observed several Shockley partials with a Burgers vector 1/6 <112> along the slip planes.” What we mean is that along the slip planes, perfect as well as partial dislocations have been observed. In the manuscript, we discuss this observation and highlight that most likely it is an artifact.

3. The nanoindentation hardness of UN couldn’t be measured at T > 473 K due to the formation of an oxidation layer on the surfaces of UN samples at higher temperatures, what kind of oxidation takes place?

The oxidation of UN has been the subject of many experimental studies, e.g., He et al. (2021) (<https://doi.org/10.1016/j.actamat.2021.116778>). However, this only pertains to our computational study in that the methodology we use to estimate the hardness can be applied at higher temperatures, at which an experimental measurement of UN’s hardness is not possible because the experiment would be measuring the hardness of the oxidation product rather than the hardness of UN.

4. The supercell is equilibrated at 1 K, and the Shockley partials transform back to a perfect edge dislocation. Please explain.

In our previous work (<https://doi.org/10.1016/j.jnucmat.2024.155247>) we showed that the Tseplyaev potential can stabilize metastable states of UN’s defective supercells (e.g., a supercell containing a dislocation) and that finite temperature equilibration (even as low as 1 K) is needed to get the correct configurations of defects. This was observed during the minimization process of the supercell containing the edge dislocation: After energy minimization at 0 K, the misfit dislocation transforms to two Shockley partials. When the supercell is equilibrated at 1 K, the Shockley partials disappear in the first few timesteps and we are left with a perfect dislocation.

5. How does an increase in stress lead to fewer fluctuations and the emergence of a nearly steady-state velocity?

Because the stress is high enough that its effect is no longer swamped by the instantaneous thermal and pressure fluctuations of the MD simulation. This is a hysteresis-like behavior usually observed in MD simulations.

Overall, the authors have done a commendable job in writing and explaining their work. The results are highly compelling and hold significant value for the scientific community, making the study well-suited for publication. I sincerely appreciate their effort.

Thanks!