Full energy range primary radiation damage model

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(Received 22 February 2021; accepted 3 May 2021; published 6 July 2021)

A full energy range primary radiation damage model is presented here. It is based on the athermal recombination corrected displacements per atom (arc-dpa) model but includes a proper treatment of the near threshold conditions for metallic materials. Both *ab initio* (AIMD) and classical molecular dynamics (MD) simulations are used here for various metals with body-centered cubic (bcc), face-centered cubic (fcc), and hexagonal close-packed (hcp) structures to validate the model. For bcc and hcp metals, the simulation results fit very well with the model. For fcc metals, although there are slight deviations between the model and direct simulation results, it is still a clear improvement on the arc-dpa model. The deviations are due to qualitative differences in the threshold energy surfaces of fcc metals with respect to bcc and hcp metals according to our classical MD simulations. We introduce the minimum threshold displacement energy (TDE) as a term in our damage model. We calculated minimum TDEs for various metal materials using AIMD. In general, the calculated minimum TDEs are in very good agreement with experimental results. Moreover, we noticed a discrepancy in the literature for fcc Ni and estimated the average TDE of Ni using both classical MD and AIMD. It was found that the average TDE of Ni should be ~ 70 eV based on simulation and experimental data, not the commonly used literature value of 40 eV. The most significant implications of introducing this full energy range damage model will be for estimating the effect of weak particle-matter interactions, such as for γ - and electron-radiation-induced damage.

DOI: [10.1103/PhysRevMaterials.5.073602](https://doi.org/10.1103/PhysRevMaterials.5.073602)

I. INTRODUCTION

Radiation damage is a very general phenomenon that affects many scientific branches and areas of application, with examples from medicine [1], particle physics [2], applied computer science [3], space and aerospace [4], and not the least nuclear energy production, where intense neutron irradiation is in many cases life limiting for components due to radiation-induced degradation [5].

The mechanism of radiation damage production in crystalline materials can be divided into two stages based on time scale. The first one is the primary damage stage. It is the atomic collision process that takes place after highly energetic particles (electrons, neutrons, or ions) interact with atoms in a material. The actual energy transfer in the initial interaction, where the transferred energy is partitioned between electronic excitation and ionic kinetic energy, is extremely rapid and not considered as part of the damage evolution stage. The initial stage is instead defined in terms of atomic displacements. The duration of the primary damage stage is typically < 10 ps, based on various experimental and simulation studies [4]. The second stage is the defect evolution stage. This is the thermally activated process which takes place over longer

time scales (from nanoseconds to years, depending on the conditions). Depending on the mechanism of damage production, a proper estimate of the damage rate induced by the radiation in the primary damage stage is an important part in studying radiation effects on materials.

The first step in generating such an estimate is to determine the number of defects (Frenkel pairs) produced in a single primary damage event. For each material, the most accurate way to know this is to perform experiments directly or run molecular dynamics (MD) simulations to get the average number of defects at different damage energies. However, this is often impractical due to the associated high cost and complexity, either in terms of experiment or in computation. Therefore, it is vital for many applications to have a simple but still reliable analytical model which gives a reasonable estimate of the number of produced defects. An analytical model to calculate the damage dose, in the canonical unit displacements per atom (dpa), was proposed by Kinchin and Pease (KP) [6]. The KP model calculates the damage dose by including the threshold displacement energy (TDE), denoted E_d , as the fundamental materials parameter. In the KP model, the number of defects is calculated as the kinetic energy divided by two times the TDE, after an initial sharp threshold, and up to a high-energy threshold where electronic stopping dominates. This model was later refined by Norgett *et al.* (NRT) [7]. Their binary collision simulations showed that $\sim 20\%$ of the vacant lattice sites are always refilled by other atoms. Hence, they added a prefactor of 0.8 to the KP model, and they also replaced the kinetic energy by the damage energy, which includes a more realistic, physically consistent, and smooth implementation of the effect of electronic stopping for higher energies. The damage energy, denoted T_d , is thus the kinetic energy available

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to cause atomic displacements after removing the electronic ionization energy. While this NRT-dpa model is more realistic than the KP model, it still significantly overestimates the defect production in collision cascades. In fact, the actual defect production is only $\sim \frac{1}{3}$ of the NRT prediction for metallic materials, based on experiments and simulations [4,8,9]. Thus, a more physically realistic model is desired. Recently, an athermal recombination corrected (arc) dpa model [9] was proposed.

Compared with the KP and NRT-dpa models, the arc-dpa model provides a more accurate estimate of the number of defects for intermediate and high damage energy collision cascades, which are typically induced by neutrons in nuclear reactors [4]. However, for low-energy events, such as those from electron and γ -ray interactions, none of the current models give reasonable estimates of the number of induced defects. This is because the damage energies of the primary knock-on atom (PKA) transferred from electron and γ rays are close to the TDE of many materials, and the effect of the sharp threshold in the KP, NRT, and arc-dpa models risk giving unphysical results. It is well known from both experiments and MD simulations [4,10–13] that each lattice direction has its own TDE. An underlying assumption in the KP, NRT, and arc-dpa models is that the TDE is a unique value in a material. This application of an averaged effect is only correct for high damage energies. The assumption is incorrect when the statistical average number of defects produced cannot be simply assumed to be 0 or 1 when $T_d < 2E_d/0.8$. In fact, it starts to be possible to produce defects when the damage energy surpasses the minimum TDE, not the average TDE, and the probability to generate a stable defect is still not unity even when the damage energy is slightly higher than the average TDE [4,10–13]. Therefore, while the arc-dpa model is already satisfactory at high damage energies, we still need a proper model for the near TDE damage events. The importance of a proper near TDE model is evident for all applications that generate energy transfer events near the threshold. One such example is γ -ray-induced damage, which may be generated due to decay of spent nuclear fuel and can produce defects in the repository materials that have to be structurally intact over hundreds of thousands of years. According to previous models, such as KP, NRT, and arc-dpa, γ -induced damage would in most cases be strictly zero, as we will see later, because of the unphysical sharp threshold. Thus, an updated model is vital for quick but accurate estimates of the effect of γ or electron irradiation of materials. Cosmic ray irradiation of space and terrestrial applications may also have significant fluxes of events near the TDE in critical materials.

In this paper, we propose a modification to the arc-dpa model to make it suitable for the full range of energies, including near TDE conditions. Classical MD simulations are performed to validate the modified model in the full energy range (both near TDE and for high damage energies), and we compare with available experimental data. *Ab initio* MD (AIMD) simulations are also performed to calculate the TDE of various body-centered cubic (bcc), face-centered cubic (fcc), and hexagonal close-packed (hcp) metal materials in specific lattice directions in comparison with TDE obtained from MD simulations and with experiments.

II. METHOD

A. Analytical damage model

The arc-dpa model is formulated as a modification on the NRT model to account for athermal recombination (recombination of defects in the primary damage stage) [9]. The number of defects (N_d) in a collision cascade calculated by the arc-dpa model is

$$N_d(T_d) = \begin{cases} 0, & T_d < E_d \\ 1, & E_d < T_d < \frac{2E_d}{0.8} \\ \frac{0.8T_d}{2E_d} \xi(T_d), & \frac{2E_d}{0.8} < T_d \end{cases}, \quad (1)$$

where T_d is the damage energy, E_d is the TDE of the material, and ξ is

$$\xi(T_d) = \frac{1 - c_{\text{arc dpa}}}{(2E_d/0.8)^{b_{\text{arc dpa}}}} T_d^{b_{\text{arc dpa}}} + c_{\text{arc dpa}}, \quad (2)$$

in which $b_{\text{arc dpa}}$ and $c_{\text{arc dpa}}$ are materials constants.

According to Eq. (1), N_d is strictly zero when $T_d < E_d$; N_d is always 1 when $T_d > E_d$ and $T_d < 2E_d/0.8$. However, E_d is not a unique value in any given material. Here, E_d is the average TDE over all lattice directions. This means that the TDE of each lattice direction can be either lower or higher than E_d . Therefore, N_d should be >0 when T_d is higher than the minimum TDE in a material, and N_d should be <1 when T_d is not much higher than E_d . Although this difference does not affect the N_d of collision cascades with high damage energy (usually neutron- or ion-induced cascades), it is vital for γ - and electron-induced collision cascades. For example, Cs-137, one of the common fission products, emits 662 keV γ rays during its decay via metastable Ba-137. There are two steps for γ rays to transfer kinetic energy to atoms in materials. Firstly, the γ rays will transfer kinetic energy to electrons due to the photoelectric effect, pair production, or Compton scattering, but for these energy ranges, Compton scattering dominates completely [14]:

$$E_e = \frac{E_\gamma^2(1 - \cos \theta)}{E_\gamma(1 - \cos \theta) + m_e c^2}, \quad (3)$$

where E_e is the kinetic energy transferred to the electron, E_γ is the energy of the γ ray, θ is the photon scattering angle, m_e is the electron mass, and c is the speed of light. After Compton scattering, the second step is that the scattered electrons will transfer kinetic energy to lattice atoms. The collisions between electrons and atoms need to be described by relativistic quantum mechanics because the energies of electrons are high enough to reach relativistic speed. The energy transfer between the atom and the relativistic electron can be described as follows [15]:

$$T_d = \frac{2E_e}{Mc^2} (E_e + 2m_e c^2) \sin^2 \frac{\phi}{2}, \quad (4)$$

where we replace the kinetic energy by the damage energy T_d , given that, in the range of 10–100 eV relevant here, electronic stopping only removes $\sim 5\%$ of the energy. Here, M is the atom mass, and ϕ is the electron scattering angle.

Based on Eq. (3), the γ rays emitted from Cs-137 can transfer at maximum ~ 477 keV kinetic energy to electrons in the material. Relativistic electrons of such energy can ultimately

transfer at maximum ~ 25 eV kinetic energy to atoms like Fe and Cu according to Eq. (4). The average TDE of Fe and Cu is >30 eV, and such γ rays would thus lead to no damage according to previous models, while the minimum TDE of Fe and Cu is ~ 20 eV [16]. Hence, the γ rays and electrons which only induce damage energies below TDE can in fact produce Frenkel pairs from scattering in lattice directions with relatively low TDEs.

Based on this, we modified the arc-dpa model by introducing the minimum TDE $E_d^{\min}$ as a parameter:

$$N_d(T_d) = \begin{cases} 0, & T_d < E_d^{\min} \\ \frac{0.8T_d}{2E_d^{\text{avr}}}, & E_d^{\min} < T_d < \frac{2E_d^{\text{avr}}}{0.8}, \\ \frac{0.8T_d}{2E_d^{\text{avr}}} \xi(T_d), & \frac{2E_d^{\text{avr}}}{0.8} < T_d \end{cases} \quad (5)$$

in which E_d^{avr} is the average TDE [same as E_d in Eq. (1)]. All other parameters are the same as in the arc-dpa model. The difference between the arc-dpa model and our modification is that the modified model shows a linear relation between N_d and T_d when the T_d is between $E_d^{\min}$ and $2E_d/0.8$. Although this adds one parameter to the model, it is a parameter that is accessible to both experiments and atomistic simulations, much more so than the average TDE.

B. Classical MD simulation

The classical MD simulations presented here consist of two parts: the near TDE simulations and the high damage energy simulations. All classical MD simulations were carried out using the code LAMMPS [17]. For the near TDE collision cascades, the simulation cell size was $12 \times 12 \times 16$ conventional lattice units. The size of the simulation cells is large enough, as has been shown earlier, for careful calculation of the TDE for Fe [13]. The simulation temperature used was 10 K. Many evenly distributed lattice directions were sampled, respecting spherical symmetries. Atoms were assigned random initial velocities with a Gaussian distribution for the simulation temperature at the beginning of the simulation and were then equilibrated for 10 ps. After equilibration, for each lattice direction, one atom was selected and given a kinetic energy impulse in each direction. These simulations for each direction and energy were repeated three times for statistics. The number of Frenkel pairs for each kinetic energy was determined after a simulation time of 6 ps. The probability of having a Frenkel pair for each energy was then calculated by averaging the number of generated Frenkel pairs in all directions. For the high energy collision cascades, the cell size was $40 \times 41 \times 42$ lattice units, and the simulation time was 10 ps. Atoms were given a kinetic energy ranging from 0.3 to 20 keV in the $\langle 135 \rangle$ direction, which is a typical low-symmetry direction that represents well randomness for simulating collision cascades [18]. Frenkel pairs were identified using Wigner-Seitz analysis implemented in OVITO [19,20].

C. AIMD simulation

In this paper, we also determine $E_d^{\min}$ in metallic materials by employing AIMD simulations. It was shown in a previous study [18] that AIMD is a powerful tool which can be applied to determine the TDE. However, due to the high complexity and computational cost, it is difficult to use

FIG. 1. Damage energy models displayed for face-centered cubic (fcc) Cu, with comparison with experiments and classical molecular dynamics (MD) simulations. When $N_d < 1$, it is the probability to produce a stable Frenkel pair in each damage event. For the experimental reference damage data, we name them as Zinkle 1993 [12]; the damage energy of the experimental data is determined from the recoil energy [9]; the Cu interatomic potential used in this work are from Ref. [25]. $E_d^{\min}$ and E_d^{avr} in our modified model were calculated from classical MD simulations for self-consistency.

AIMD to search for the global $E_d^{\min}$ of various materials over all lattice directions. Nevertheless, since $E_d^{\min}$ usually exists in high-symmetry directions, we can with good confidence determine $E_d^{\min}$ of any material by only calculating the TDE of several high-symmetry directions. Furthermore, we can minimize the number of samplings in the threshold search by using experience from classical MD simulations. All AIMD simulations were performed in the microcanonical (NVE) ensemble using the Vienna *Ab initio* Simulation Package (VASP) [21] with the projector augmented-wave method [22]. The generalized gradient approximation with the Perdew-Burke-Ernzerhof exchange-correlation functional [23] was used for all calculations. For bcc metals, noncubic $7 \times 6 \times 6$ supercells containing 504 lattice sites were constructed. This size of supercell is large enough to sample the TDE according to previous studies [18]. For fcc and hcp metals, noncubic $6 \times 5 \times 5$ supercells with 600 lattice sites were constructed. We used the standard pseudopotential for Al and semicore pseudopotentials for all other metals to have proper short-range interactions and yield more correct TDEs [18,24]. All calculations were carried out using the Γ point in the Brillouin zone. The search for the TDE was done by successively increasing the kinetic energy of the PKA until a stable Frenkel pair was seen after a simulation time of 2 ps, as in Ref. [18]. This minimum kinetic energy for having a stable Frenkel pair is the TDE for a particular direction. Even though the simulation time of AIMD is 4 ps shorter here than that in classical MD, no recombination of defects was observed in the classical MD simulations between 2 and 6 ps. This is because near TDE collision cascades cool down quickly due to low damage energy. Once stable Frenkel pairs are formed, just a few picoseconds are not enough for them to thermally migrate and recombine.

FIG. 2. Damage production in body-centered cubic (bcc) metals. Classical and *ab initio* molecular dynamics (MD) simulations, as well as the athermal recombination corrected displacements per atom (arc-dpa) model and our low-energy extension are compared. For our own classical MD simulations, the reference numbers are the interatomic potentials used in this work; for the reference damage data using classical MD simulations, we name them as last name of the interatomic potential developer and publication year of the potential for better comparison; for the density functional theory (DFT) reference data, we name them as last name of first author and publication year. The reference numbers for reference classical MD data contain both simulation works and potential development works (some of the potential developers also performed simulations). Reference data: V: Johnson 1989 [28,29]; Fe: Calder 1993 [31,32], Marinica 2007 [33], Olsson 2016 [18]; Nb: Lin 2017 [35]; W: Ackland 1987 [9,38]; Björkas 2009 [9,39]. Interatomic potentials used in this work: V [30], Fe [34], Nb [36,37], W [40,41]. $E_d^{\min}$ and E_d^{avr} were calculated from classical MD simulations for self-consistency. The error bars correspond to standard deviation.

III. RESULTS AND DISCUSSION

A. Near TDE damage in fcc Cu

In Fig. 1, we show the damage production as a function of damage energy in fcc Cu. Copper is chosen here as a first illustration of the model because there are both experimental results and simulations to compare with. As we shall see later, the step function of the earlier models, here exemplified with the arc-dpa model, does not compare well with available data for near-threshold events. According to Fig. 1, both experimental and simulation results are better explained by the modified model than by the arc-dpa model. The modified model can provide an overall more reasonable estimation of damage production in Cu when the damage energy is near the TDE, even though it is very simple. However, while both the modified model and experimental results show that the increase of damage production probability is essentially linear,

there is a nonlinear relationship in the MD simulation results. The reason for this will be discussed in Sec. III B.

B. Defect production in bcc, fcc, and hcp metals

Figures 2–4 show the comparison between the modified model and MD simulation results for various bcc, fcc, and hcp metals, respectively. In Figs. 2 and 4, it is seen that the modified model generally shows excellent agreement with bcc and hcp metals. For fcc metals in Fig. 3, even though there are nonlinearities in the simulation results, the modified model still agrees well with simulation results. Hence, we can conclude that our modified model is general for metals and completes the arc-dpa model to cover the full energy range.

The reason for the nonlinearities in the fcc results is that the TDE surfaces of fcc metals obtained from MD simulations are qualitatively different from the other metal structures. In our

FIG. 3. Damage production in face-centered cubic (fcc) metals. Classical molecular dynamics (MD) simulations, experimental data, as well as the athermal recombination corrected displacements per atom (arc-dpa) model and our low-energy extension are compared. For our own classical MD simulations, the reference numbers are the interatomic potentials used in this work; for the reference damage data using classical MD simulations, we name them as last name of the interatomic potential developer and publication year of the potential for better comparison; for the experimental reference data, we name them as last name of first author and publication year. The reference numbers for reference classical MD data contain both simulation works and potential development works. Reference data: Al: Ercolessi 1994 [42,43]. Ni: Cleri 1993 [45,46]; Cu: Zinkle 1993 [12], Averback 1998 [8], Sabochick 1991 [9,48]; Ag: Merkel 1977 [49]. Interatomic potentials used in this work: Al [44], Ni [36,47], Cu [25], Ag [50,51]. $E_d^{\min}$ and E_d^{avr} were calculated from classical MD simulations for self-consistency. The damage energy in the experimental data was determined from the recoil energy for Cu [9] and Ag [27]. The error bars correspond to standard deviation.

modification, it is assumed that the distribution of TDEs from minimum to maximum is uniform, meaning that the cumulative distribution function (CDF) for TDEs should increase linearly with energy. For bcc and hcp metals, this assumption is relatively accurate. Figure 5 illustrates such uniform TDE distribution for bcc Fe. It is seen that, while the increase of the CDF is not completely linear, the TDE distribution is still relatively uniform and fits well with the assumption of our modified model. For fcc metals, there are two types of TDE surfaces for explaining the kinks in the results. The first type is demonstrated in Fig. 5 for Ag. It has a similar shape with the simulation result of Ag, meaning that the threshold energies for this metal in all directions are either very low or rather high, i.e., there are almost no directions with near-average level TDEs. Therefore, the number of defects will first increase rapidly with damage energy and produce defects in

the low-TDE directions, then it will stop increasing until the damage energy is high enough to produce defects in high-TDE directions, opening a new regime. The second type of TDE surface is shown in Fig. 5 for Cu (the classical MD simulation result), where the number of defects first increase rapidly with damage energy in a similar shape with the corresponding CDF of the TDE. When the damage energy is high enough, there will on average be >1 defect produced in a single collision in the low-TDE directions. Hence, an abrupt increase of number of defects appears, as shown in Fig. 3 for Cu. For the fcc metals studied here, Ag and Al have the first type of TDE surface, and Cu and Ni have the second type of TDE surface, based on classical MD simulations. The two types of TDE surfaces are also observed in experiments. Figure 3 compared the experimental TDE distributions with the simulated TDE distribution in Cu. Experimental results in Refs. [11] and [10] have first

FIG. 4. Damage production in hexagonal close-packed (hcp) metals. Classical molecular dynamics (MD) simulations, as well as the athermal recombination corrected displacements per atom (arc-dpa) model and our low-energy extension are compared. For our own classical MD simulations, the reference numbers are the interatomic potentials used in this work; for the reference damage data using classical MD simulations, we name them as last name of the interatomic potential developer and publication year of the potential for better comparison. The reference numbers for reference classical MD data contain both simulation works and potential development works. Reference data: Ti: Ackland 1992 [52,53]; Zr: Ackland 1995 [52,55]. Interatomic potentials used in this work: Ti [53,54], Zr [47]. $E_d^{\min}$ and E_d^{avr} were calculated from classical MD simulations for self-consistency. The error bars correspond to standard deviation.

and second type of TDE surfaces, respectively. Based on both experimental and simulation results, we conclude that TDE surfaces of fcc metals are qualitatively different from those of bcc and hcp metals. This difference causes the nonlinearities in the simulation results. Nevertheless, since the overall agreement between simulation results and the modified model is still good, it should still be very useful for damage production estimation also in fcc metals.

For the high energy damage events ($T_d > 300$ eV), we also performed many simulations of collision cascades and compared them with other available experimental and simulation results in Figs. 2–4. For bcc and fcc metal materials, $b_{\text{arc-dpa}}$ and $c_{\text{arc-dpa}}$ parameters in Eq. (2) are taken from Refs. [9,26]. However, we note that the $c_{\text{arc-dpa}}$ values are not so well fitted for hcp Ti and Zr in Ref. [26], see the dashed lines for Ti and Zr in Fig. 4. Therefore, by following the method in Ref. [26], we refitted $c_{\text{arc-dpa}}$ of Ti and Zr. Table I shows the

refitted $c_{\text{arc-dpa}}$ values for Ti and Zr, while $b_{\text{arc-dpa}}$ is unchanged. Based on Ref. [26], it is in principle reasonable to assume that $b_{\text{arc-dpa}} = -1$ for most materials, including Ti and Zr. Figures 2–4 demonstrate that the arc-dpa model excellently agrees with bcc, fcc, and hcp metals at high T_d .

C. AIMD calculation of minimum TDEs of metals

Because we note that the minimum TDE carries particular importance for near-threshold events, and we therefore introduced the term $E_d^{\min}$ in Eq. (5), we have calculated the minimum TDEs for various metal materials using both AIMD and classical MD. These are listed in Table II in comparison with experimental data. Based on the classical MD results, it is illustrated that, generally, the minimum TDE direction is one of the specific high-symmetry lattice directions, such as $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$, or the global minimum TDE is only ~ 2 eV

FIG. 5. The cumulative distribution function (CDF) of threshold displacement energy (TDE) distributions in Fe, Ag, and Cu. For our own classical molecular dynamics (MD) simulations, the reference numbers are the interatomic potentials used in this work. The dashed black lines are the CDF of uniformly distributed TDEs, which is the ideal assumption used in the modified model. The dashed gray lines are the average TDE calculated from classical MD simulations. The interatomic potentials are Fe [34], Ag [50], Cu [25]. The experimental references are King 1981 [10] and King 1983 [11].

TABLE I. Comparison of reference and refitted c_{arcdpa} for Ti and Zr.

c_{arcdpa}	Ti	Zr
Reference [26]	0.83	0.70
Refitted	0.35	0.32

lower than that of the lowest high-symmetry direction. Hence, we conclude that AIMD simulations can be a very powerful predictive tool here. As described in Sec. II C, we only try to find minimum TDEs in several high-symmetry lattice directions but expect these to either be the actual minima or be very near them. The AIMD results are demonstrated in Table II. In general, the AIMD results agree very well with the available experimental results. These results support our assumption that minimum TDEs usually exist in specific high-symmetry directions.

D. Revising the TDE of fcc Ni

For fcc Ni, we note that the calculated average TDE from classical MD simulations is 64 eV [47] and 82 eV [36], both of which are significantly different from the commonly used literature value of 40 eV from American Society for Testing and Materials (ASTM) [60]. We also note that experiments and AIMD simulations of the minimum values in Table II are significantly lower than those of classical MD simulations.

Ni-based alloys exhibit considerably interesting mechanical properties and good radiation tolerance [61], which make them promising candidates as structural materials in Gen-IV fission reactors. Hence, finding the correct TDE of Ni is an important step for studying Ni and Ni-based alloys under irradiation. The TDE of Ni has been determined using both experiments and simulations [16,56,60,62]. However, different methods yield significantly different results. The TDE of Ni thus needs to be more accurately determined. We utilized AIMD calculations to determine the TDEs in three specific lattice directions in Ni where experimental references exist. The TDEs in these specific lattice directions can be compared with other results to estimate the actual average TDE of Ni. We also used two more interatomic potentials to calculate TDEs of Ni. The results are listed in Table III. The TDEs obtained using different potentials are very different. This is, however, quite expected because the TDEs are significantly influenced by the potential fitting methods applied. While all potentials give different TDEs, they all suggest that the average TDE is much higher than 40 eV. This is further supported by AIMD calculations. Even though AIMD simulations present some differences with respect to the experimental results, they still clearly support the general levels and level differences present in the experimental results and, consequently, that the low ASTM value is unreasonable. We conclude that the 40 eV recommendation for Ni from ASTM should be updated in future work and that ~ 70 eV, as indicated

TABLE II. Minimum TDEs of various metals, both experimental and simulation results.

Crystal structure	Metal	Experiment (eV)	AIMD (eV)	Classical MD	
				Minimum (eV)	Specific directions (eV)
bcc	V ^a	25 ^b , 30 (100) ^c	26 (100)	12	12 (100)
	Fe ^d	20 ^c	18 ^e	18	20 (100)
	Nb ^f	28 ^b	28 (100)	20	20 (100)
	W ^g	42 (100) ^h	48 (410) ⁱ	36	36 (100)
fcc	Al ^j	16 ^b	19 (100)	14	16 (100) (110)
	Ni ^k	23 ^b , 22 (110) ^c	27 (100)	38	40 (110)
	Cu ^l	19 (110) (100) ^c	25 (100)	18	20 (100)
	Ag ^m	23 (110) ^c	24 (100)	20	22 (100)
hcp	Ti ⁿ	23 (0001) ^o	23 (0001)	12	12 (0001)
	Zr ^p	21 ^q	20 (0001)	16	22 (1120)

^aReference [30].

^bReference [56].

^cReference [16].

^dReference [34].

^eReference [18].

^fReference [36].

^gReference [40].

^hReference [57].

ⁱReference [24].

^jReference [44].

^kReference [47].

^lReference [25].

^mReference [50].

ⁿReference [54].

^oReference [58].

^pReference [47].

^qReference [59].

TABLE III. Average TDE and TDEs in specific directions for Ni. For MD simulations, the potentials used are named as last name of first author and publication year.

	Reference (eV)		This paper (eV)				
	ASTM ^a	Experiment	AIMD	Wilson 2015 ^b	Zhang 2016 ^c	Ko 2015 ^d	Bonny 2013 ^e
$\langle 100 \rangle$		38 ^f	27	46	50	28	52
$\langle 110 \rangle$		21 ^f	30	40	44	32	52
$\langle 111 \rangle$		>60 ^f	70	70	80	40	80
E_d^{avr}	40	69 ^g		65	82	49	100

^aReference [60].

^bReference [47].

^cReference [36].

^dReference [63].

^eReference [64].

^fReference [16].

^gReference [56].

by experiments, seems to be a more consistent and reasonable value.

IV. CONCLUSIONS

In this paper, we modified the arc-dpa model with a low-energy extension to make it suitable for near TDE primary damage events and thus provide a simple analytical damage model valid for all energy ranges. Classical MD simulations were used to validate the modified model. It is shown here that these provide predictive data that can be used generally for a wide implementation of the model. In general, the modified model agrees very well with simulation results on metallic materials. For fcc metals, the TDE surfaces are qualitatively different from bcc and hcp metals, which is the reason for the larger deviation between the model and simulation results. We also used AIMD simulations to determine the minimum TDEs for metallic materials in a few high-symmetry directions. The AIMD results are in excellent agreement with experimental results. This means that AIMD can be used to calculate the minimum TDEs of metallic materials with reasonable computational cost and very good accuracy. In addition, the

average TDE of Ni is estimated using both MD and AIMD. By comparing the simulation data with experimental results, it is indicated that the commonly used literature TDE of Ni (40 eV) is incorrect, and the true average TDE of Ni is closer to 70 eV.

ACKNOWLEDGMENTS

The financial support by the China Scholarship Council (No. 201807930008), Svensk Kärnbränslehantering AB and the EUROfusion Consortium through the Euratom research and training programme 2019-2020 under Grant Agreement No. 633053 is acknowledged. The views and opinions expressed herein do not necessarily reflect those of the European Commission. The computational resources were provided by the Swedish National Infrastructure for Computing (SNIC) and by the CINECA HPC center in Italy. The authors gratefully thank Elin Toijer, Luca Messina, and Zhongwen Chang for inspiration as well as Kai Nordlund at University of Helsinki for fruitful discussions. This paper contributes to the Joint Program on Nuclear Materials (JPNM) of the European Energy Research Alliance (EERA).

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