**Comments from the editors and reviewers:**  
-**Reviewer 1**  
  
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The authors present their work on threshold displacement energies (TDE) in uranium metal. This work is interesting and valuable, as TDEs are a fundamental property of that material that can also be of great importance to parameterise mesoscale or macroscopic models. I also think that this will be of interest to JNM readers. Overall, I recommend this article to be published provided that the authors address the points below.

p.4: It would be useful to have the approximate physical lengths of the simulation boxes, particularly considering that the lattice parameters of alpha-U and gamma-U are not mentioned in that paper.

The supercell sizes have been included: 25x12x15 for alpha U, 20x20x20 for gamma U. Each supercell is approximately a cube of 70 Å along each side. These supercell sizes were found to be sufficient to encapsulate even the largest possible cascades included in this study based on preliminary testing.

p.4: The authors mention a range of 35.3º for phi, divided into 4º intervals, surely at least one of these numbers is inaccurate.

The 35.3 is divided into 4-degree intervals, with the final interval of 3.3 degrees. This has been added.

p.6: It is mentioned that the simulations have been done at 800 K and 1000 K. Why have these temperatures been chosen?

The following text has been included: “These temperatures are within the operational temperature ranges for UZr fuel. In addition, the potentials are limited in the range of temperature available for investigation, and as such the temperatures chosen allowed for comparisons across potentials and between phases without going beyond the means of each individual potential. Below 800 K, the bcc phase is considered to be unstable while above 1000K, the thermal fluctuations make it difficult to separate irradiation produced defects and thermally produced defects.”

p.6: A standard arithmetic average over the different directions is problematic from a statistical point of view. Using the scheme presented in p.4, the directions are not uniformly distributed. If the authors have used the correct averaging presented in Nordlund et al. 2006, they should make it explicit, if only to help readers doing it properly in the future.

An arithmetic average is taken in this work. The directions are uniformly distributed except for the last direction and the error introduced is minimal. The method developed by Nordlund et al in 2006 would perhaps be a more accurate method for averaging; however, we do not believe it would change the average value much because the directions in this work are uniformly distributed.

The angular scheme was designed in such a way as to generate consistent solid angles between each direction, and thus uniformly distribute the directions. Each individual direction samples a solid angle of the same given area. The only exception is for the single direction in the bcc phase that has an interval of 3.3 degrees in phi, compared to the rest of the directions which have an interval of 4 degrees. The error introduced by overweighting this single direction (by approximately 18%) among the 55 directions is negligible to the overall results.

p.6: I am not entirely sure why a polynomial was fitted to the average data. I assume that this was done to calculate the TDE more accurately, but this is unclear. It would be interesting to have the data points along with the polynomial on figure 3, to show the quality of the fit.

As the referee surmises, the polynomial fits were introduced to calculate the TDE value more precisely. Polynomial fits were utilized to determine the median points of the data and to better average the data. This statement is included in the manuscript. Data points have also been included on Fig. 3.

p.6: The authors make the point that the Frenkel pair (FP) formation probability is not a step function at finite

temperature. Then, it would be nice to show the curves for the two considered temperatures in figure 3.

We thank the referee for the suggestion. Changes in temperature have been included in Fig 7. This figure now shows the effect of temperature on the displacement energy for each of the interatomic potentials.

p.9: The authors discuss direction-dependent changes in TDE. It would be interesting to discuss this in terms of the crystal structure (neighbour and interstitial sites positions). As it is, the numbers do not give much insight on why specific directions have particularly large or low TDEs.

We thank the referee for this suggestion. The discussion of the contour plots has been expanded to provide greater insight into the crystallographic features that result in variable displacement energy with PKA direction.

p.9: The authors emphasize the importance of selecting a good potential, but in the following sentence explain that because of the lack of experimental data it is impossible to assess the quality of the potentials. It seems that instead of arguing for selecting the right potential that reproduces experimental numbers, the authors really argue for using different potentials to try to estimate systematic error caused by one particular potential.

The following sentence has been added: “When calculating properties such as displacement energy in uranium where there is no experimental data available for comparison, utilization of multiple interatomic potentials is important in order to determine possible sensitivities of data related to the choice of interatomic potential. Thus the property being calculated is verified by different potentials to be consistent even if it cannot be validated against available experimental data.”

p.10: The authors have done the simulations at two temperatures, they should show the resulting averaged probabilities on figure 5, this would give more information than simply the TDE reported in table 2.

A figure has been included (now fig 7), that summarizes results for three potentials and two temperatures in graphical form.

p.10: Discussions on the ZBL potential do not really belong in the results section. I would suggest adding a section describing the potentials before the results section. It would also be useful to have the functional forms of the different potentials, and possibly the exact potential parameters used, in the interest of helping other people reproduce these results. Alternatively, the LAMMPS definitions of the potentials used would be valuable supplementary information. It would also be useful for context to provide basic materials properties predicted by the three potentials such as lattice parameters and cohesive energy of the considered structures when appropriate. To be honest, the dimer energy predicted by the UMo ADP potential as shown in figure 6 does not inspire much confidence.

An appendix outlining and discussing the MEAM and ADP potential formalisms, with a brief comparison of basic properties of gamma U calculated by each of the potentials is now included in the manuscript. The dimer-dimer work has been included in the computational details. The results text has been appropriately modified.

p.11: The way the error ranges have been calculated and the authors obtained the 68% confidence energy intervals is unclear and should be detailed. In any case, the intervals reported in table 2 are not centred on the mean, and therefore are not confidence intervals in the standard sense.

This paragraph has been modified, with an included figure to try to provide clarity. For a given PKA energy, the error bars are symmetric. For each data point, upper and lower bound probability curves are generated with the +/- standard error. The resultant median of the +/- curves need not be symmetric around the original curve median. Thus, the discussion has attempted to highlight that the curves represent a 68% confidence interval for the data, not necessarily a 68% confidence interval for Ed.

p.12: It might be useful to clarify that the FP energy calculated that way correspond to unbound FP, which is not necessarily the case of the FP formed during the TDE simulations.

Correct. This distinction has been included.

p.13: The uncertainties should be added to the defect energies in table 3.

As suggested, uncertainties in the form of +/- deviation from average values have been added to the table.

p.18: The temperatures considered for alpha-U are 600 K and 800 K. The authors should explain why these values have been chosen, and why are they different from the temperatures chosen for gamma-U.

The discussion of choice of temperature was included in computational details. “Temperatures of 800 K and 1000 K are investigated for gamma U and temperatures of 600 K and 800 K are investigated for alpha U. These temperatures are within the operational temperature ranges for UZr fuel. In addition, the potentials are limited in the range of temperature available for investigation, and as such the temperatures chosen allowed for comparisons across potentials and between phases without going beyond the means of each individual potential. For example, below 800 K, the bcc phase is considered to be unstable while above 1000K, the thermal fluctuations make it difficult to separate irradiation produced defects and thermally produced defects.”

p.18: As in the case of gamma-U, standard, unweighted arithmetic averaging is probably inaccurate.

This point was addressed above. Directions were designed to be equal solid angles, allowing for direct arithmetic averaging.

p.19: Figure 11 shows peaks for some of the FP formation probability (notably around 30 eV, with one reaching 0.9 before decreasing below 0.8). This should be discussed and linked with structural features (concerned directions and mechanisms involved). This figure also shows local minima (e.g around 100 eV and 120 eV) which suggest sampling issues.

These simulations have statistical noise and thus one would expect fluctuations, although the specific extreme fluctuations referenced are rare. Additionally, this is the probability of defect formation, not the number of defects produced per PKA. # of defects per PKA would show a more monotonic increase with increasing energy, as it is possible to create multiple defects from a single PKA, however it is the probability that is the target in these simulations. Thus, the probability will bounce around 0.7-0.9 until higher PKA energies (energies beyond the scope of this study). With greater samples, yes, this noise should cancel out. By analyzing many directions, the noise from a single direction is nullified. Also, considering the scope of this work, and that over 400k simulations have been performed, we feel that the current sampling of the crystal systems is sufficient, even though there will be some statistical noise for a given direction. More discussion along these lines has been included.

p.20: As in gamma-U, the direction dependence of the TDEs should be discussed in terms of crystal features.

Similar to the added discussion in gamma U, the section discussing the contour plots for alpha U has been expanded to more directly refer to the crystallographic orientations of the alpha structure.

p.21: The uncertainties should be added to the defect energies in table 5.

Error bars have been added to the table.

p.22: It would be useful to add the DFT defect formation energies from the literature to the tables 5 and 6 where they could be directly compared with the MD results.  
DFT formation energies have been added to table 3 and table 5.

Finally, there were a couple of minor typos and awkward sentences that could benefit from additional proofreading.

Manuscript has been proofread again in order to identify and correct such errors. We will be happy to work with editors to proofread further.

-**Reviewer 2**  
  
  - I recommend the paper for publication after minor corrections in accordance with the following remarks.

1. Page 6, lines 5-6 of item 3.1. It is reasonable to point out that results shown in Fig.2 were obtained for temperature of 800K.

It has been added that these results are for 800 K.

1. Page 13, line 6. The units of energy should be given.

Units added.

1. Page 15, lines 1-3. It is desirable to give more details what r2 is and how D0 and Em are calculated.

This section has been expanded to define r2 and explicitly state how D0 and Em are determined.

1. Page 15, second line below Eq.(2). Are cintand cvac really energies?

The referee is correct, these are not energies but concentrations. This has been corrected.

1. Page 18, third line of item 3.2. Only one potential is used for α-U.

This sentence has been modified to reflect that fact.

1. Page 19, Fig. 11. Sharp peaks are observed in probability curves for many directions. What is the cause? Some curves cross the line of probability of 0.5 several times. How was displacement energy evaluated in such cases? There are a few resembling peaks in Fig.2. But they are not so sharp there.

These simulations have statistical noise and thus one would expect fluctuations. With greater samples this noise should cancel out. By analyzing many directions, the noise from a single direction is nullified. Additionally, this is the probability of defect formation, not the number of defects produced per PKA. # of defects per PKA would show a more monotonic increase with increasing energy, as it is possible to create multiple defects from a single PKA, however it is the probability that is the target in these simulations. Thus, the probability will bounce around 0.7-0.9 until higher PKA energies (energies beyond the scope of this study).

For a single direction, the Ed would be determined by fitting a polynomial and calculating where this polynomial crossed 0.5. For the average system, this raw data is utilized and averaged. In the aggregate, any such fluctuations are canceled out. More discussion along these lines has been included.

1. Page 22, lines 2-4 below Table 6. In my opinion, formation energy can be easily calculated for zero temperature to compare with DFT results.

Results have been compared to DFT results. 0 K alpha defects have been included on the table.