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Dear Editor,

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled “Molecular-dynamics study of diffusional creep in uranium mononitride”, for publication in the Journal of Nuclear Materials.

In this paper, molecular dynamics (MD) simulations are used to study UN’s diffusional creep. Nanometer-sized polycrystals are used to simulate diffusional creep and to calculate an effective GB width. It is found that Nabarro-Herring creep is not dominant in the temperature range of 1700–2000 K and that the dominant diffusional creep mechanism is Coble creep with an activation energy of 2.28 eV. A method is proposed to calculate the diffusional GB width and its temperature

dependence in polycrystals. The effective GB width of UN is calculated as 2.69 nm. This value fits very well with the prefactor of the phenomenological Coble creep formula. It is demonstrated that the most comprehensive thermal creep model for UN can be represented as the combination of our Coble creep model and the dislocation creep model proposed by Hayes et al.

To the best of our knowledge, this study is the first computational investigation of the Coble creep behavior UN, and the most thorough investigation of the mechanisms of creep in UN. This paper has clarified discrepancies in historical creep experiments through a combined creep model, providing a useful tool for fuel performance modeling. We believe our research offers valuable insights into the behavior of UN and adds greatly to the scientific community.

Sincerely,

Benjamin Beeler