

Calculation of Threshold Displacement Energies in UO_2

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Abstract

Despite the extensive utilization of uranium dioxide (UO_2) as a fuel in commercial nuclear reactors, there is only minimal information regarding the fundamental nature of radiation damage at high temperatures, such as those experienced by the fuel under operation. In this work, molecular dynamics simulations have been performed to determine the threshold displacement energy (E_d) for oxygen and uranium in UO_2 at 1500 K. Three definitions of displacement energy were employed to fully study the nature of low energy radiation damage: 1) the probability of having the primary knock-on atom (PKA) leave its original lattice site, 2) the probability that the PKA will permanently displace atoms from their original lattice site, and 3) the probability of forming a stable Frenkel pair. Additionally, four unique interatomic potentials were utilized to investigate uncertainties associated with potential choice in high temperature radiation damage studies in UO_2 . This work provides critical insight into the high temperature behavior of radiation damage in UO_2 , as well as the variation in behavior between oxygen and uranium PKAs.

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1. Introduction

Due to its usage as a nuclear fuel, uranium dioxide ([..¹¹]UO₂) has been thoroughly studied both theoretically and experimentally over the the last half-century. Utilization of this data can provide correlations for a range of thermo-mechanical behaviors, and such correlations can serve as inputs to continuum-level fuel performance modeling. Such fuel performance models [? ? ? ? ?] have shown impressive accuracy in their ability to describe fuel behavior. However, fuel performance models that rely on empirical correlations are inherently limited in their applicability to the scope of the data used to construct those empirical models. In order to predict fuel behavior in scenarios outside of the existing experimental data regimes, the underlying physics of the material systems needs to be included into the fuel performance models. This can be done by informing continuum level simulations with mesoscale and atomistic data taking into account the microstructural evolution of the material.

In addition to very high neutron flux and fluence during operation, nuclear fuels are exposed to high energy fission fragments and alpha particles released during radioactive decay of fission products. The ability to quantify the damage resulting from this radiation is a critical step in describing and understanding microstructural evolution of nuclear fuel. The threshold displacement energy ([..¹²]E_d) is a critical measure of a material's response to radiation damage. The amount of damage that a material system experiences under irradiation is typically described in displacements per atom (dpa). Models such as the Norgett-Robinson-Torrens (NRT) [?] utilize a threshold displacement energy to calculate a given *dpa* based on the material and irradiation condition. For a multicomponent system an effective displacement energy needs to be utilized in the NRT model [?], while the more rigorous approach by Parkin and Coulter [?] requires a displacement energy for each component. It is thus critical to possess an accurate description of [..¹³]E_d in order to accurately assess the number of *dpa* the material system of interest experiences.

There have been several investigations over the past three decades studying [..¹⁴]E_d in UO₂. Using transmission electron microscopy on room temperature [..¹⁵]UO₂ samples, Soullard [? ?] determined that the threshold displacement energies in [..¹⁶]UO₂ are 20 eV for oxygen primary knock-on atoms (PKAs) and 40 eV for uranium PKAs. However, this work makes usage of a variety of assumptions, including the validity of the Kinchin-Pease model, extrapolation of dislocation loops to the number of point defects and that the oxygen [..¹⁷]E_d is half that of the uranium [..¹⁸]E_d. Additionally, Soullard only reports that the

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uranium ^[.19] E_d is “on the order of 40 eV.” These are the only known experimental studies on ^[.20] E_d in UO_2 . Therefore there are no experimental studies on the value of E_d for O PKAs in UO_2 .

Computationally, Meis and Chartier [?] used the sudden approximation method within the Mott-Littleton approach [?] in order to determine ^[.21] E_d . They determined that the value of ^[.22] E_d for oxygen PKAs (^[.23] $E_d[\text{O}]$) is approximately 20 eV, and ^[.24] E_d for uranium PKAs (^[.25] $E_d[\text{U}]$) is approximately 50 eV. Molecular dynamics simulations have also been employed to investigate radiation damage in ^[.26] UO_2 , although not specifically ^[.27] E_d . Van Brutzel [?] and Martin et al [?] performed radiation damage simulations for PKA energies of up to 100 keV at 300 K and compared their results to the NRT correlation for an ^[.28] E_d value of 30 eV (averaged over the experimental ^[.29]approximations of 20 eV for O and 40 eV for U). It is interesting to note that Van Brutzel determined that the linear NRT ^[.30]correlation was not valid at higher energies due to the recombination of defects and that the number of defects instead follows a power law, but Martin showed that a linear relationship is retained at high PKA energies. Devanathan [?] conducted 1 keV cascade simulations at 300 K utilizing five different interatomic potentials and extrapolated the displacement energy from the modified Kinchin-Pease equation [?]. Martin [?] studied the effect of temperature on displacement cascades using the Morelon [?] potential. The authors are unaware of any attempts to investigate the nature of ^[.31] E_d in UO_2 at high temperatures. We note that all these studies employ the basic monoatomic NRT model which is not rigorously applicable to the diatomic UO_2 , which has two constituents that have very different Z values and thus very different charged particle scattering cross sections.

Although ^[.32] E_d has been extensively studied computationally, there still exist some discrepancies with regard to how individual researchers define ^[.33] E_d . Meis and Chartier [?] define ^[.34] E_d as the “minimum energy transferred to a lattice atom along a given crystallographic direction yielding the creation of a stable Frenkel defect”. However, other authors such as Devanathan [?] define the threshold displacement energy as “the minimum energy needed to displace an atom from its lattice site.” This definition from Devanathan is yet unclear with respect to how displacement is defined. For instance, the energy required to remove an

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atom from a lattice site *permanently* is higher than the energy required to remove an atom from its lattice site and have it eventually return. [..³⁵] Perhaps a more precise definition is described by Motta [?] where [..³⁶] E_d is "the minimum energy required to sufficiently move the atoms so that they do not return to their initial sites". It should be noted that this definition from Motta does not necessarily indicate the generation of a stable Frenkel pair. It is worth investigating all three definitions (generation of a Frenkel pair, displacement off initial lattice site, permanent displacement off initial lattice site) of the threshold displacement energy separately in order to ascertain the differences in the [..³⁷] hope of implementing the correct definition for the correct application.

In this study we will determine the threshold displacement energy for uranium and oxygen PKAs in [..³⁸] UO_2 at 1500 K. [..³⁹] Four different interatomic potentials will be utilized to determine uncertainties associated with potential choice in high temperature radiation damage studies in [..⁴⁰] UO_2 . The threshold displacement energy is investigated through the following definitions: 1) the probability [..⁴¹] that a primary knock-on atom (PKA) [..⁴²] leaves its original lattice site, 2) the probability that a PKA permanently displaces an atom from its original lattice site, and 3) the [..⁴³] probability of forming a stable Frenkel pair. It is worth pointing out that the self-diffusion energy of an atom from its lattice site into an interstitial configuration is closely related to the second E_d , however E_d depends on the actual barrier in the crystallographic direction of displacement, while for the self-diffusion the minimum barriers are considered. This work provides the first high temperature investigation into the threshold displacement energy of [..⁴⁴] UO_2 .

2. Interatomic potentials

Molecular dynamics (MD) solves Newton's equations of motion on a collection of particles utilizing a potential energy function that defines the ways in which the particles interact. In this study, molecular dynamics are used to determine the threshold displacement energies. Although it is possible to determine [..⁴⁵] E_d from other methods like density functional theory (DFT), such *ab initio*-MD methods are deemed far too computationally expensive at this stage and there exist a plethora of interatomic potentials available for the [..⁴⁶] UO_2 system that are in common usage, particularly with regard to radiation damage simulations.

This work makes use of [..⁴⁷] four distinct UO_2 interatomic potentials to govern particle interactions.

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The Basak [?], [..⁴⁸]Yakub [?], Morelon [?], and Cooper [?] potentials have all been demonstrated to reproduce certain experimental properties when tested at temperatures and pressures of interest [? ? ?]. The [..⁴⁹]Yakub potential was selected specifically because of [..⁵⁰]its close approximation of physical properties of [..⁵¹]UO₂ at 1500 K, such as the lattice parameter [..⁵²] a_0 , specific heat [..⁵³] C_p , and the Bulk modulus K [?]. The Basak potential was selected because it is an improved fitting of the Yamada potential, created by using isothermal compressibility data in order to better model the lattice parameter and lattice expansion [?]. The Morelon potential has been used extensively and was specifically fit to better approximate experimental point defect formation and migration energies. The Cooper potential is a more recent potential that combines a pair potential with a many body embedded atom method description and shows excellent prediction of thermophysical properties and Frenkel pair energies.

These potentials in their native form do not contain a repulsive potential sufficient to model small distance interactions between atoms. For this reason, the Ziegler-Biersack-Littmark (ZBL) [?] potential was splined to the three separate potentials so that high energy atoms would interact with other atoms in a more physical manner. This ZBL spline occurred between 0.35 and 1.34 Å for the O-O interaction, 1.7 and 2.12 Å for the U-U interaction, and 0.64 and 1.09 Å for the U-O interaction. At these interatomic separation distances the respective potential energy contributions well exceed the thermal energies at the temperatures of interest. [..⁵⁴]Additionally, the potential energy at the outer ZBL cutoff exceeds point defect energies. As such, this splining does not affect the properties of the potentials for non-irradiation observables[..⁵⁵].

3. Computational details

Molecular dynamics simulations are performed with the LAMMPS [?] software package. Threshold displacement energies are typically obtained through supplying a primary knock-on atom (PKA) with an additional amount of kinetic energy and the subsequent interaction of the PKA with other atoms in a lattice. By systematically increasing the PKA energy over a prescribed range of energies, the relationship of the number of defects produced to PKA energy can be developed. In a system at 0 K utilizing low energy PKAs, this relationship would be a step function, where below a critical PKA energy zero defects are generated and above that critical energy a single defect is generated. However, in a system at high temperature the thermal fluctuations smooth out this step function and create a continuous probability

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curve. Thus, a range of PKA energies are required to adequately sample the probability distribution for defects as a function of PKA energy.

Simulations were performed at low PKA energies in the 5-65 eV range in increments of 5 eV and a subset of simulations were performed at higher PKA energies in the ⁵⁶100-200 eV range in order to fully investigate the breadth of atomic displacements in the system. ⁵⁷These energies are sufficiently low that electronic stopping can be neglected. The simulations consisted of 32,928 atoms⁵⁸. Systems were initialized and minimized at 0 K. The temperature was then increased to 1500 K and the system was equilibrated in an NPT ensemble. This temperature was chosen as it is a realistic fuel temperature. A PKA is introduced into the equilibrated system, the timestep is reduced to ⁵⁹ 5×10^{-5} ps and the system is allowed to evolve in an NVE ensemble for 20000 timesteps (1 ps), after which the timestep is increased to ⁶⁰ 5×10^{-4} ps and the simulation is allowed to evolve for another 9000 timesteps (4.5 ps), for a total post-PKA relaxation time of 5.5 ps. Subsequently, the systems are quenched to 0 K over approximately ⁶¹10 ps and their configurations energetically minimized using a conjugate gradient minimizer for ease of post-processing. This reduction in system temperature is required due to the thermal motion of atoms at 1500 K in UO₂ leading to spurious defect populations. The quench undertaken in these simulations is sufficiently rapid to ensure no change in defect populations.

PKAs were initialized in the following directions: [100], [110], [⁶²111], [⁶³130], [⁶⁴141], [232], and ⁶⁵a set of random directions. These directions were selected because they offer a range of both low and high symmetry directions. Additionally, both U and O atoms were utilized as the PKA in each of these directions. For each unique simulation setup for a given direction, PKA species, PKA energy and ⁶⁶interatomic potential, 100 independent simulations were performed via random number initialization of velocities to ensure the statistical significance of the data set. ⁶⁷Convergence testing was performed to ensure that 100 simulations were sufficient. In Fig. ??, the results are shown for an example run in which a 60 eV PKA in a random direction for the Morelon potential, tracking the number of Frenkel pairs formed. The running average is displayed as a function of the number of simulations performed, and the average plus or minus twice the standard error (yielding a 95% confidence interval) is shown as a dashed line above and below the average. It is observed that above approximately 75 simulations, the results are converged and that minimal additional

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accuracy is obtained by extending to 200 simulations. It was deemed that 100 simulations are sufficient to obtain, with reasonable certainty, a converged result. In total, approximately 70,000 simulations were performed in the course of this work, using approximately 2.5 million cpu-hours.

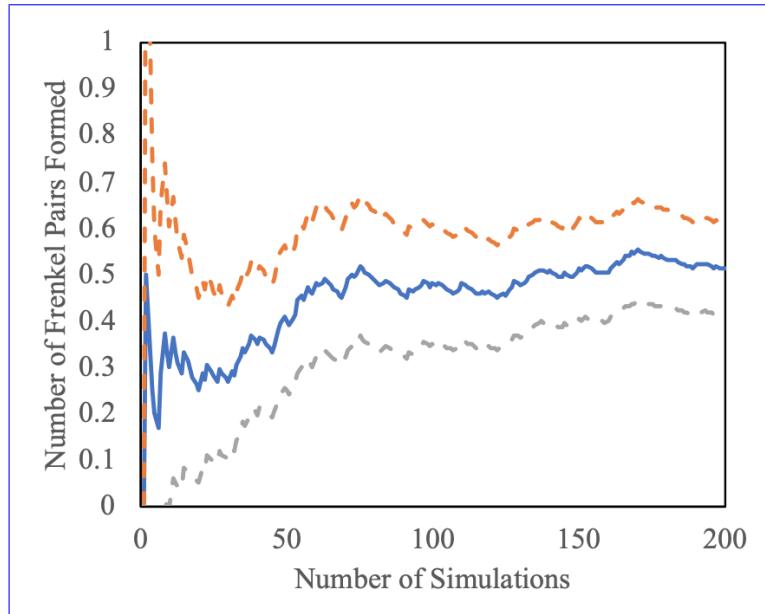


Figure 1: The number of Frenkel pairs as a function of the number of simulations. Twice the standard error of the mean is shown as dashed lines above and below the running average.

Atomic positions were output at various times throughout the simulation in order to accurately investigate all three definitions of the E_d displacement energy. For the first E_d and the second definitions of E_d (probability PKA is displaced from its lattice site, probability of permanently displacing atoms), atomic positions were output once the system reached a thermal state, indicating the end of the thermal spike. It should be noted why atomic positions were output immediately after the return to a thermal state and not at the end of the simulation. Oxygen interstitials diffuse rapidly within these systems, and when one is trying to determine the number of atoms that have been displaced in a system, rapid O interstitial diffusion will artificially inflate this number E_d due to dumbbell diffusion moving atoms in a chain-like fashion E_d]. Thus, in order to obtain the number of displaced atoms due solely to the damage cascade, systems are quenched immediately following the dissipation of the thermal spike. The specification for the determination

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of a thermal state is when the sum of excess kinetic energy ^[..72](KE_{xs}), defined by equation 1, is less than 5 eV^[..73],

$$KE_{xs} = \sum_i (KE_i - 1\text{eV}) \quad (1)$$

where KE_i is the kinetic energy of atom i , and KE_{xs} is summed over all atoms. These specifications are sufficiently strict to ensure that the PKA energy spike has dissipated. Figure 2 shows the total excess kinetic energy of atoms above 1 eV as a function of time following the introduction of the PKA. The thermal state is reached ^[..74]at a time of 0.25 ps, ^[..75]where the sum of excess kinetic energy of all particles above 1 eV was ^[..76]less than 5 eV. The figure is made from ^[..77]a 50 eV ^[..78]U PKA in a random direction with the Basak potential, hence the initial energy of approximately 50 eV.

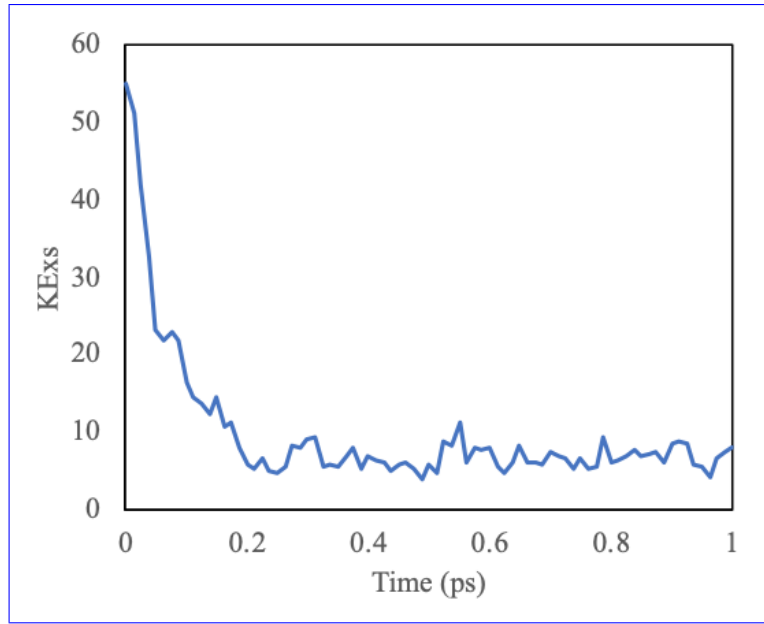


Figure 2: Total ^[..79]excess kinetic energy for all atoms above 1 eV versus time following the introduction of ^[..80]a PKA.

4. ^[..81]

3.1. ^[..82]

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For the third definition of E_d (generation of a Frenkel pair), the Voronoi package within the LAMMPS code [? ?] was utilized. This package creates a Voronoi tessellation at an initial stage and determines if additional atoms are present in the cell (or atoms have left the cell) at the end of the simulation, allowing for a direct way to determine vacancies and interstitials.

[..⁸³]
[..⁸⁴][..⁸⁵][..⁸⁶][..⁸⁷][..⁸⁸][..⁸⁹][..⁹⁰][..⁹¹][..⁹²][..⁹³][..⁹⁴][..⁹⁵][..⁹⁶]
[..⁹⁷]For each definition of E_d , a distribution is generated for the probability as a function of PKA energy.
[..⁹⁸]

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⁸⁴removed: The probability of Frenkel pair formation as a function of energy for U PKAs is shown in Fig. 9. Probabilities are observed to be zero up to approximately 25 eV for all interatomic potentials and directions. Above 20 eV, probabilities become non-zero and there is a clear directional dependence in the probability curves. The
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⁹⁰removed: directions consistently have the highest probability of Frenkel pair formation. Thus, it is easiest to generate defects from PKAs in the
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⁹⁶removed: direction. Generally, excellent agreement is observed between the potentials. Utilizing the definition of E_d as the lowest energy at which defect formation occurs, the displacement energy for uranium PKAs ($E_d[U]$) is 30 eV for the Basak and Yakub potentials, and 25 eV for the Yamada potential. This is substantially lower than the experimentally reported value of 40 eV [? ?].
⁹⁷removed: It can often be valuable to generate an average probability curve and analyze the median of this curve (the point where the probability becomes greater than 0.5). This value for E_d is not a quantity directly comparable to experiment, but is likely the more appropriate value for usage in the NRT equation [? ?]. Thus, the results for the six PKA directions are linearly averaged to create a single probability curve for Frenkel pair formation
⁹⁸removed: The median value for $E_d[U]$ is 54 eV for Basak, 54 eV for Yakub, and 55.5 eV for Yamada. Interestingly, this interpretation for E_d compares very favorably to the computational studies of Meis [?]. It should be noted that given this limited set of PKA directions, a true crystallographically averaged Frenkel pairformation probability curve would likely be different in nature. However, this simplified exercise can still provide a valuable approximation for the average behavior of U PKAs in the UO_2 system.

[⁹⁹] [¹⁰⁰] [¹⁰¹] [¹⁰²] [¹⁰³] [¹⁰⁴] [¹⁰⁵] [¹⁰⁶] [¹⁰⁷] [¹⁰⁸] [¹⁰⁹] [¹¹⁰] [¹¹¹]

[¹¹²] In order to extract a value for the E_d for each of these distributions, E_d is determined as the energy at which the probability is equal to, or greater than, 0.5. This indicates that it is likely to either displace a PKA from its lattice site, permanently displace an atom, or create a Frenkel [¹¹³] pair, respectively. Additionally, for the second and third definitions of E_d , the *total number* of displaced atoms and the *total number* of Frenkel pairs produced are determined as a function of [¹¹⁴] PKA energy. A secondary value of E_d is defined as when it is likely to displace one atom or to create one Frenkel pair. This secondary formalism of E_d may or may not necessarily match the value for the primary formalism. Although both characterizations will be investigated, only the first formalism based on probabilities will be utilized for comparisons among different definitions of E_d .

[¹¹⁵] A discussion on the meaning of the [¹¹⁶] terms permanent and stable needs to be undertaken. These terms are relative and defined in this manuscript on a picosecond timescale. The permanent displacement of an atom from its lattice site means that the atom has been moved from its original lattice site and exists at a different lattice site at the end of the thermal spike. A stable Frenkel pair means that a Frenkel pair exists at the end of the simulation (after 5.5 ps at 1500 K). The authors are aware that additional recombination, defect clustering, and migration is possible. However, given the constraints of molecular dynamics timescales, this work provides a reasonable result for the defect population produced from cascades that can then be utilized in higher timescale modeling methodologies such as kinetic Monte Carlo and cluster dynamics to investigate further defect

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¹¹⁴removed: energy for O PKAs is shown in Fig. 11. Probabilities are consistently below 0.1 for all PKA energies investigated in this range. Oxygen PKAs at these low energies are unable to transfer sufficient energy to displace uranium atoms, thus only O defects can be formed. Albeit very minimal, probabilities do become non-zero near a PKA energy of 20 eV. Utilizing the definition of E_d as the lowest energy at which defect formation occurs, the displacement energy for oxygen PKAs ($E_d[O]$) is 20 eV for the Basak potential and 30 eV for both the Yakub and Yamada potentials. This can be viewed as in concordance with the experimentally observed $E_d[O]$ of 20 eV [? ?]. No observable directional dependence can be elucidated from these results, as the statistical noise from this sample is equal to the magnitude of the probabilities. Similarly, comparisons of potentials is untenable due to the rare Frenkel pair formation events.

¹¹⁵removed: Given that the probability of Frenkel pair formation does not exceed 0.1 for the range of PKA energies,

¹¹⁶removed: construction of a directionally-averaged probability curve (in order to obtain the PKA energy where the probability becomes greater than 0.5) is meaningless

evolution. A more complete discussion on the investigation of Frenkel pair recombination distance and lifetime was undertaken by Van Brutzel [?] and can be consulted for extrapolation of these results.

[¹¹⁷] [¹¹⁸] [¹¹⁹] [¹²⁰] [¹²¹] [¹²²] [¹²³] [¹²⁴] [¹²⁵] [¹²⁶] [¹²⁷] [¹²⁸] [¹²⁹]

4. Results

4.1. Probability of [¹³⁰] PKA displacement

[¹³¹]

4.1.1. Uranium PKA

The probability of the PKA leaving its lattice site in [¹³²] UO_2 for uranium PKAs is shown in Fig. [¹³³] 3 for all sets of PKA directions and all four interatomic potentials. It is observed that U PKAs can be displaced from their lattice site at an energy as low as [¹³⁴] 10 eV. It should be emphasized that this does not denote the generation of a defect or a permanent displacement of an atom off of its lattice site, simply that the PKA achieved a maximum displacement sufficient to be classified as no longer on its original lattice site. [¹³⁵] The highest probability of PKA displacement [¹³⁶] is observed for the [¹³⁷] [¹³⁸] [¹³⁹] [¹⁴⁰] 100 [¹⁴¹] [¹⁴²] direction, while the lowest probability is observed for the [110] direction [¹⁴³]. This relationship is present for all potentials analyzed. It is likely that this is due to the proximity of the nearest neighbor in the

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¹³⁵removed: It makes qualitative sense, provided the nature of the definition, that the observed energies for non-zero probabilities in Fig. ?? are much lower than in Fig. 9. The highest probabilities

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¹⁴³removed: exhibits the lowest probability of PKA displacement. Thus one can conclude from Fig. 9 and Fig. ?? that although it is more difficult to displace an U atom from its lattice site in the

specific PKA direction. In the $[\bar{1}100]$ direction, ¹⁴⁴the nearest neighbor is at a distance of one full lattice parameter, while in the $[\bar{1}110]$ direction, ¹⁴⁵the nearest neighbor is only at a distance of $\sqrt{2}/2$ times the lattice parameter, which is a significantly closer neighbor. Such a variability in the local environment produces such changes in PKA displacement probability. For the random set of directions, the PKA has a greater than 90% probability of being displaced for PKA energies of at least 35 eV for all potentials except the Morelon, which requires 50 eV of kinetic energy to yield a 90% probability of displacing the PKA. Utilizing the random set of directions as approximating average behavior and taking a probability of ¹⁴⁶50% to represent E_d , the value of E_d for U PKAs ($E_d[U]$) is determined to be 25 eV for the Basak ¹⁴⁷and Yakub potentials, 35 eV for the Morelon potential and 20 eV for the Cooper potential.

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¹⁴⁶removed: 214

¹⁴⁷removed: where is it moderately easy to displace an atom from its lattice site, but that atom is very unlikely to form a stable Frenkel pair. Excellent agreement is shown across all three potentials for the magnitude and the relative probabilities of PKA directions. Linearly averaging over the set

¹⁴⁸removed: PKA directions in Fig. ?? allows for the creation of a single probability curve for PKA lattice site displacement as a function of PKA energy. The single probability curve enables us to obtain the PKA energy where it is probable to displace a U atom from its lattice site. This formalism of $E_d[U]$ is 23.1 eV, 25.5 eV and 24.6 eV

¹⁴⁹removed: , Yakub and Yamada potentials, respectively

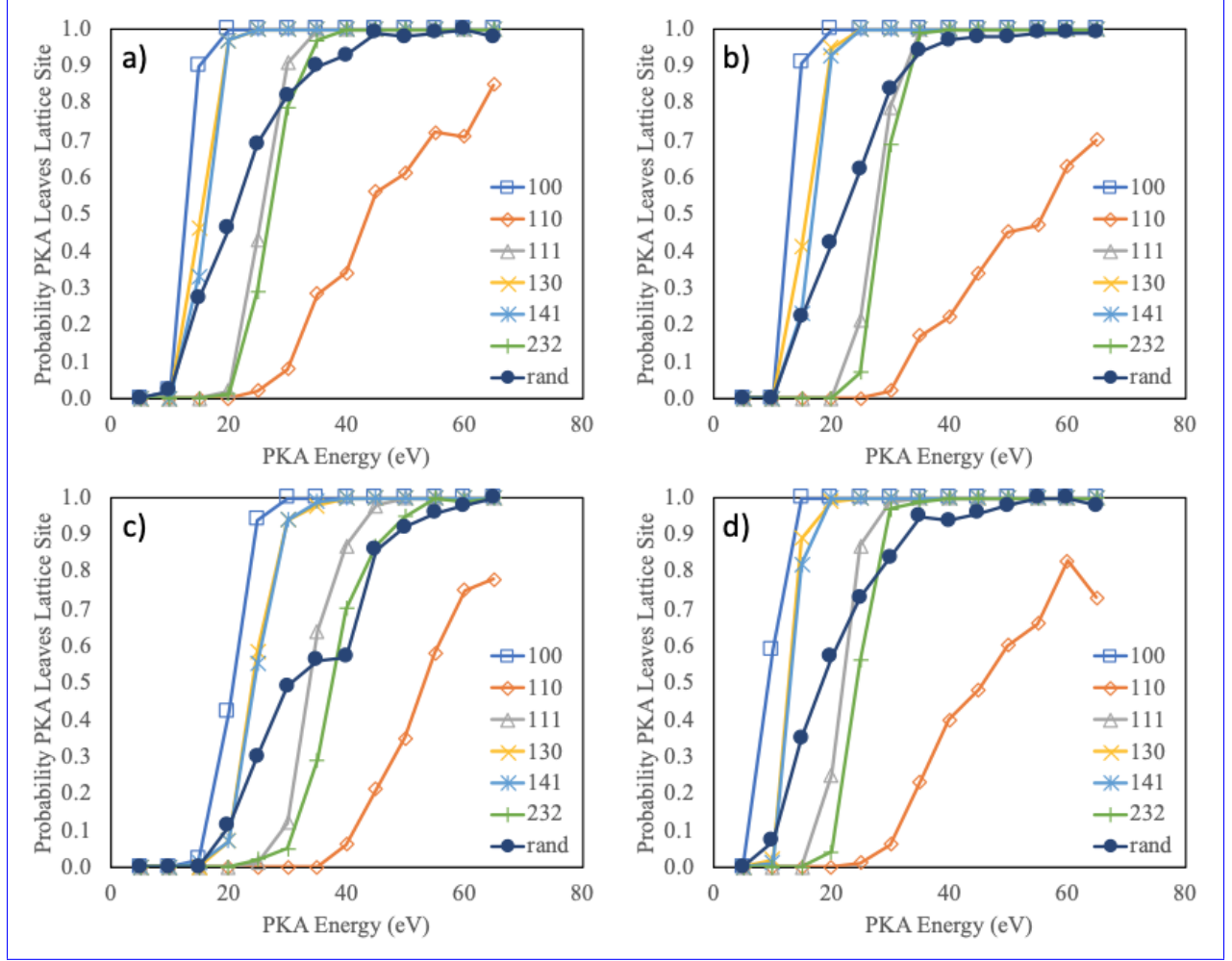


Figure 3: Probability of PKA leaving lattice site in $^{157}\text{UO}_2$ for uranium PKAs in the $[100]$, $[110]$, $[111]$, $[130]$, $[141]$, $[232]$ and random directions for the a) Basak, b) Yakub¹⁶², c) Morelon¹⁶³, and d) Cooper potentials.

4.1.2. Oxygen PKA

The probability of the PKA leaving its lattice site in $^{164}\text{UO}_2$ for oxygen PKAs is shown in Fig. ¹⁶⁵4 for all sets of PKA directions and all four interatomic potentials. It is observed that O PKAs can be displaced from their lattice site at an energy as low as 10 eV. ¹⁶⁶Analyzing the different directions, it is observed that the highest probability is for the $[110]$ direction, while the lowest probability ¹⁶⁷is for the $[100]$ direction. This ¹⁶⁹is in direct contrast to the U PKAs, but perfectly corresponds to nearest neighbor distances

¹⁶⁴removed: UO_2

¹⁶⁵removed: ??

¹⁶⁶removed: The highest probability of PKA displacement is observed

¹⁶⁷removed: of PKA displacement is observed

¹⁶⁸removed: 232

¹⁶⁹removed: directional dependence is consistent over the three interatomic potentials. However, there is a noticeable difference in the magnitude of the displacement probabilities for the Yamada potential when compared to the

in the crystal structure. Oxygen atoms are organized on a simple cubic sublattice inside the U face-centered cubic sublattice, comprising the UO_2 fluorite structure. As such, the closest nearest neighbor distance for O atoms is along the $[100]$ direction, which exhibits the lowest probability of PKA displacement. Utilizing the random set of directions as approximating average behavior and taking a probability of 0.5 to represent E_d , the value of E_d for O PKAs ($E_d[\text{O}]$) is determined to be 15 eV for the Basak and Yakub potentials [..¹⁷⁰] and 10 eV for the Morelon and Cooper potentials.

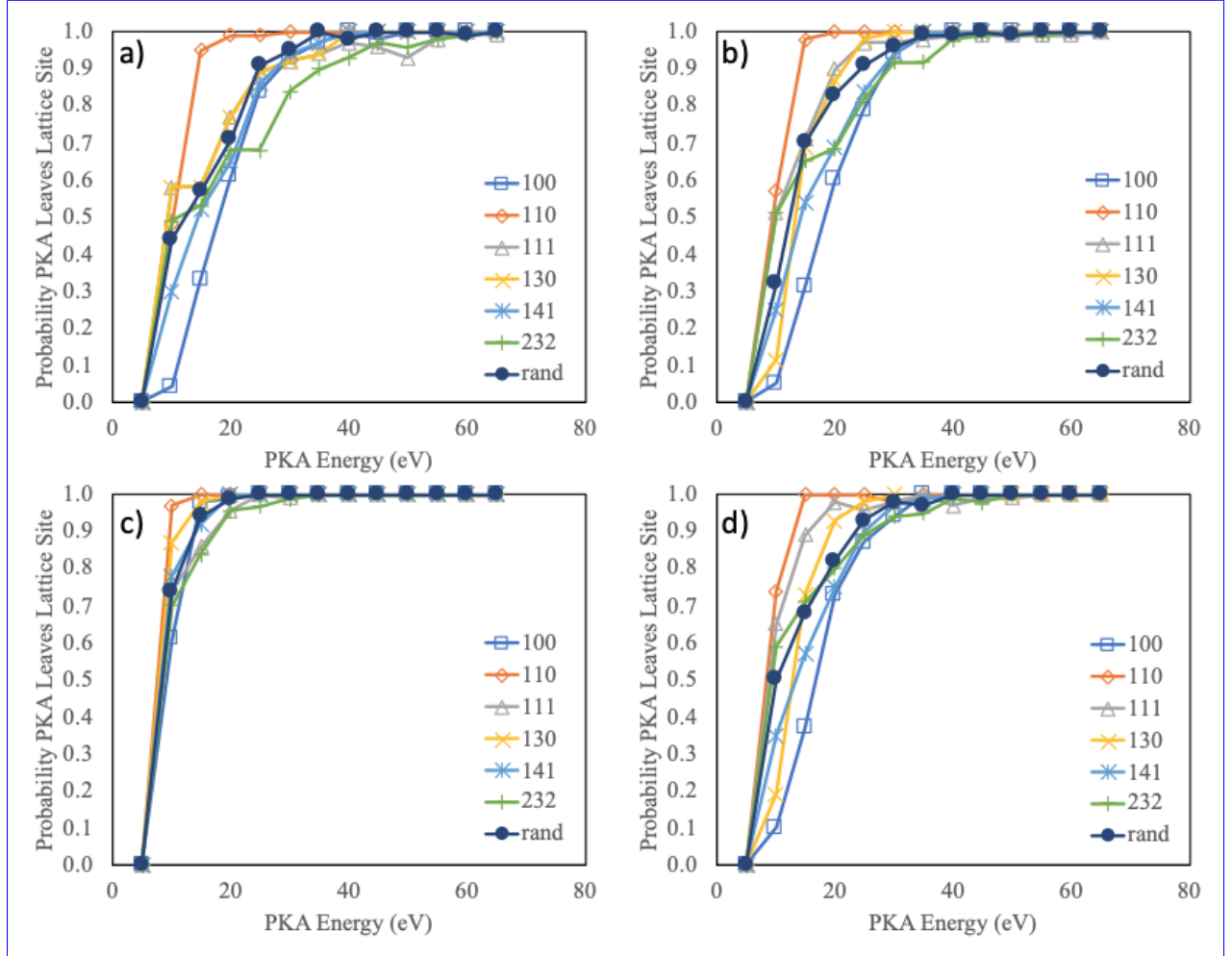


Figure 4: Probability of PKA leaving lattice site in UO_2 for oxygen PKAs in the $[100]$, $[110]$, $[111]$, $[130]$, $[141]$, $[232]$ and random directions for the a) Basak, b) Yakub, c) Morelon, and d) Cooper potentials.

4.2. Permanent displacement of atoms

4.2.1. Uranium PKA

¹⁷⁰removed: . The PKA displacement probability curves are shifted to the right for the Yamada potential, suggesting a greater difficulty of moving the O PKA from its lattice site. The data

The probability of the U PKA causing permanent displacement of atoms is shown in Fig. [..¹⁷¹]5 for all sets of PKA directions and all four interatomic potentials. It is observed that U PKAs begin to permanently displace atoms at 15 eV for the Basak, Yakub and [..¹⁷²]Cooper potentials and at 10 eV for the Morelon potential. Similar crystallographic relatedness is observed to the results in Fig. 3, where the [110] direction generally displays the lowest probability of displacement and the [100] generally displays the highest probability of displacement. The value of $E_d[U]$ is determined to be 45 eV for all four interatomic potentials investigated.

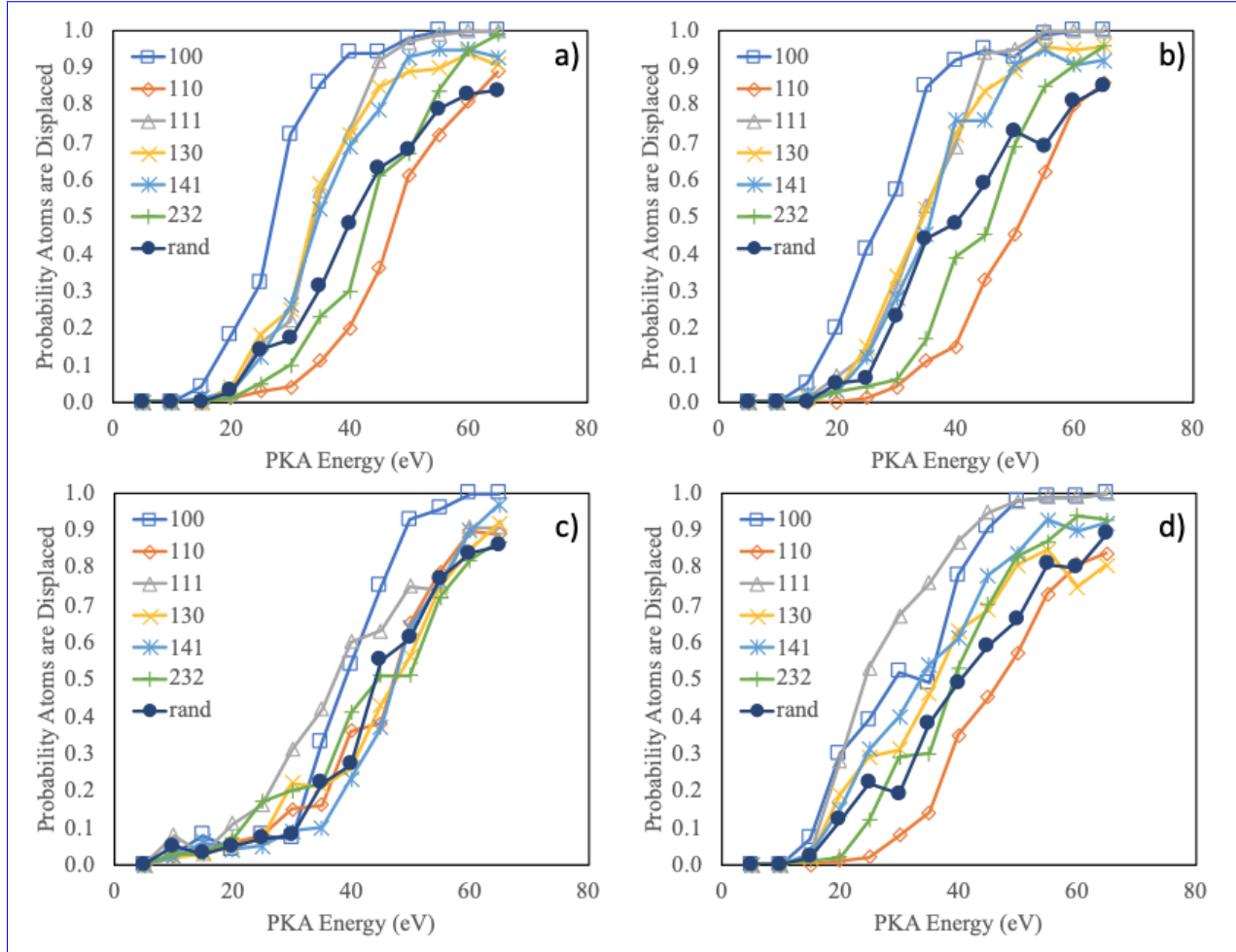


Figure 5: Probability of U PKA [..¹⁸²] permanently displacing atoms in [..¹⁸³] UO_2 for [..¹⁸⁴] PKAs in the [100], [110], [..¹⁸⁵] [111], [..¹⁸⁶] [130], [..¹⁸⁷] [141], [232] and [..¹⁸⁸] random directions for the a) Basak, b) Yakub [..¹⁸⁹], c) [..¹⁹⁰] Morelon, and d) Cooper potentials.

¹⁷¹removed: ?? is utilized to construct a single probability curve for PKA lattice site displacement as a function of PKA energy. Taking the median of this data, the $E_d[U]$ is 14.6 eV , 16.4 eV and 19.5 eV

¹⁷²removed: Yamada potentials , respectively. This more clearly illustrates the shift right of the data of the Yamada potential.

4.3. [..¹⁹¹]

4.2.1. [..¹⁹²]

[..¹⁹³]

[..¹⁹⁴]In addition to the probability of displacing atoms, the total number and type of atoms [..¹⁹⁵]displaced provides information relevant to the effects of radiation damage. Fig. 6 displays the total number of atoms displaced, along with the individual number of U and O atoms displaced as a function of PKA energy for U PKAs. For all interatomic potentials, [..¹⁹⁶]the majority of the displaced atoms are O atoms, with a ratio of O atoms displaced to U atoms displaced from approximately 4:1 up to 6:1. The total number of atoms displaced follows the same crystallographic trends as the probability that atoms are displaced from Fig. 5. Utilizing the random set of directions to approximate average behavior and utilizing the secondary formalism of E_d (when a PKA displaces on average one atom), the value of $E_d[U]$ is 35 eV for the Basak, Yakub and [..¹⁹⁷]Cooper potentials and 40 eV for the Morelon potential. This formalism of E_d , although it investigates the same type of local atomic changes due to a PKA, yields slightly lower values for $E_d[U]$ than for the first formalism extracted from Fig. 5.

Finally, it can be observed from Fig. 6 the different U PKA energies at which a O atom or a U atom is displaced. O atoms typically begin to be displaced at U PKA energies of 20 eV and U atoms tend to begin to be displaced at U PKA energies of 30 eV. Thus even though the PKA is U, it still requires approximately 10 eV less energy to displace a O atom, than a U atom.

[..²¹¹]

¹⁹¹removed: Permanent displacement of atoms

¹⁹²removed: Displaced oxygen atoms

¹⁹³removed:

¹⁹⁴removed: The average number of oxygen atoms permanently displaced per U PKA as a function of PKA energy is shown in Fig. ???. Permanent displacement of O

¹⁹⁵removed: begins at a PKA energy of approximately 20 eV. Although there exist directional dependencies for each individual potential, a general trend for high or low displacement directions across all potentials is not observable. A clear observation is the distinct differences between the three potentials. The Basak and Yamada potentials display similar behavior, while the Yamada potential predicts significantly more displaced O atoms for a U PKA of a given energy. To more clearly illustrate this phenomenon, the results for each potential are averaged over the investigated directions . At a U PKA energy of 60 eV, the directionally-averaged number of displaced O atoms per UPKA is 4.5

¹⁹⁶removed: 3.4 and 8.1

¹⁹⁷removed: Yamada potentials , respectively. It should be emphasized that this does not necessarily indicate the generation of a Frenkel pair, but only the permanent displacement of an atom off of its original lattice site.

²¹¹removed: The average number of oxygen atoms permanently displaced per O PKA as a function of PKA energy is shown in Fig. ???. Permanent displacement of atoms begins at an O PKA energy of approximately 20

[..198][..199][..200][..201][..202][..203][..204][..205][..206][..207][..208][..209][..210]

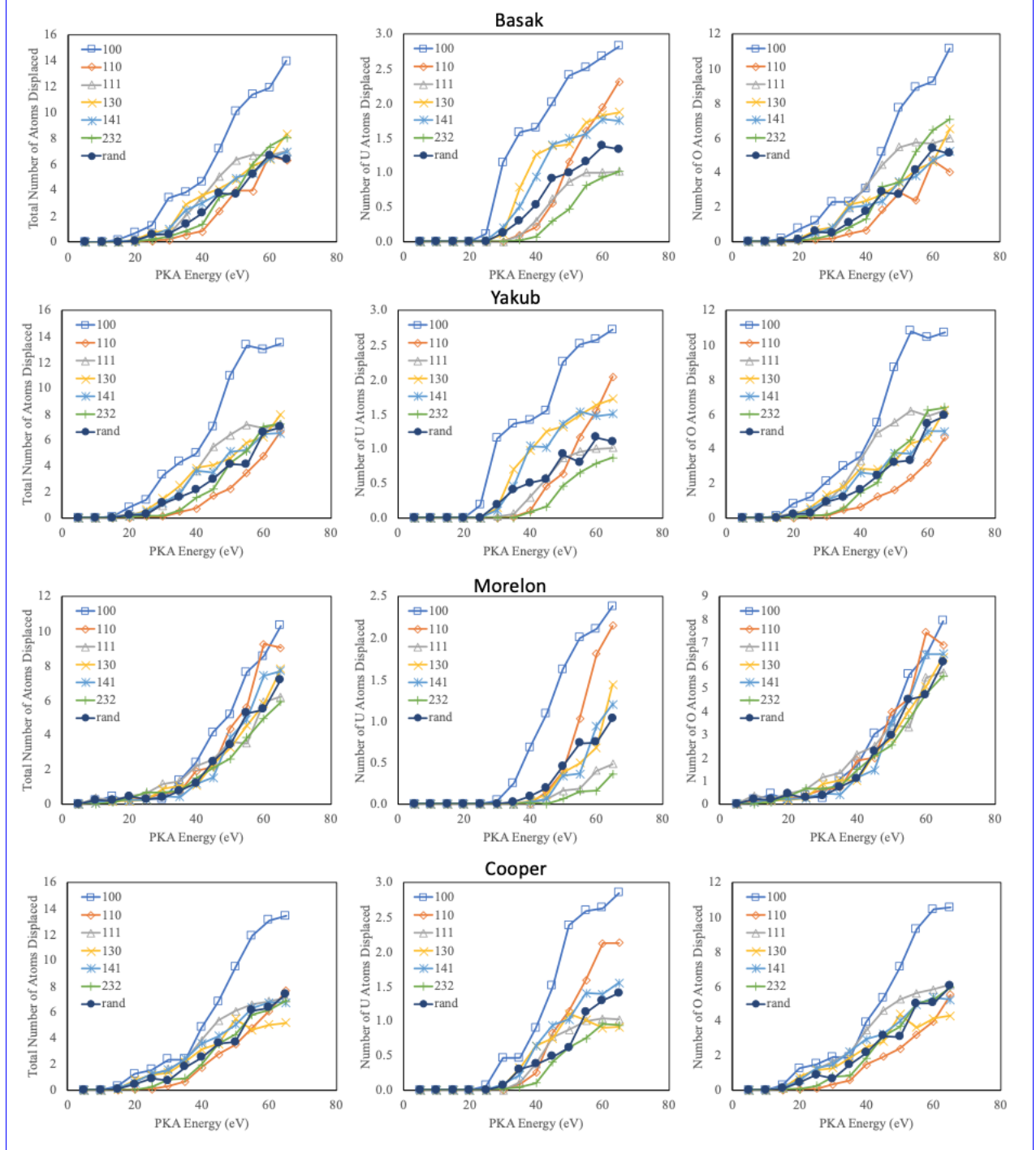


Figure 6: The number of atoms permanently displaced in UO_2 by U PKAs in the [100], [110], [111], [130], [141], [232] and random directions for the Basak, Yakub, Morelon, and Cooper potentials. The total number of displaced atoms, as well as the number of U and O atoms displaced is displayed.

4.2.1. Oxygen PKA

The probability of the O PKA causing permanent displacement of atoms is shown in Fig. 7 for all sets of PKA directions and all four interatomic potentials. It is observed that O PKAs begin to permanently displace atoms at approximately 15 eV ^[.212] ^[.213] ^[.214] ^[.215] ^[.216] for the Basak^[.217], Yakub and Cooper potentials and at 10 eV for the Morelon potential. It is difficult to discern crystallographic variation, as the data are relatively closely bunched. This indicates at minimum a weak dependence upon PKA direction. The value of $E_d[\text{O}]$ is determined as 60 eV for the Basak potential, 45 eV for the Yakub and Cooper potentials, and 20 eV for the Morelon potential. This is a wide disparity in the values for $E_d[\text{O}]$ that was not present for the definition of $E_d[\text{O}]$ in section 4.1.

²¹²removed: . It is interesting to note that the minimum required energy to permanently displace an O atom from its lattice site is independent of whether the PKA is a U or an O atom. The

²¹³removed: 232

²¹⁴removed: direction consistently exhibits the fewest number of oxygen atoms displaced per PKA across all potentials. The

²¹⁵removed: 110

²¹⁶removed: O PKA direction leads to the highest number of displaced O atoms

²¹⁷removed: and Yakub potentials, while no single high displacement direction exists for the Yamada potential. Additionally, the magnitude of the displaced O atoms is less for the Yamada potential than for the Basak and Yakub potentials. The results for each potential are averaged over the investigated directions. At

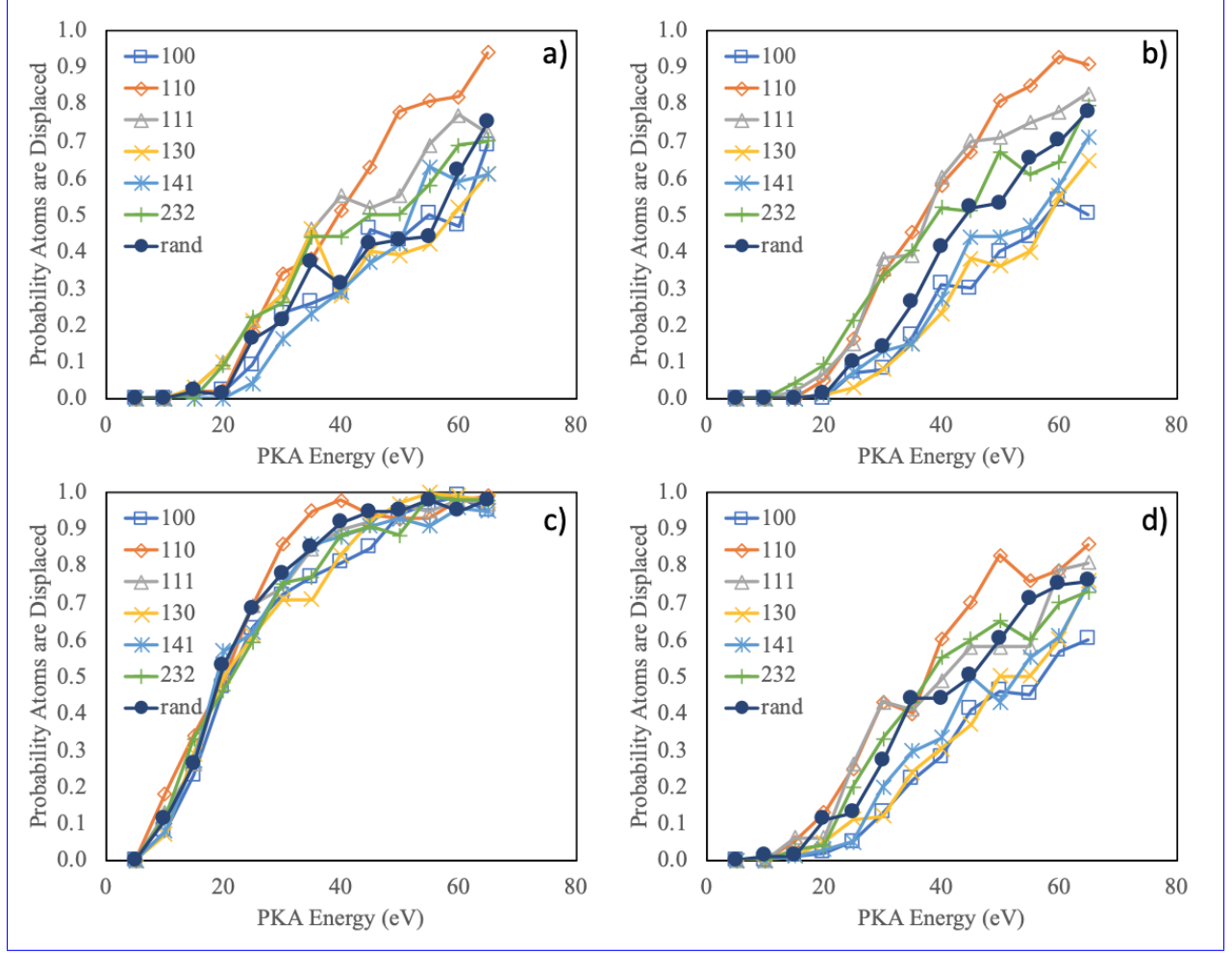


Figure 7: Probability of O PKA permanently displacing atoms in UO_2 for PKAs in the [100], [110], [111], [130], [141], [232] and random directions for the a) Basak, b) Yakub, c) Morelon, and d) Cooper potentials.

Fig. 8 displays the number of O atoms displaced due to an O PKA^[.218]. Oxygen atoms at these energies are not moving rapidly enough to displace U atoms, and as such the number of O atoms displaced in Fig. 8 is also the total number of atoms displaced. There is a general linear trend for the number of O atoms displaced as a function of PKA energy over this energy range, with the interatomic potential determining the slope of the linear relationship. It should be emphasized that the scale on the axes is different for the Morelon potential in Fig. 8c. Utilizing the random set of directions to approximate average behavior and utilizing the secondary formalism of E_d , the value of $E_d[\text{O}]$ is ^[.219] 30 eV for the Basak ^[.220] potential, 35 eV for the Yakub and Cooper potentials and ^[.221] 15 eV for the Morelon potential. The relative ordering of the interatomic potentials is identical to the

²¹⁸removed: energy of 40 eV, the directionally-averaged number of displaced O atoms per O PKA

²¹⁹removed: 1.6, 1.5 and 1.1

²²⁰removed: , Yakub

²²¹removed: Yamada potentials , respectively.

relative ordering for the primary formalism of $E_d[\text{O}]$, however the magnitudes are reduced slightly compared to the values of $E_d[\text{O}]$ from Fig. 7.

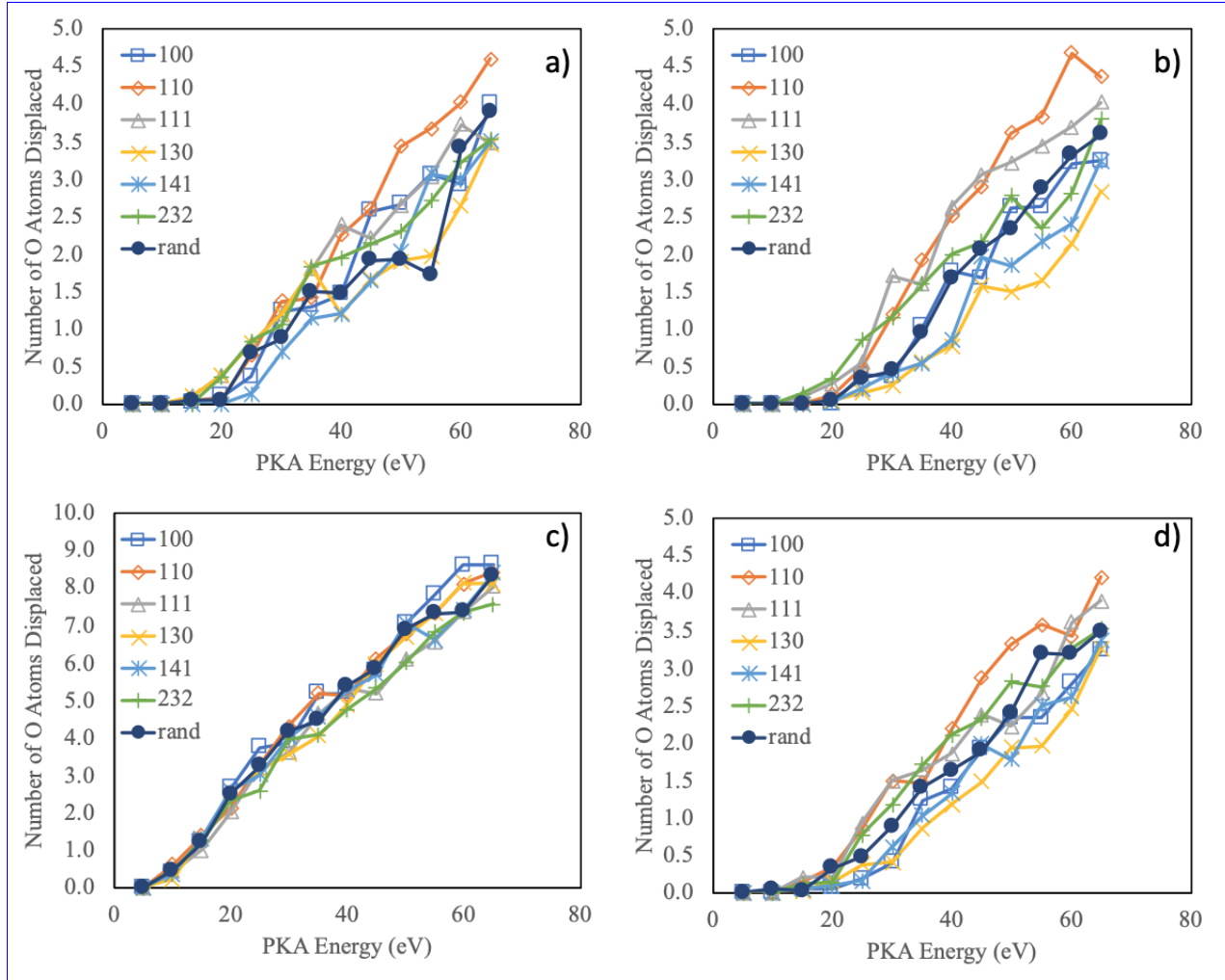


Figure 8: [..²³³] The number of [..²³⁴] O atoms permanently displaced in UO_2 by [..²³⁵] O [..²³⁶] PKAs in [..²³⁷] the [100], [110], [..²³⁸] [111], [..²³⁹] [130], [..²⁴⁰] [141], [232] and [..²⁴¹] random directions for the a) Basak, b) Yakub[..²⁴²], c) [..²⁴³] Morelon, and d) Cooper potentials. U atoms are not displaced by O PKAs in this energy range..

4.2.2. [..²⁴⁴]

[..²⁴⁵]

4.3. Probability of Frenkel pair formation

[..²⁴⁶]

²⁴⁴removed: Displaced uranium atoms

²⁴⁵removed:

²⁴⁶removed: The average number of uranium atoms permanently displaced per U PKA

4.3.1. Uranium PKA

The probability of Frenkel pair formation as a function of PKA energy for U PKAs is shown in Fig. ²⁴⁷9. Probabilities are observed to be zero up to approximately 20 eV for all interatomic potentials and directions. Above 20 eV, probabilities become non-zero and there is a clear directional dependence in the probability curves. Similar to the results in both section 4.1 and section 4.2, the highest probability is observed for the ²⁴⁸[100] ²⁴⁹direction. The value of E_d ²⁵⁰[U] ²⁵¹is determined to be 60 eV for each of the Basak, Yakub and Cooper potentials and is determined to be greater than 65 eV for the Morelon potential. The Morelon potential yields a maximum probability for the random directions of 0.42 for U PKAs with an energy of 65 eV.

²⁴⁷removed: ?? . Permanent displacement of atoms begins at a PKA energy of approximately 30 eV . Comparing to Fig. ??, it requires an additional 10 eV of kinetic energy for a U atom to permanently displace another U atom, than for that U atom to displace an O atom. The

²⁴⁸removed: 130

²⁴⁹removed: and

²⁵⁰removed: 141

²⁵¹removed: directions show the highest number of displaced U atoms, which is in agreement with the results in Fig. 9 on Frenkel pair generation. The fewest U atoms are displaced for PKAs in the

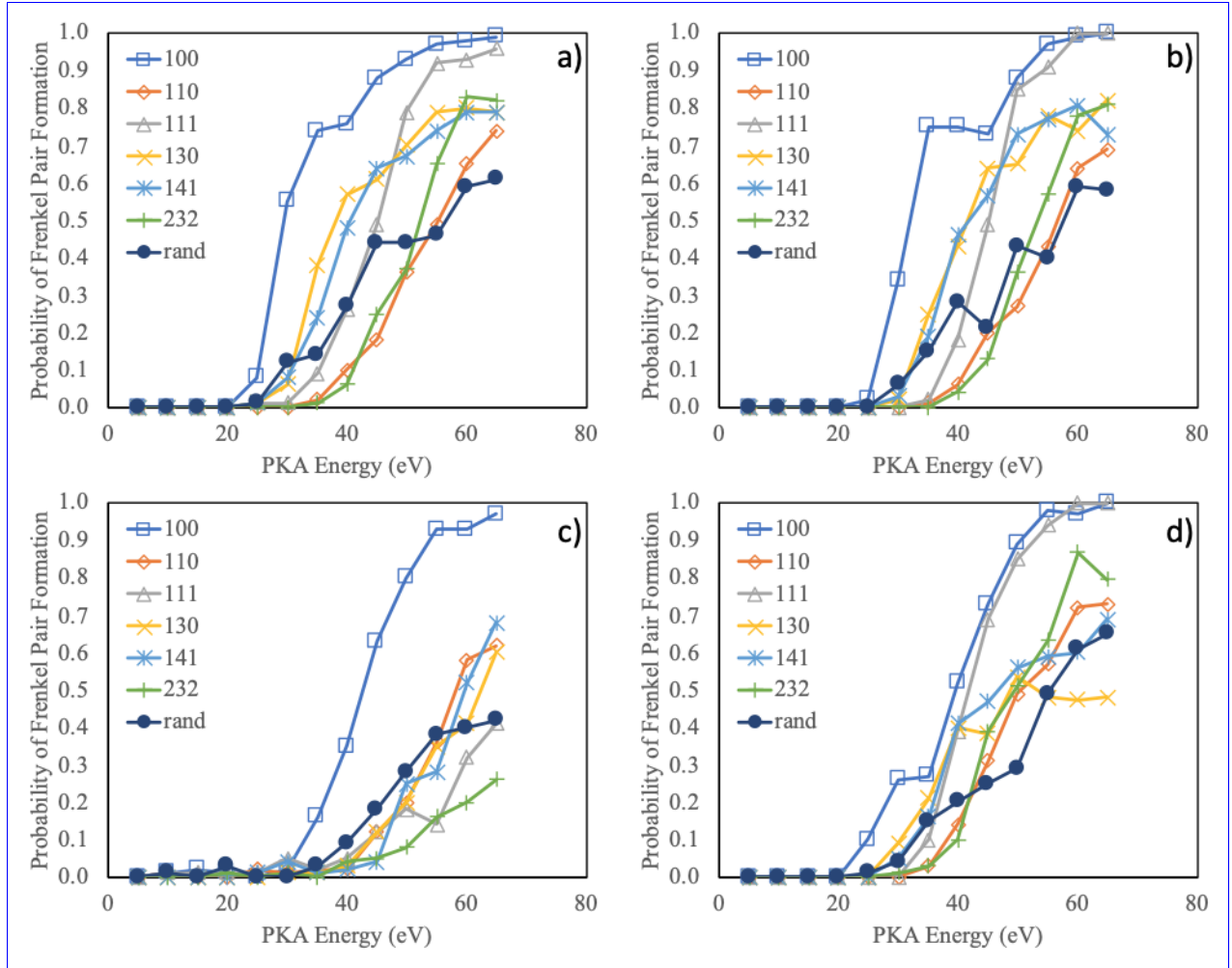


Figure 9: Probability of Frenkel pair formation as a function of PKA energy in UO_2 for U PKAs in the [100], [110], [111], [130], [141], [232] and random directions for the a) Basak, b) Yakub, c) Morelon, and d) Cooper potentials.

In addition to the probability of generating Frenkel pairs, the total number of Frenkel pairs is relevant to understanding a material's radiation response. Fig. 10 displays the total number of Frenkel pairs created. As expected, the total number of Frenkel pairs follows the same crystallographic trends as the probability to form Frenkel pairs from Fig. 9. Utilizing the random set of directions to approximate average behavior and utilizing the secondary formalism of E_d (when a PKA creates on average one Frenkel Pair), the value of E_d [..²⁵²]U [..²⁵³] is 60 eV [..²⁵⁴] for the Basak and Cooper potentials and greater than 65 eV for the Yakub the Morelon potentials. The maximum number of Frenkel pairs per PKA for a 65 eV U PKA is [..²⁵⁵]0.94 for the Yakub

²⁵²removed: 214

²⁵³removed: direction, which is also in agreement with Fig. 9. There is a general agreement on directional dependence and on the magnitude of displacements for all three potentials. For a U PKA of

²⁵⁴removed: , the directionally-averaged number of displaced U atoms per

²⁵⁵removed: 1.3, 1.1 and 1.2 for the Basak, Yakub and Yamada potentials, respectively. Comparing to Fig. ??, a U PKA of 60 eV will permanently displace approximately 4 times, 3 times or 8 times as many O atoms as U atoms for

potential and 0.61 for the Morelon potential. This formalism for $E_d[U]$ yields identical results for the Basak and Cooper potentials, but increases the magnitude of E_d for the Yakub and Morelon potentials.

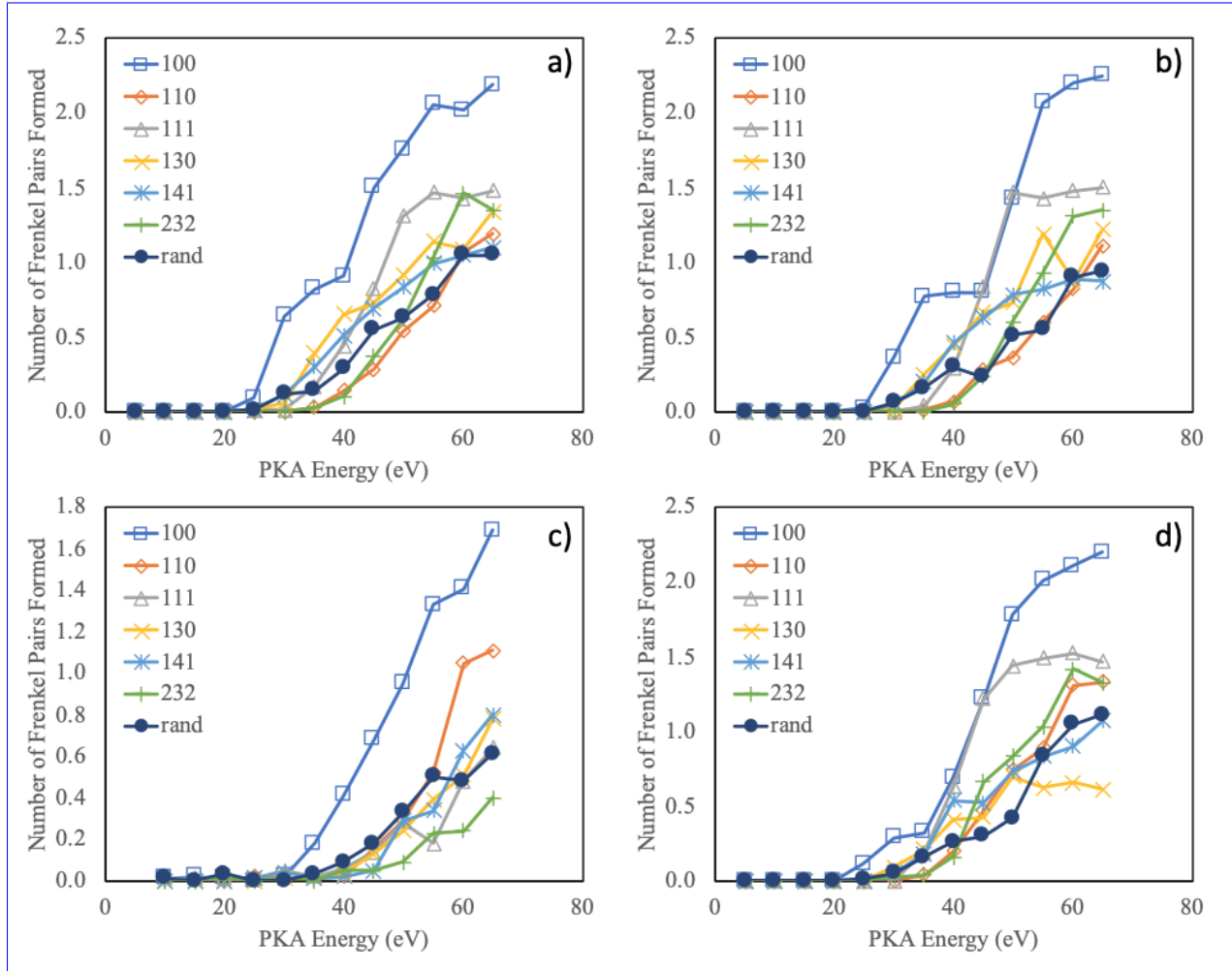


Figure 10: Total number of Frenkel pairs formed as a function of PKA energy in UO_2 for U PKAs in the [100], [110], [111], [130], [141], [232] and random directions for the a) Basak, b) Yakub, c) Morelon, and d) Cooper potentials.

4.3.2. Oxygen PKA

The probability of Frenkel pair formation as a function of PKA energy for O PKAs is shown in Fig. 11. Probabilities do not exceed 0.1 for any PKA energy with the Basak, Yakub and [..²⁵⁶]

[..²⁵⁷] Cooper potentials, and do not exceed 0.33 for the Morelon potential. Thus, it is never probable to form a Frenkel pair for O PKAs for energies below 65 eV. As such, $E_d[O[..²⁵⁸]]$ is undefinable, other than to note that it is greater than 65 eV. In this energy range, O PKAs are unable to transfer sufficient energy to displace

²⁵⁶removed: Yamada potentials, respectively.

²⁵⁷removed: Permanently displaced U atoms due to an O PKA are not shown in this section, as the low energy

²⁵⁸removed: PKAs did not possess sufficient kinetic

[..²⁵⁹] uranium atoms, thus only a minimal number of O defects are formed. Albeit very minimal, probabilities do become non-zero at a PKA energies greater than 20 eV.

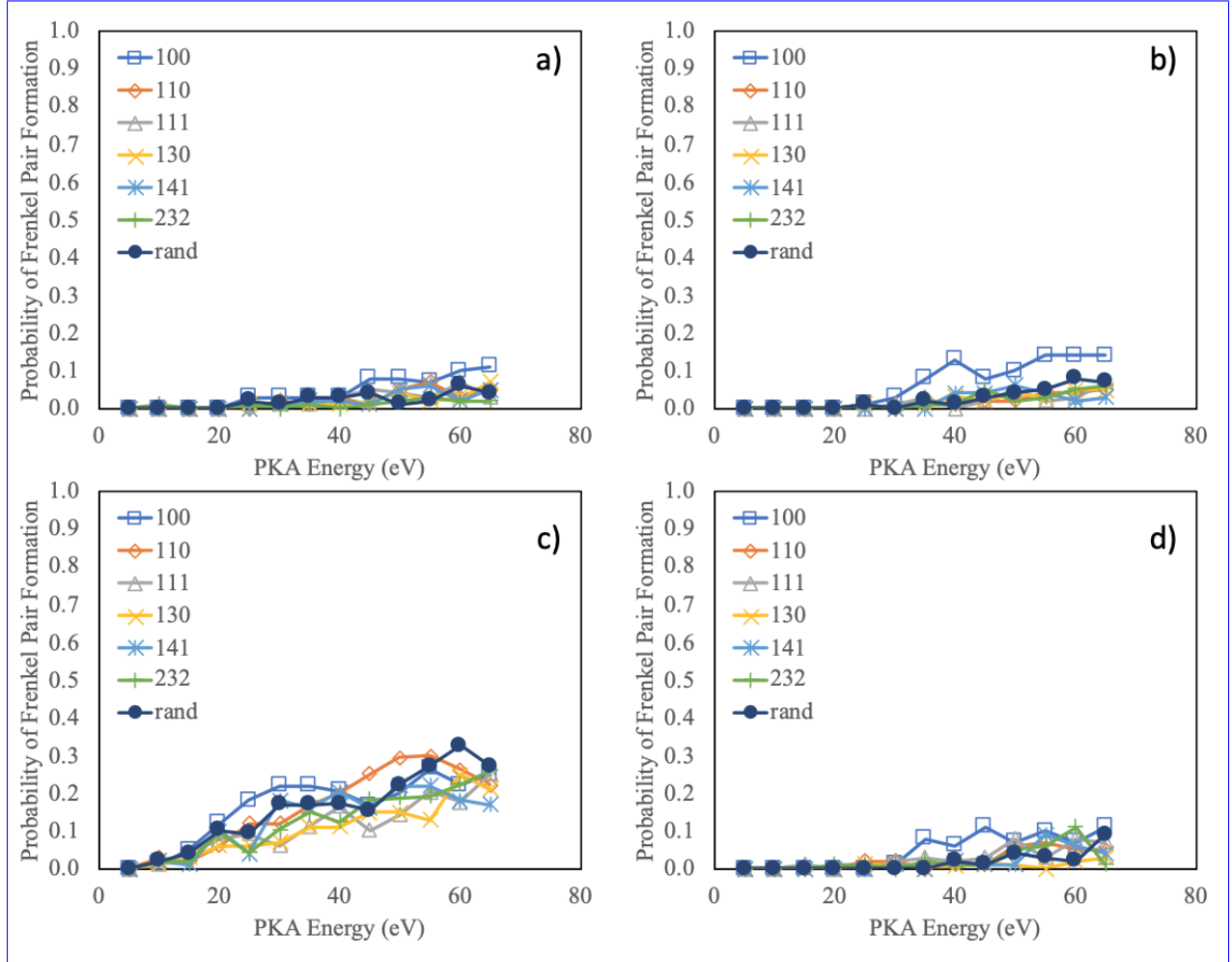


Figure 11: [..²⁶⁹] Probability of [..²⁷⁰] Frenkel pair formation as a function of PKA energy in [..²⁷¹] UO_2 for O PKAs in the [100], [110], [..²⁷²] [111], [..²⁷³] [130], [..²⁷⁴] [141], [232] and [..²⁷⁵] random directions for the a) Basak, b) Yakub[..²⁷⁶], c) [..²⁷⁷] Morelon, and d) Cooper potentials.

4.4. [..²⁷⁸]

[..²⁷⁹]

In order to investigate the potential displacement of uranium atoms from an oxygen PKA, [..²⁸⁰] higher energy O PKAs of up to 200 eV were utilized. [..²⁸¹] Figure 12 shows the probability of Frenkel pair formation

²⁵⁹removed: a U atom from its original lattice site.

²⁷⁸removed: High energy oxygen PKA

²⁷⁹removed:

²⁸⁰removed: high energy (150-200 eV) oxygen PKAs

²⁸¹removed: As such, a full analysis of each formalism of the displacement energy was performed for the high energy O PKAs.

as a function of O PKA energy [..²⁸²]for the random direction and all four interatomic potentials. There is a positive trend of increasing defect probability with increasing PKA energy. [..²⁸³]For the Basak, Yakub and Cooper potentials, the probability of generating a Frenkel pair from an O PKA of 200 eV [..²⁸⁴]does not exceed 0.3. Thus, even for relatively high energy O PKAs, it is still unlikely to form a Frenkel pair. However, for the Morelon potential, the probability to create a Frenkel pair is significantly higher. A value for $E_d[\text{O}]$ can be defined at 125 eV, where it becomes probable to create a Frenkel pair. It should be noted that these defects are almost entirely on the O [..²⁸⁵]sublattice. Thus, even though the kinetic energy of O atoms in Fig. 12 [..²⁸⁶]is much higher than that of U atoms in Fig. 9, it is [..²⁸⁷]much more probable to create Frenkel pairs from a U PKA.

[..³¹⁸][..³¹⁹][..³²⁰][..³²¹]

²⁸²removed: . For each potential, there is a slight

²⁸³removed: Significantly, the Yamada potential predicts a dramatically higher Frenkel pair formation probability than either the Basak or Yakub potentials. At

²⁸⁴removed: , average probability of defect formation is 0.28, 0.26, and 0.72 for the Basak, Yakub and Yamada potentials, respectively. Thus, the Yamada potential predicts that a

²⁸⁵removed: PKA will produce approximately 2.5 times more Frenkel pairs than the same O PKA as predicted via the Basak or Yakub potentials. This substantial difference underlines the importance of understanding a given potential's behavior when conducting radiation damage simulations, given that similar potentials can produce dramatically different results. When comparing higher energy O PKAs

²⁸⁶removed: to lower energy U PKAs

²⁸⁷removed: observed that low energy U PKAs are still more likely to produce Frenkel pairs over these energy ranges (with the exception of results concerning the Yamada potential)

³¹⁸removed: Table ?? shows the average number of displaced uranium atoms due to the high energy oxygen PKA. No uranium atoms were displaced in the

³¹⁹removed: 110

³²⁰removed: ,

³²¹removed: 130

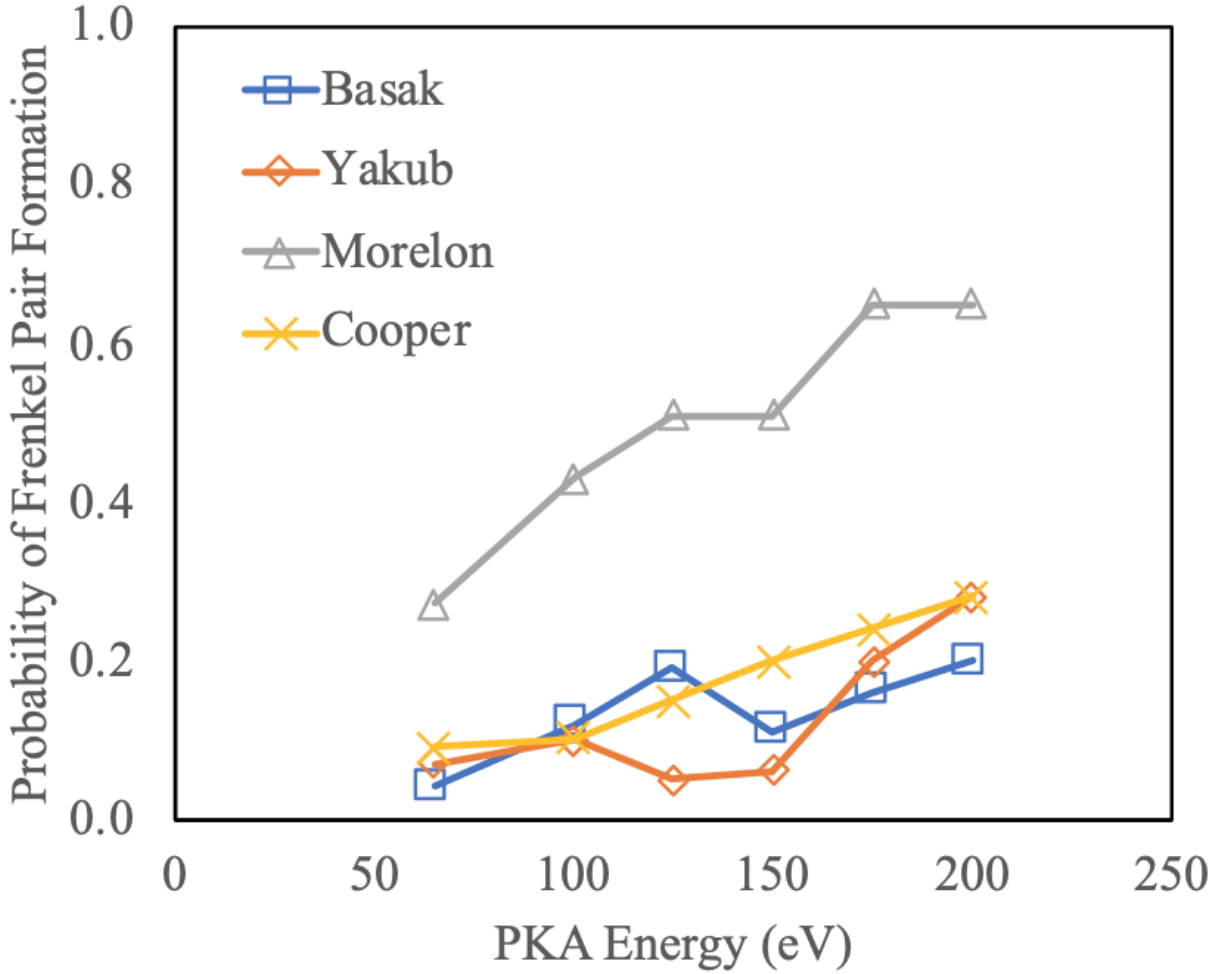


Figure 12: Probability of Frenkel pair formation as a function of PKA energy ^[.303] for higher energy O PKAs in UO_2 in the ^[.304] ^[.305] ^[.306] ^[.307] ^[.308] ^[.309] ^[.310] ^[.311] ^[.312] ^[.313] ^[.314] ^[.315] random direction for the a) Basak, b) Yakub^[.316], c) ^[.317] Morelon, and d) Cooper potentials.

5. Discussion

A more clear comparison can be made by extracting the data for each set of random directions for each interatomic potential, PKA type, and E_d definition. The consolidated results are shown in Table 5, with the probability distributions shown for U PKAs in Fig. 13 and for O PKAs in Fig. 14. In the table, the different definitions of E_d are labeled E_d^1 , E_d^2 and E_d^3 , for the definitions of 1) the probability that a primary knock-on atom (PKA) leaves its original lattice site, 2) the probability that a PKA permanently displaces an atom from its original lattice site, and 3) the probability of forming a stable Frenkel pair. It is observed that results for the Basak, Yakub and Cooper potentials generally agree very well with one another, which the Morelon potential tends to exist as

an outlier. The Morelon potential predicts lower probabilities for all three definitions of $E_d[U]$ [..³²²] [..³²³] [..³²⁴] [..³²⁵] and predicts higher probabilities for all three definitions of $E_d[O]$ [..³²⁶].

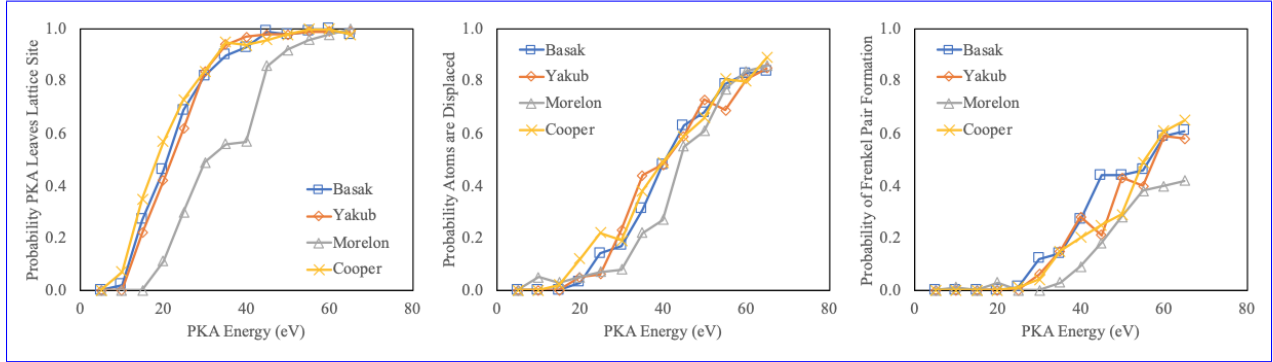


Figure 13: Probability PKA leaves lattice site, Probability atoms are displaced and Probability of Frenkel pair production as a function of U PKA energy for four interatomic potentials.

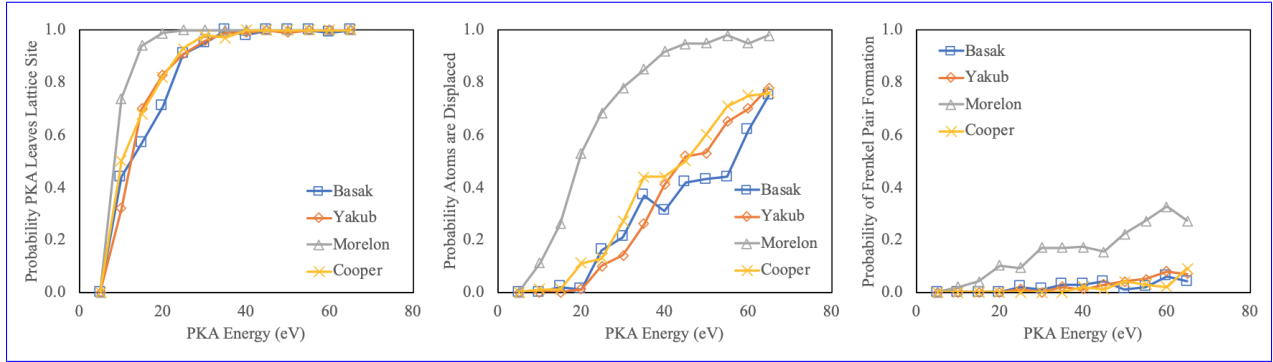


Figure 14: Probability PKA leaves lattice site, Probability atoms are displaced and Probability of Frenkel pair production as a function of O PKA energy for four interatomic potentials.

[..³⁹¹] The relative magnitude of the different definitions of E_d make qualitative sense, in that it should be easiest to simply displace the PKA off of its lattice site and it should be most difficult to create a stable Frenkel

³²²removed: , and

³²³removed: 141

³²⁴removed: PKA directions, thus they are excluded from the table. The O PKA energy range tested encompasses the minimum energy needed to transfer approximately 50 eV to the uranium atoms (with a direct collision). Due to this fact, the average number of uranium atoms displaced is very small, as at most a single uranium atom can be displaced in a given simulation. Additionally, there is not a monotonic increase of displacement probability . As U displacements from this energy range of O PKAs are rare events and thermal fluctuations are high in these systems (simulation temperature of 1500 K) , it is reasonable that there is significant statistical noise in the results . Although not statistically significant, the most likely PKA direction for U displacements is the

³²⁵removed: 232

³²⁶removed: direction, and it is found that the Yakub potential is the most likely to show U displacements from these high energy OPKAs

³⁹¹removed: Fig.?? shows the average number of displaced oxygen atoms due to the high energy oxygen PKAs. Similar to Fig. 12 and Fig. ??, there is a positive trend of increasing number of displaced O atoms with increasing O PKA energy.

Table 1: The calculated displacement energies for four interatomic potentials, two PKA types and three different definitions of E_d .

[.. ³²⁷]	[.. ³²⁸] E_d^1	[.. ³²⁹] E_d^2	
Basak E_d [U]	[.. ³³¹]25	[.. ³³²]45	
[.. ³³⁴]Basak E_d [O]	[.. ³³⁵]15	[.. ³³⁶]60	[.
[.. ³³⁸][.. ³³⁹][.. ³⁴⁰]Yakub E_d [U]	[.. ³⁴¹]25	[.. ³⁴²]45	
[.. ³⁴⁴]Yakub E_d [O]	[.. ³⁴⁵]15	[.. ³⁴⁶]45	[.
[.. ³⁴⁸][.. ³⁴⁹][.. ³⁵⁰]Morelon E_d [U]	[.. ³⁵¹]35	[.. ³⁵²]45	[
[.. ³⁵⁴]Morelon E_d [O]	[.. ³⁵⁵]10	[.. ³⁵⁶]20	[
[.. ³⁵⁸][.. ³⁵⁹][.. ³⁶⁰]Cooper E_d [U]	[.. ³⁶¹]20	[.. ³⁶²]45	
[.. ³⁶⁴]Cooper E_d [O]	[.. ³⁶⁵]15	[.. ³⁶⁶]45	[.. ³⁶⁷][.. ³⁶⁸][.. ³⁶⁹][.. ³⁷⁰][.. ³⁷¹][.. ³⁷²][.. ³⁷³][.. ³⁷⁴][.. ³⁷⁵][.. ³⁷⁶
[.. ³⁸⁷][.. ³⁸⁸][.. ³⁸⁹]			
	[.. ³⁹⁰]		

pair. When comparing to the typically utilized values for E_d [U] of 40 eV and E_d [O] of 20 eV, [..³⁹²]

[..³⁹³][..³⁹⁴][..³⁹⁵][..³⁹⁶][..³⁹⁷][..³⁹⁸][..³⁹⁹][..⁴⁰⁰][..⁴⁰¹][..⁴⁰²][..⁴⁰³][..⁴⁰⁴][..⁴⁰⁵]

6. [..⁴⁰⁶]

Furthermore, the Yamada potential shows the highest number of displaced O atoms, while the Basak and Yakub show generally similar quantities of displaced O atoms. For a 200 eV PKA, the average number of displaced O atoms is 19

³⁹²removed: 15 and 25 for the Basak, Yakub and Yamada potentials, respectively.

³⁹³removed: Average number of oxygen atoms displaced by an O PKA as a function of PKA energy in UO_2 in the

³⁹⁴removed: 110

³⁹⁵removed: ,

³⁹⁶removed: 130

³⁹⁷removed: ,

³⁹⁸removed: 141

³⁹⁹removed: ,

⁴⁰⁰removed: 214

⁴⁰¹removed: ,

⁴⁰²removed: 232

⁴⁰³removed: and

⁴⁰⁴removed: 313

⁴⁰⁵removed: directions for the a) Basak, b) Yakub and c) Yamada potentials.

⁴⁰⁶removed: Discussion

[⁴⁰⁷] the [⁴⁰⁸] only set of results that provides a near match is for the [⁴⁰⁹] E_d^2 definition and the [⁴¹⁰] Morelon potential, which as stated previously is the outlier in this dataset. However, the authors do believe the most relevant definition when comparing to these experimental results is likely E_d^2 , which simply looks at permanent displacement of atoms, regardless of the production of defects. For this definition of E_d , this work points to values of $E_d[\text{O}]$ and $E_d[\text{U}]$ of approximately 45 eV. However, this number alone is not sufficient to understand the nature of the atoms that are displaced, as there are typically 5x more O atoms displaced than U atoms. Sublattice-specific displacements are important information, particularly because O atoms have been shown to be able to self-heal. It was also found that the minimum energy to displace a U atom is approximately 30 eV (from a U PKA) and the minimum energy to displace an O atom is approximately 10 eV (from a O PKA).

The authors believe the most relevant definition of E_d when trying to actually understand the results of radiation damage and potential deleterious effects on the material is E_d^3 , which indicates the actual production of point defects. For this definition, $E_d[\text{U}]$ is approximately 60 eV, and $E_d[\text{O}]$ is higher than 200 eV. The authors believe this value, which allows for instantaneous (<5 ps) recombination of defects, is the appropriate value for utilization in the NRT equation for the calculation of radiation-induced damage.

6. Conclusion

Molecular dynamics simulations of low energy PKAs have been performed to investigate the threshold displacement energy ([⁴¹¹] E_d) in UO_2 at 1500 K. The Basak, Yakub[⁴¹²], Morelon and Cooper interatomic potentials were utilized. The [⁴¹³] E_d was evaluated under three distinct definitions: 1) the probability that a primary knock-on atom (PKA) leaves its original lattice site, 2) the probability that [⁴¹⁴] a PKA permanently displaces an atom from its original lattice site, and 3) the probability of forming a stable Frenkel pair. Both U and O PKAs were utilized to [⁴¹⁵] develop species dependent values of E_d . It was found that the minimum

⁴⁰⁷removed: This work has shown a consistency regarding the variation among the three interatomic potentials, in that they are in concordance when considering U PKAs, but the radiation damage properties vary significantly for the Yamada potential when considering O PKAs and the O sublattice. This is likely due to the oxygen sublattice properties defined by the Yamada potential. The Yamada potential exhibits properties of a more fluid oxygen sublattice, with significant distortion of O atoms off of the sublattice, in addition to rapid O interstitial diffusion. This was visually confirmed to be the case by use of Ovito [?]. Because the Basak potential is considered an improvement of

⁴⁰⁸removed: Yamada potential [?], and the Basak results generally agree with the Yakub potential,

⁴⁰⁹removed: Yamada potential is viewed as producing inaccurate oxygen sublattice behavior, and the authors would discourage the use of

⁴¹⁰removed: Yamada potential in high temperature radiation damage studies

⁴¹¹removed: E_d in UO_2

⁴¹²removed: and Yamada

⁴¹³removed: E_d was studied by looking at the probability of Frenkel pair production,

⁴¹⁴removed: the PKA leaves its lattice site and the number of permanently displaced atoms due to the PKA. Both uranium and oxygen

⁴¹⁵removed: investigate a broad scope of potential radiation damage in UO_2 . Utilizing the definition of E_d as the minimum energy required to form a stable Frenkel pair, it was found that the E_d for U PKAs is 25-30 eV and the E_d for O PKAs is 20-30

energy [..⁴¹⁶] to displace a U atom is approximately 30 eV (from a U PKA) and the minimum energy to displace an O atom [..⁴¹⁷] is approximately 10 eV (from a O PKA). For U PKAs, it becomes probable to displace an atom above an energy of approximately 45 eV and it becomes probable to create a defect at approximately 60 eV. For O PKAs, it becomes probable to displace an atom above an energy of approximately 45 eV and it does not become probable to create a defect at energies analyzed up to 200 eV. This work has provided the first insight into the high temperature nature of the [..⁴¹⁸] displacement energy in [..⁴¹⁹] UO_2 .

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eV, depending on the interatomic potential utilized. These results are in agreement with experimental results for O atoms, but suggest a lower E_d than the experimental value of 40 eV for U atoms. For utilization of the NRT equation, a median, directionally-averaged E_d for U PKAs was calculated as approximately 55 eV. This quantity was not determined for O PKAs.

It was found that the PKA

⁴¹⁷removed: from its lattice site is approximately 20 eV , regardless of the PKA type. Additionally, it requires 30 eV of

kinetic energy for a U PKA to permanently displace a U atom from its lattice site. The minimum PKA energy observed for an O atom to displace a U atom is 150 eV. The results for the Basak and Yakub potentials were consistent for both U and O PKAs and showed only minimal variance across all simulated systems. The Yamada potential showed significant differences when compared to the Basak and Yakub potentials regarding O PKAs and properties of the O sublattice

⁴¹⁸removed: threshold

⁴¹⁹removed: UO_2

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