Reviewer #1: The reliability of molecular dynamics (MD) simulations critically depends on the accuracy of the empirical interatomic potentials employed. Therefore, it is essential that these potentials be thoroughly validated against more accurate methods such as density functional theory (DFT) calculations. Unfortunately, this important aspect, raised in the first review of this manuscript, remains insufficiently addressed after revision. The authors assert that the angular dependent potential (ADP) used for the U-Mo system has been shown to reasonably reproduce several material properties for both pure U and U-Mo alloys. However, the supporting references they provide (Refs. 38-41) predominantly focus on applications of the ADP potential in MD simulations, rather than on rigorous validation against DFT or experimental benchmarks. Notably, Ref. 38 does not employ the ADP potential for U-Mo at all and is therefore not relevant in this context; it should be removed from the list of supporting references. Furthermore, in Figures 1A and 1B, the formation energies of both interstitials and vacancies exhibit a significant variation over the temperature range of 600 K to 1200 K. Such behavior may be an artifact of the empirical potential rather than a reflection of true physical trends. Without additional validation or discussion, it is difficult to assess the physical realism of these temperature-dependent results. To strengthen the manuscript, the reviewer recommend that the authors provide validation of the ADP potential through direct comparison with DFT data, either from the literature or new calculations.

We acknowledge the need to properly establish the credibility of the interatomic potential. In the original manuscript presenting the potential, density functional theory data was used for alpha, gamma and liquid phases of U, bcc and liquid phases of Mo, and gamma, gamma’, and delta phases of U-Mo. The potential reproduced ab initio reference data with the average accuracy of 281.97 meV/Å for the forces, 35.18 meV for the energies, and 0.42 GPa for the stresses. This is considered excellent agreement. Due to their computational expense, there is very limited additional DFT or AIMD data on U-Mo alloys. The only relevant DFT work is by Landa [https://doi.org/10.1016/j.jnucmat.2011.02.019] which looked at enthalpy of mixing curves, which the original ADP manuscript cited and compared against, showing reasonable results. To the knowledge of the authors, there are no studies on point defects using DFT in bcc U-Mo alloys. Such an undertaking is itself a manuscript, would require months of computational effort, and is outside of the scope of this work. Additionally, there are even fewer experimental efforts for which to benchmark against, beyond those listed in the original ADP manuscript. Thus, we have more completely explained the background of the interatomic potential, the data with which it was fit to, and the utilization cases. We have also provided additional context.

The prior reference 38 has been removed as it uses an EAM potential, not the ADP in question. We thank the reviewer for catching this mistake.

The updated paragraph discussing the potential is below in latex formatting.

MD simulations are performed utilizing the LAMMPS \cite{plimpton1995} software package and a U-Mo angular dependent potential (ADP) \cite{starikov2018,beelerumoxe}. This potential was fit to density functional theory data including multiple phases of U, Mo, and U-Mo, and reproduced \textit{ab initio} reference data with the average accuracy of 281.97 meV/Å for the forces, 35.18 meV for the energies, and 0.42 GPa for the stresses, which is considered excellent agreement. The potential has been shown to reasonably predict a number of material properties and phenomena in both pure U and U-Mo alloys, including phase stability/distortion \cite{starikov2018,starikov2023,kolotova2020}, $\alpha$-U diffusivity and grain boundary energetics \cite{wang2023,mahbuba2025}, and $\gamma$U-Mo grain boundary properties \cite{hasan2024}. Unfortunately, there are limited additional \textit{ab initio} or experimental data available for further potential validation. However, in the authors' opinion, this potential is currently the most accurate tool for the description of the U-Mo phase in classical molecular dynamics.

Reviewer #3: [Since some of the equations are difficult to read, I have attached a PDF version for clarity. The content remains the same.]

In this paper, the authors investigate various properties related to point defects in U-Mo alloys under pressure using molecular dynamics simulations. U-Mo alloys are important fuel materials, and the analysis conducted in this paper is also essential. The employed analysis methodology appears generally reasonable, except for the issues listed below. In addition, the manuscript contains several inappropriate analyses and lacks sufficient discussion in critical areas, as outlined below. Therefore, I do not recommend this manuscript for publication in the Journal of Nuclear Materials in its current form and suggest major revisions.

1. Throughout the manuscript, various properties are evaluated without distinguishing between U and Mo atoms. However, properties such as formation energies and diffusion coefficients are different for U and Mo and should be evaluated separately. If such a distinction is not made, the authors should clearly explain why it is appropriate to treat U and Mo as indistinguishable in their analysis.

We agree that U/Mo properties are unique. The approach we have taken is to provide an averaged defect behavior for the specific U-Mo compositions. With no *a priori* knowledge of the concentration of types of defects, we have inserted random defects in such a manner as to maintain the composition of the U-Mo system. Thus, the interstitial formation energy of U-10Mo (~22 at.%) consists of 22% Mo defects and 78% U defects. This is in line with the approach of random solid substitutional alloys presented in [https://doi.org/10.1016/j.commatsci.2021.110308]. We have refined the methods section to hopefully more clearly inform the reader of these distinctions and what the paper does or does not attempt to compute.

2. U-Mo alloys exhibit a miscibility gap, and phase separation is expected at high Mo concentrations. Nevertheless, the authors carry out all calculations assuming a completely homogeneous solid solution, even at high Mo concentrations. The significance for using this assumption should be clearly explained.

Per the phase diagram of U-Mo from Okamoto [https://doi.org/10.1007/s11669-012-0095-z], U-Mo at elevated temperatures exists in a random solid solution bcc phase for up to approximately 40 at% Mo. Irradiation of U-Mo alloys has constantly shown a random solid solution [https://doi.org/10.5516/NET.07.2014.706]. Effects of irradiation are likely to induce a randomization effect, limiting the appearance of short-range order. Therefore, we believe the most appropriate and technically relevant exploration is of a random solid solution U-Mo alloy in the bcc structure with varying Mo content. Additional sentences have been included to emphasize this point.

3. The formation energy is defined in Eqs. (1) and (2), but the reference states used in these definitions are unclear to me. For instance, if the formation energy of a U interstitial is defined as E\_f^(U\_int )=E^(U\_int )-E^bulk-E\_U, it is understood that a U atom has moved from a pure U reservoir into the U-Mo alloy as a interstitial atom. Alternatively, a reasonable definition would be E\_f^int=E^int-〖(1+N)/N E〗^bulk, where one atom in U-Mo alloy is taken from the bulk to form an interstitial. Here, the energies on the right-hand side are directly obtained from MD, not as defined by Eq. (2). The definitions given in Eqs. (1) and (2) appear more complicated and less transparent. A more detailed explanation is necessary to clarify these points.

The one critical aspect missing from the reviewer’s formulation is the inherent formation energy of the alloy itself. In the aggregate, we believe that the formation energies from the reviewer’s formulation and the formulation presented in this manuscript would result in effectively the same answer, with some statistical variation. However, this methodology applies for the insertion of a given defect of one species and performs an averaging over all defect types inserted. This is very similar to the robust approach of Zhang [https://doi.org/10.1016/j.commatsci.2021.110308], as indicated in a prior response. We believe that the formulation presented here is more complete than simply taking a reference state, without accounting for the underlying alloy formation energy.

4. If my understanding is correct, the formation volume is calculated as (∂E\_f)/∂p instead of (∂H\_f)/∂p in this paper. This approach is incorrect, as E\_f=H\_f only holds at zero pressure. Since finite pressure conditions are considered in this work, the formation volume should be determined typically via NPT-MD simulations of defective structures, which does not appear to have been performed in this study. If this understanding is incorrect, a clearer explanation of how the formation volume is computed should be provided.

We apologize for any misunderstanding, the formation volume is in fact determined from the slope of the formation enthalpy with respect to pressure. We have slightly modified the wording in the methods to ensure that this is clear.

5. The elastic dipole tensor is defined in Eq. (4) as the first-order coefficient in the strain expansion of defect energy. Under this definition, the elastic dipole tensor is independent of strain or pressure. However, in this study, the pressure dependence of the elastic dipole tensor is analyzed, probably suggesting a generalization of the above definition. The authors should explicitly define the version of the elastic dipole tensor used in this work and clarify how it differs from the conventional definition (Eqs. 4 and 5).

Check this… que saco

6. The authors claim that the elastic dipole tensor for interstitial defects is isotropic. However, in bcc structures, interstitials typically adopt dumbbell configurations, which result in anisotropic elastic dipole tensors. If the dipole tensors are averaged without accounting for specific interstitial configurations, isotropy may appear artificially. The authors should consider the actual geometry of interstitials in their calculations. It is possible that dumbbell orientations fluctuate rapidly at high temperature, leading to effective isotropy. In such a case, the authors should verify and demonstrate whether this dynamic averaging occurs in their simulations.

It probably does…

7. The temperature used in the pressure gradient simulations is not specified. This information should be included.

The temperature used in the pressure gradient simulations (1200 K) is now included in the computational details section. (Section 2.2)

8. In the simulations involving pressure gradients, the analysis of defect travel distance and spatial spread is insufficient. Given that pressure-dependent diffusion coefficients, the evolution of defect density could be estimated by solving the diffusion equation　∂ρ/∂t=∂/∂x D(x) ∂ρ/∂x. 　Such an analysis should be included to support the discussion.

The evolution of defect density has been estimated by solving the diffusion equation. The analysis is now included in section 3.4. A plot of the estimated defect densities is added to Figure 9. (Page 16-17)

9. In the radiation damage simulations, the number of defects is reported to be the largest at 1200 K. However, it is generally expected that defect recombination becomes more efficient at higher temperatures, leading to a lower net defect population. The results presented here contradict this common understanding, yet no sufficient explanation is provided. A more thorough discussion is necessary to reconcile this discrepancy.

Additional explanation is now included in the manuscript. While additional recombination will take place at higher temperatures, this leads only to a lower fraction of residual defects compared to that found at lower temperatures. However, the magnitude of the residual defects is dependent upon the temperature, as a ballistic event induces a pseudo-localized melting, which becomes easier/larger as the temperature approaches the melting point of the system. Thus, the peak number of defects is dramatically higher at 1200 K than at 400 K, leading to a higher number of residual defects, despite the recombination efficiency being higher.

Reviewer #4: In the revised manuscript, the authors has addressed the majority of the reviewers' comments. While the general topic is of interest, there are still a few issues that the authors should address:  
1) If possible, please compare the calculation results of this article, especially the formation energy of defects, with the previously published DFT or experimental results.

To do.

2) Fig.1 is taken from a published paper Ref.[23] by the same authors, and the according discussion is similar. The author should expound on its necessity although the authors mentioned in the manuscript that This figure is updated from [23].

Further statistics, minor edits, expand here.

3) The defect formation energies initially decrease and subsequently increase with the increasing Mo content. However, the underlying physical mechanisms and contributing factors responsible for this trend were not discussed by the authors.

It is not known… related to mixing enthalpy? Related to mechanics?

4) In cascade displacement simulations, excess kinetic energy is removed through temperature rescaling. However, this approach may influence the defect evolution process and the number of surviving defects, both of which are temperature-dependent.

This is correct. This approach has been validated previously [cite Yongfeng’s paper] and was further analyzed here. Minor effects, comparable to statistical fluctuations, are observed for simulations with temperature rescaling versus systems with an NVE ensemble and a heat sink. The lack of a statistically significant difference indicates that this approach is suitable, and avoids the potential of cascades interacting with a boundary layer which can modify their behavior. It should also be noted that the temperature scaling rate imposed in this work is much more conservative (less frequent) than that in XXX [cite Yongfeng again], thus, we have confidence in the robustness of this work.