Cascade morphology transition in bcc metals

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Abstract

Energetic atom collisions in solids induce shockwaves with complex morphologies. In this paper, we establish the existence of a morphological transition in such cascades. The order parameter of the morphology is defined as the exponent, $b$, in the defect production curve as a function of cascade energy ($N_F \sim E_{MD}^b$). Response of different bcc metals can be compared in a consistent energy domain when the energy is normalized by the transition energy, $\mu$, between the high- and the low-energy regime. Using Cr, Fe, Mo and W data, an empirical formula of $\mu$ as a function of displacement threshold energy, $E_d$, is presented for bcc metals.

Keywords: displacement cascade, morphology transition, threshold energy, morphology classification, sub-cascade, molecular dynamics simulation, tungsten molybdenum iron chromium

(Some figures may appear in colour only in the online journal)

1. Introduction

An energetic particle entering a solid metal will initiate a collision cascade upon scattering with an atomic nucleus and this process often induces complex shockwaves. The morphology of the cascade depends on the energy of the primary knock-on atom (PKA). At high energies, a single PKA may induce multiple damage regions. These damage regions are generally referred to as sub-cascades. After the 1990s, molecular dynamics (MD) simulations of displacement cascades with millions of atoms have become computationally affordable. A good collection of some MD data in metals can be found in the review articles [1–3]. Examples include, but not limited to, Al [4], Cu [5–8], Fe [9, 10], Fe–Cr [11–13], Mo [14], Ni [4, 5], Ni3Al [15], Ti [16], V [17–19], W [19–24] and Zr [16]. Nevertheless, the majority of the MD data is limited to PKA energies of 10 or 20 keV, which is not high enough to investigate the sub-cascade phenomenon and often times the data are sparse.

Due to the importance of steel in nuclear technologies, Fe has been one of the most studied materials [3, 25]. For Fe, Stoller et al simulated cascades up to 200 keV [26]. There are also some results at 200 keV and 500 keV by Zarkadoula et al [27, 28]. In Fe, sub-cascades are routinely observed at 20 keV and above. The plot of the number of surviving defects versus energy on a log–log scale shows a bilinear curve with a kink at around 20 keV. This shows that the defect production behavior is affected by the underlying cascade morphology. From our own simulations and recent MD data by Sand et al at 150 keV [29, 30], a different kind of cascade morphology is observed in W. In this case, the sub-cascades are interconnected. The implication of such morphology on the defect production trend is even more prominent than in Fe. In fact, extended defects such as loops of self-interstitial atoms (SIAs) [29, 31] can form in a single cascade in W. Given the important implication of different cascade morphologies on defects and their subsequent microstructural evolution, it is of interest to study the transition energy between these morphologies. This manuscript is primarily concerned with the determination of the transition energies along with an empirical formula to estimate them for a group of body-centered cubic (bcc) metals Cr, Fe, Mo and W.
In 1991, Heinisch et al. [32] determined the threshold energy for sub-cascade break up in face-centered cubic (fcc) Al, Cu, Ag, Au, in addition to bcc Fe, Mo and W. This study was performed within the binary collision approximation (BCA) [33]. The sub-cascade break up energy for Fe, Mo and W was determined to be 50, 130 and 300 keV, respectively. They reported that these energies scale linearly with the value of the screened Coulomb potential at the screening radius for each metal. Some important discrepancies are found between BCA and MD results. For example, the sub-cascade break up energy in Fe from BCA simulation is 50 keV, while in MD it is around 20 keV as previously mentioned. Within BCA, W cascades do not exhibit any morphology change until 300 keV, while MD simulations show that the morphology changes at around 30–40 keV as presented here. One of the reasons for these discrepancies is presumably inherent with the approximation itself. Within BCA, each collision is assumed to involve only two atoms. While in reality, a collision may concurrently involve many atoms. Even though BCA is expected to be less realistic than MD, the BCA results do indicate that a morphology transition is not exclusive to a certain material but a common phenomenon, at least among fcc and bcc metals that have been investigated.

Indeed, because of the computational cost, we are only beginning to explore in a systematic way the high-energy regimes of displacement cascades using MD. In this manuscript, we present and compare cascades in Cr, Fe, Mo and W as a function of cascade energy. We include energies up to 70, 200, 100 and 150 keV for Cr, Fe, Mo and W, respectively. We show the existence of a morphological transition and determine the transition energy in these bcc metals. We explore how the transition point can be predicted from materials properties related to radiation damage such as mass and displacement threshold energy.

2. Methods

The MD simulations are performed using the LAMMPS code [34]. The forces are derived mostly from Finnis–Sinclair potentials [35] with further improvements, particularly the repulsive parts, that are suitable for cascade simulations; Fe by Calder et al [9], Mo by Salonen et al [36, 37] and W by Juslin et al [37, 38]. For Cr, the embedded-atom-method potential by Bonny et al is taken [39] with short-range extension done by Juslin for this work.

Before a cascade simulation is started, the atoms are thermalized at 300 K and zero pressure with a Nosé–Hoover thermostat to obtain a proper distribution of positions and velocities. The cascade is initiated by giving a random primary-knock-on-atom (PKA) near the center of the cell an initial velocity with a random direction. In keeping with our comparison to previous simulations [25, 26, 31, 40], the simulations did not treat electronic stopping. To first order, neglecting electronic losses amounts to an energy difference between the true PKA energy and the MD cascade energy; the latter of which is essentially equivalent to the damage energy in the Norgett–Robinson–Torrens (NRT) displacement model [26, 41, 42]. However, the effects of electronic energy losses are complex [43–45] and beyond the scope of the current effort. We shall return to this effect in the Discussion section.

The PKA initial kinetic energy is denoted by $E_{\text{MD}}$. An adaptive time step is used with a maximum displacement of 0.005 Å per step. The cascades in Cr and W have been simulated in an NVE ensemble for all atoms except the border atoms. The border atoms are those within one lattice unit from the box edges. A Nosé–Hoover thermostat at 300 K with 50-fs time constant is applied to the border atoms to extract heat from the system. With this setting, the temperature of the system is $< 400 \text{K}$ at the end of the simulation. Such an increase of the temperature has negligible effect on the results presented here. Therefore, the choice of the time constant is appropriate. The simulations are stopped when the number of surviving Frenkel pairs, $N_F$, does not change for more than 10 ps. Note that for all other metals, unless otherwise specified, the cascade simulations were performed with this default procedure. Some of the cascade data for W are taken from our earlier study [31], in which NVE was used for the first 10 ps, then NVT was applied to all atoms and the simulation was followed up to 55 ps. We have verified that the two simulation settings yield the same results within statistical error. For Fe and Mo, the simulations were performed at 100 K and 300 K, respectively, as described in [26, 40]. Detailed information on which data points are obtained from previous simulations and which ones are calculated in this study is presented in the Appendix. Sufficiently large simulation cells are used to ensure no interaction between displaced atoms across the periodic boundaries. A self-interstitial atom or a vacancy is determined from the occupancy of the Wigner–Seitz cells of a reference lattice.

For our analysis, a consistent determination of displacement threshold energy for each potential, $E_d$, is essential. Therefore, all values of $E_d$ in this study are calculated using the same method, as described here. Periodic boundaries are applied along all axes. An orthorhombic box of $20 \times 18 \times 16$ supercell is used to avoid the self-interaction of the SIA moving along the $<1 1 1>$ directions. The box contains 11,520 atoms. In test runs using 10 PKAs in each direction along $[1 0 0]$, $[1 1 0]$, $[1 1 1]$ and $[1 3 6]$, a smaller box size of $18 \times 16 \times 14$ is used and the results are the same within the standard error as with the $20 \times 18 \times 16$, giving confidence that the $20 \times 18 \times 16$ box is sufficient. We have also visually verified that replacement events are contained within the box when an SIA is created.

For threshold energy simulation, the system is equilibrated at 10 K and zero pressure for 20 ps before a displacement is initiated. Then, low-energy displacements are simulated using the same setting as described previously. In this case, the border atoms are equilibrated at 10 K to extract heat. From visualization, it is evident that 3 ps is appropriate for observing defect creation. Therefore, the simulation is followed up to 3 ps. In the test runs, we also verified that simulations up to 5 ps give the same results. Since the high-energy cascades that are analyzed in this study involve collisions along random
directions, the appropriate $E_d$ is the average value over all directions [46]. The average value is defined as

$$E_d = \frac{1}{4\pi} \int_0^{4\pi} E_d(\Omega) d\Omega,$$

where $\Omega$ is the direction in space and $d\Omega$ is the solid angle. Due to symmetry, only $E_d(\Omega)$ that are within the irreducible crystal directions (ICD) are needed. The ICD and the PKA direction grid used in this study are shown in figure 1(a).

If ICD are employed, it is necessary to account for the different multiplicity of each direction to correctly calculate the average. The multiplicity represents the number of equivalent directions of a grid point. In figure 1(b), the multiplicity of grid point-$i$, denoted as $P_i$, is shown as the number following the x character given in parentheses. The grids are constructed with a Miller index increment of 1/24 resulting in a total of 325 points. Note that these points are not located on the surface of a sphere centered at the origin. Therefore, an appropriate weight due to the different solid angle of each point needs to be taken into account. The solid angle of point-$i$, denoted as $\Delta\Omega_i$, is calculated as the solid angle enclosing a small sphere with a diameter $D = 1/24$ (i.e. the diameter is the same as the side length of the grid cube) centered at grid point-$i$, as illustrated in figure 1(a). Finally, equation (1) becomes

$$E_d = \sum_i E_{d,i} P_i \Delta\Omega_i \left/ \sum_i P_i \Delta\Omega_i \right.,$$

$$\Delta\Omega_i(h, k, l) = 2\pi \left( 1 - \frac{\sqrt{h^2 + k^2 + l^2}}{\sqrt{h^2 + k^2 + l^2 + D^2/4}} \right),$$

where $h, k, l$ are the Miller indices. For each direction, $E_{d,i}$ is averaged from 10 simulation runs, each using a different PKA chosen from near the box center. To search for the threshold energy, the PKA energy is incremented by 5 eV until a defect is detected, then decremented by 1 eV until no defects are detected. The minimum energy where a defect is detected is taken as the threshold for this specific run.

3. Results and discussion

For each data point, the number of simulation runs ($N_r$), the number of surviving Frenkel pairs ($N_F$) and the standard error of the mean (STE) of $N_F$ are presented in the Appendix. The standard error is calculated as $STE = STD/\sqrt{N_r}$, where STD is the standard deviation. Figure 2 shows plots of $N_F$ versus $E_{MD}$ for each metal on a log–log scale. The data points exhibit remarkably clear linear regimes on this scale ($N_F \sim E_{MD}^b$). It is evident from the W and Fe curves that two linear regions exist, characterized by different slopes, $b$. It is logical then to expect similar behavior for Cr and Mo, which is observed albeit with a less pronounced change in slope. To consistently determine the characteristic slopes, the data are fit as follows. Only data points where $N_F > 1$ are included in the fit. This is motivated by the fact that in the energy regime where $N_F < 1$, the probability of creating a Frenkel pair is normally either 1 or 0. In such a regime, cascade-like behavior does not occur. A linear regression is performed to fit the data with two lines. The determination of which line segment the data points should be assigned is based on a minimization of the total norm of the residuals from the two fit lines. The value of $E_{MD}$ at the intersection (inflection) of the fit lines is defined as the transition energy, $\mu$. We note that the slopes determined in this way are slightly different from those obtained by the original authors for Fe [26] and Mo [40].

Due to the different displacement threshold energies of each metal, perhaps a better way to compare different materials is to use a reduced energy $E^* = E_{MD}/E_d$. Table 1 summarizes the values of $E_d$ calculated with equation (2). Figure 3(a) shows the plots of $N_F$ versus $E^*$. The standard NRT model, $N_F = 0.4 E^*$, is included for reference [41]. The deviation of MD results from the NRT model is evident. The deviation arises from the fact that the efficiency of in-cascade SIA-vacancy recombination is energy dependent. In the low-energy regime ($E_{MD} < \mu$), in-cascade recombination increases with energy. This leads to sub-linear behavior with a characteristic
Figure 2. Plots of $N_F$ versus $E_{MD}$. The error bars represent the standard errors of the mean. The fit lines reveal two energy regimes with a transition energy $\mu$.

Table 1. Displacement threshold energy, $E_d$, calculated using equation (2) as described in the text and using normal or variable atomic masses, as described later in the text.

| Interatomic potential | $E_d$ (eV) | Note |
|-----------------------|------------|------|
| Cr                    | 34.4 ± 1.5 | As is. |
| Fe                    | 41.8 ± 1.6 | As is. |
| Mo                    | 78.7 ± 2.9 | As is. |
| W                     | 122.6 ± 4.4| As is. |
| Cr                    | 33.8 ± 1.4 | With W mass. |
| Cr                    | 18.9 ± 1.1 | With W PKA mass. |
| W                     | 123.6 ± 4.4| With Cr mass. |
| W                     | 170.9 ± 6.7| With Cr PKA mass. |
| W-hjörkas             | 98.0 ± 3.7 | As is. |

Figure 3. (a) Plots of $N_F$ versus $E_{MD}/E_d$. The error bars represent the standard errors of the mean. The range of the transition energy, $\mu$, is shown as a vertical gray bar. (b) Average size of the largest SIA clusters, revealing the formation of large SIA clusters in tungsten after the transition energy.

Identifying the underlying physical origin of the change in slope of defect production is non-trivial due to the complex nature of the cascade process. This has previously been associated qualitatively with the onset of sub-cascade formation [26, 32]. Here we seek a more detailed explanation based on the cascade damage production process. The size distribution of the surviving defect clusters provides a hint.Interstitial clusters are identified with a cutoff of the third nearest-neighbor distance (NN3) [31]. Varying the cutoff from NN1 to NN3 does not alter the qualitative results presented here [31]. Figure 3(b) shows the average size (over all simulations) of the largest SIA clusters, $S_{\text{SIA}}^{\text{max}}$. A clear correlation can be seen between $\mu$ and the onset of the rapid increase in the $S_{\text{SIA}}^{\text{max}}$ curve for W. For $E_{MD} < \mu$, the $S_{\text{SIA}}^{\text{max}}$ for W is similar to that for other metals, consistent with the similarity in the slopes of the defect production in this regime. For $E_{MD} > \mu$, the $S_{\text{SIA}}^{\text{max}}$ increases rapidly for W while for Cr, Fe and Mo it increases only gradually. The fact that Cr, Fe, Mo exhibit a common gradual increase in the $S_{\text{SIA}}^{\text{max}}$ rather than a rapid change, is consistent with the similarity in the slopes
Figure 4. Colormap of coordination number within 1.4\(a_0\) revealing three different cascade morphologies (a) single-shock (SS), (b) non-interacting or separate multiple-shock (sMS) and (c) interacting multiple-shock (iMS). Surviving SIAs (green atoms) and vacancies (black) are superimposed to show the associated defect clustering.

of the defect production in these metals; \(b < 1\) below the transition which increases only moderately to \(b \approx 1\) above the transition. The overall correlation suggests the existence of three cascade morphologies as a function of energy, namely (i) \(E_{MD} < \mu\) (\(b < 1\)), (ii) \(E_{MD} > \mu\) of Cr, Fe and Mo (\(b \approx 1\)) and (iii) \(E_{MD} > \mu\) of W (\(b > 1\)).

To reveal the cascade morphology, a colormap of atom density (number of neighbors within 1.4\(a_0\), \(a_0\) is the lattice constant) is analyzed as in [47] using the OVITO code [48]. Figure 4(d) shows the number of displaced atoms, \(N_{DA}\), versus \(t\) from a typical high-energy (75 keV) cascade in W. Displaced atoms are those beyond 0.3\(a_0\) from any lattice site and are useful to reveal the pressure wave progression (note that displaced atoms create pressure variation within the materials). At the beginning, up to \(\sim 0.18\) ps, \(N_{DA}\) increases with time as \(\sim t^3\), suggesting that the wave front moves at a constant speed. For a 75 keV PKA, the speed\(^4\) is \(2.8v_L\) (where \(v_L = 5220\) m s\(^{-1}\) is the speed of a longitudinal sound wave in W). Clearly, the cascade is governed by supersonic shocks at this stage, which ends at \(t_1\). The cascade energy is then dissipated elastically via a sonic wave until 2 ps. The middle of the sonic stage is labeled with \(t_2\).

Figure 4(a) shows a density map representing the case of \(E_{MD} < \mu\). All metals in this regime exhibit a similar morphology consisting of one low-density region (core), even though the core shape is irregular. This figure depicts a single supersonic shock. Hence the cascade exhibits a single-shock (SS) morphology. For brevity throughout this article, the term shock is used to denote a supersonic shock. For \(E_{MD} > \mu\), the PKA energy is sufficiently high to create multiple shocks. Figure 4(b) shows the morphology associated with Cr at \(E_{MD} > \mu\), which is also representative of Fe and Mo. The shocks are separate from each other with a distance similar to the size of the shocks. At \(t_2\) (bottom panel), three shock domains are evident. Due to the separation, each shock progresses independently. The surviving SIAs (green atoms) and vacancies (black) are superimposed with the density map (bottom panel) to show how SIAs are distributed at the shock periphery. This morphology is referred to as non-interacting or separate multiple-shock (sMS). Meanwhile, figure 4(c) shows the morphology associated with W at \(E_{MD} > \mu\). In this case, the shock fronts are interconnected. The location of the large final SIA cluster is marked by a rectangle. It can be seen that the SIA cluster is located at a low-density region. By following the evolution of such a plot, it is apparent that this cluster originates from the nearby shock fronts as indicated by the arrow. The connectivity among the shocks enables the formation of a high atomic density region and simultaneously provides a place for these atoms to readily form a large cluster. The morphology is referred to as interacting multiple-shock (iMS). We summarize

\(^4\) The speed of the wave front, \(v_w = \frac{r_c}{t_1}\), is approximated by equating the number of bcc lattice sites in a sphere of radius \(r_c\) to the number of displaced atoms.
the cascade morphology classification as:

- **single-shock (SS) morphology**, occurs at \( E_{\text{MD}} < \mu \). The exponent of the \( N_f \) curve is \( b < 1 \) due to the energy-dependence of in-cascade SIA-vacancy recombination.

- **separate multiple-shock (sMS) morphology**, occurs at \( E_{\text{MD}} > \mu \) e.g. in Cr, Fe and Mo. The high defect survival efficiency in regions in between the shocks balances the in-cascade recombination resulting in \( b \approx 1 \).

- **interacting multiple-shock (iMS) morphology**, occurs at \( E_{\text{MD}} > \mu \) e.g. in W. The shocks are closely interconnected allowing the formation of large SIA clusters resulting in \( b > 1 \).

Calder et al investigated defect clustering in Fe [47]. Using a single Fe PKA, they did not observe interacting multiple shocks. However, when they employed a molecular Bi\(_2\) PKA (two Bi atoms), interacting multiple shocks were induced due to high energy deposition associated with the more massive PKA. They reported that the Burgers vectors of the SIA loops are not oriented radially from the cascade core. We confirm their observation in our W simulations. The loop formation mechanism in an interacting multiple-shock cascade is different from other models which describe the formation of dislocation arrays and dislocation loops from a single shock wave [49–52]. A good visualization of these models can be found in [53]. For these single shock wave models, Smith proposed an array of edge dislocations at the shock front to accommodate the compressed lattice behind the shock front [49]. Hornbogen modified the Smith model by replacing the edge dislocation array with an array of dislocation loops [50]. Meyers proposed a more complicated model in which part of the shock wave outruns the edge dislocations creating another set of dislocations [51]. Armstrong, Miller and Sandusky proposed reactions of these dislocations to produce dislocation pairs [52, 54, 55]. Diaz de la Rubia and Guinan reported the prismatic loop punching mechanism in Cu, which produced loops with Burgers vector aligned radially from the cascade core [56].

Correspondingly, when the cascade morphology is quantified in terms of the presence of supersonic shocks and their connectivity, the characteristic slope of \( N_f \) curve can be correlated with the underlying cascading morphology. In this sense, the transition energy \( \mu \) that marks the beginning of the multiple-shock morphology has a physical importance. While the transition energy falls in a narrow range as previously described, more data points are needed to obtain a more reliable scaling, possibly as a function of mass and/or \( E_d \). Thus, we performed additional simulations using the interatomic potentials of Cr and W (representing the lightest and heaviest element in this study, respectively), but applied these potentials to simulation cells that had different atomic mass, as described below (and listed in table 1). We also performed simulations of cascades in tungsten using a different potential labeled as W-björkas.

- **Cr/W-mass**, with Cr potential and W mass for all atoms.
- **Cr/W-PKAmass**, with Cr potential and mass for all atoms except the PKA, which was given mass equal to W.

![Figure 5. Transition energy, \( \mu \), as a function of displacement threshold energy, \( E_d \), showing a good linear scaling.](image-url)

- **W/Cr-mass**, with W potential and Cr mass for all atoms.
- **W/Cr-PKAmass**, with W potential and mass for all atoms except the PKA, which was given a mass equal to Cr.
- **W-björkas**, simulation using the W potential developed by Björkas et al [19].

For each of the above systems, the threshold energy has been calculated following the procedure outlined previously. The resulting values of the threshold displacement energy are also provided in table 1. Changing the effective mass of all atoms in the simulation for a given interatomic potential appears to have little to no effect on the threshold energy. However, changing just the mass of the initial PKA atom does result in significant changes, presumably as a result of the scattering efficiency. For W, the threshold energy increases from 122.6 eV to 170.9 eV when the PKA mass is decreased from that of W to that of Cr. Notably, this change is reasonably consistent with the decreased scattering efficiency of the energy transfer between Cr and W (\( \Lambda = 4m_nu_2/(m_1 + m_2)^2 \approx 0.69 \)). Increasing the PKA mass has an opposite effect. For Cr, \( E_d \) decreases from 34.4 eV to 18.9 eV if the PKA mass is changed from W to Cr.

High-energy cascades were then simulated for these additional systems to determine the transition energy using the default procedure as described previously. Figure 5 shows the plot of the transition energy as a function of the threshold energy for all systems. Overall, the value of \( \mu \) shows a remarkable linear correlation with \( E_d \). This finding confirms the narrow range of \( \mu^* \). A linear fit is performed with a constraint to pass through the origin. The scaling is found to be \( \mu = (284 \pm 16) \times E_d \). Note that if the fit is done using only the Cr, Fe, Mo and W data, we obtain \( \mu = (310 \pm 24) \times E_d \).

The effect of PKA mass on threshold energy seems to be carried over to the transition energy. Increasing the PKA mass, Cr \( \rightarrow \) Cr/W-PKAmass, causes the transition to occur at a lower energy. Likewise, decreasing the PKA mass, W \( \rightarrow \) W/Cr-PKAmass, increases the transition energy. Despite these shifts, the reduced value of \( \mu \) remains unchanged. This indicates that
The factors determining energy nor the lattice parameter. Cohesive energy is one of changing the mass of all atoms changes neither the cohesive if the mass is smaller. For a given interatomic potential, similar, the dynamics of the cascade evolution occurs faster shown as a vertical gray bar.

The transition energy is closely related to the threshold energy. For a given PKA energy, increasing the PKA mass causes more damage since \( E_d \) is smaller. The probability of forming multiple shocks increases with the damage level. Therefore, the transition energy occurs at a lower value.

When the mass of all atoms is changed altogether, we do not observe a consistent trend in the shift of \( \mu \). Increasing the mass, Cr \( \rightarrow \) Cr/W-mass, slightly decreases \( \mu \). However, decreasing the mass, W \( \rightarrow \) W/Cr-mass, also decreases \( \mu \). This leads us to conclude that the effect on \( \mu \) is insignificant if the mass of all atoms is varied. Note from the threshold simulation that \( E_d \) also does not change in such cases. If all atoms still have the same mass, the kinematics of the collisions remains similar, i.e. the scattering angles and energy partitioning in each collision. This leads to an insignificant change in \( E_d \) and thus \( \mu \). Note that while the cascade kinematics is similar, the dynamics of the cascade evolution occurs faster if the mass is smaller. For a given interatomic potential, changing the mass of all atoms changes neither the cohesive energy nor the lattice parameter. Cohesive energy is one of the factors determining \( E_d \). Various migration pathways with the associated activation energies, defect formation energies and the detail of the collision process itself are all important factors.

Figure 6 shows the \( S_{\text{MAX}}^{\text{SIA}} \) for all systems. For the Cr potential, there is a slight increase from Cr to Cr/W-PKAmass. Likewise, for the W potential, there is a slight decrease from W to W/Cr-PKAmass. Above the transition energy, the curves for Fe, Mo and all cases of Cr still show the behavior characteristic of separate multiple-shock cascade morphology. While those for W-björkas and all cases of W show the strong clustering associated with the interacting multiple-shock morphology.

For Cr, Fe and Mo, the morphology transition can be directly inferred from the cascade visualization because the multiple shocks are separated. On the other hand, the morphology transition in W can be inferred from the clustering behavior. From this point of view, the existence of the transition is evident in all of these metals. Therefore, it is suggested to fit the defect production curve separately for each morphology. With the available data, we may compare the goodness of the bilinear curve fit (two-line fit) to that if the data are fit only with one line (one-line fit). One may use the standard \( R^2 \), the norm of the residual, or other parameters to measure the goodness. Even though the least-square method maximizes the \( R^2 \), or equivalently, minimizes the norm of the residual to find the best fit, these parameters often times are not informative. Thus, for the comparison purposes, we calculate the root-mean-square of the relative error, \( \delta_{\text{rms}} \), given in percentage as follows:

\[
\delta_{\text{rms}} = 100 \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{y_i - y_{i,\text{fit}}}{y_{i,\text{fit}}} \right)^2}
\]

where \( y_i \) is the \( N_F \) data point, \( y_{i,\text{fit}} \) is the \( N_F \) value from the fit and \( N \) is the total number of data points in the set. The results are presented in table 2. The two-line fit gives \( \delta_{\text{rms}} \) of \( \sim 5\% \) across all systems. The one-line fit gives about 20\% for Fe and W and 10\% for Cr and Mo. It is important to note that the one-line fit error will be increasingly larger if higher-energy data points were available.

It is worth mentioning that for W, both vacancy and SIA loops are observed in our simulations. Whereas in a self-ion irradiation experiment [57], it was suggested that only vacancy loops were formed from a single cascade, while SIA loops were observed only at higher doses presumably as a result of loop interactions from, or reactions with, multiple cascades. The discrepancy could arise from the fact that the ion irradiation experiment was performed on a thin foil. Given that the mean range of ions is typically only \( \sim 100 \) Å, any small SIA loops which are mobile, are usually assumed to have migrated and are lost to the surface [58, 59].

Sand et al recently reported the results of cascade simulations in W at 150 keV [29, 30]. In their simulations, a velocity-dependent frictional force is added to the equation of motion to model the electronic stopping [60]. The frictional

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**Table 2.** Root-mean-square of the relative error, \( \delta_{\text{rms}} \), of \( N_F \) given in percentage, calculated using equation (4).

| System               | Two-line fit | One-line fit |
|----------------------|--------------|--------------|
|                      | \( \delta_{\text{rms}}(\%) \) | \( \delta_{\text{rms}}(\%) \) |
| Cr                   | 5.1          | 10.2         |
| Fe                   | 5.9          | 18.8         |
| Mo                   | 5.0          | 9.3          |
| W                    | 3.3          | 19.9         |
| Cr/W-mass            | 5.8          | 12.4         |
| Cr/W-PKAmass         | 5.3          | 18.4         |
| W/Cr-mass            | 5.6          | 24.2         |
| W/Cr-PKAmass         | 5.5          | 11.8         |
| W-björkas            | 6.3          | 34.0         |

Note: Two-line fit denotes that the fit is performed using a bilinear curve as described in the text, while one-line fit uses only one line to fit all the data points of \( N_F \) versus energy.
force is applied to atoms whose kinetic energy is above a cutoff energy, $T_c$. They performed the simulations with the Ackland–Thetford (A–T) potential [37], which is similar to the Juˇslin potential in our simulations and the modified Dudarev–Derlet (D–D) potential [19, 61], which is the same as the Björkás potential in our study. With $T_c = 1$ eV, only little defect clustering occurs, which is inconsistent with the experiment where vacancy loops are seen [57]. Thus, $T_c = 1$ eV was considered as an incorrect choice. With $T_c = 10$ eV, the A–T potential shows the same trend as the D–D potential in which both SIAs and vacancies form large clusters and loops, although the cluster sizes are smaller than those with the D–D potential. They reported that the cascade morphology exhibits no sub-cascade break up, producing a massive, unbroken molten area, which facilitates the formation of large defect clusters; an observation that is consistent with ours. In terms of defect production, they reported that the A–T potential produced $N_F = 124 \pm 16$. The total electronic loss was calculated to be $\sim 40$ keV, thus the damage energy was $\sim 150–40 = 110$ keV. In our simulation, $N_F = 116 \pm 8$ at 100 keV and the fit formula gives $N_F = 0.257 \times (110)^{1.335} = 137$ at 110 keV, which is within the statistical error of the calculation with electronic loss. Using the Björkás potential, they reported $N_F = 179 \pm 21$, while in our simulation, $N_F = 171 \pm 20$ at 100 keV and the fit gives $N_F = 0.216 \times (110)^{1.467} = 213$ at 110 keV. Note that the error estimates are all taken from the standard errors of the mean. The number of simulations to calculate these errors is four (for the A–T and D–D potentials in their study), 20 (Juˇslin potential in our study) and 15 (björkás potential in our study).

Zarkadoula et al simulated cascades in Fe at 200 and 500 keV in which the electronic stopping was also modeled as a frictional force. In this case, they used $T_c = 8.5$ eV [27]. They reported that the number of surviving defects at 200 and 500 keV follows the trend of the defect production curve of the lower energies, i.e. the curve for Fe above $\mu$ in our study. This comparison is plotted in figure 4 of [27]. Unfortunately, the amount of energy loss was not reported, thus it was unclear whether they were comparing the same amount of damage energy. We acknowledge that excluding electronic loss may lead to an overestimate of the number of stable defects, defect clustering and the transition energy. However, based on the available data, the impact on our analysis appears to be either small or inconclusive (because of the scarcity of the data for comparison). The possible magnitude of any correction cannot be determined without a more extensive investigation of electronic energy losses which includes a two-temperature model [28, 44, 62] across a similar range of cascade energies.

Before we leave the discussion, we note that when a cascade exhibits a sMS morphology, the formation of sub-cascades can be clearly observed. Therefore, the $\mu$ in a SS $\rightarrow$ sMS transition corresponds to the threshold energy for sub-cascade formation. Evidently, this is not the case for W. In fact, the question becomes whether or not at some higher energy, W will exhibit another transition, namely iMS $\rightarrow$ sMS (sub-cascade formation). Within the binary collision approximation, sub-cascade formation is predicted, regardless of the metal [32, 63]. However, because of the limitation of this approximation to describe realistic cascades, MD simulations at even higher energies are needed in the future to verify the BCA predictions.

4. Conclusions

In conclusion, we have shown that there exists a transition energy in the defect production curve, $N_F \sim E^{*\text{MD}}_b$, of bcc metals. Below the transition energy, $\mu$, only a single supersonic shockwave forms. The value of the exponent is $b < 1$. Above the transition, the cascade energy is sufficient to induce multiple supersonic shockwaves. In Cr, Fe and Mo, the shockwaves are separated from each other. This leads to a value of the exponent, $b \approx 1$. The transition energy scales reasonably well with the threshold displacement energy. The empirical fit is found to be $\mu = (284 \pm 16) \times E_d$. All values of $E_d$ have been calculated using a consistent procedure. The procedure takes into account proper weighing factors that include point symmetry and solid angle coverage for each direction grid. For a given potential, the effect of mass on $E_d$ is negligible. However, increasing the PKA mass while keeping the mass of other atoms unchanged decreases $E_d$ and vice versa. Due to the linear scaling of $\mu$ with $E_d$, the effect of mass on $\mu$ is inherently included in its effect on $E_d$. Based on the results of this study, renormalizing the cascade energy with $E_d$ is suggested when comparing defect production among different bcc metals.

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Appendix A.

In this appendix, we present the list of the number of simulation runs ($N_r$) for each data point along with the number of surviving defects ($N_F$) and the standard error of the mean (STE) of $N_F$. The standard error is calculated as $\text{STE} = \text{STD}/\sqrt{N_r}$, where STD is the standard deviation.
| $E_{\text{MD}}$ (keV) | Cr$^a$ | Fe$^b$ | Mo$^c$ | W$^d$ |
|-----------------|------|------|------|------|
|                | $N_r$ | $N_F$ | STE  | $N_r$ | $N_F$ | STE  | $N_r$ | $N_F$ | STE  |
| 0.1             | 20   | 1.1  | 0.2  | 40   | 1.4  | 0.1  |      |      |      |
| 0.15            |      |      |      |      |      |      |      |      |      |
| 0.2             | 20   | 2.2  | 0.2  | 32   | 2.1  | 0.1  | 20   | 1.1  | 0.2  |
| 0.3             | 20   | 2.7  | 0.3  | 128  | 2.5  | 0.1  | 20   | 1.8  | 0.2  |
| 0.5             | 20   | 3.6  | 0.3  | 16   | 3.9  | 0.2  | 20   | 1.8  | 0.2  |
| 0.75            |      |      |      |      |      |      | 40   | 2.2  | 0.2  |
| 1               | 20   | 6.9  | 0.5  | 12   | 6.1  | 0.4  | 20   | 2.8  | 0.1  |
| 1.5             |      |      |      |      |      |      |      | 15   | 2.7  |
| 2               | 20   | 10.7 | 0.7  | 10   | 10.1 | 0.8  | 20   | 4.4  | 0.2  |
| 3               | 20   | 13.9 | 0.8  |      |      |      | 20   | 5.5  | 0.5  |
| 5               | 20   | 21.5 | 1.0  | 9    | 22.0 | 0.7  |      |      |      |
| 7.5             | 20   | 25.0 | 1.1  |      |      |      | 15   | 12.1 | 0.9  |
| 10              | 20   | 33.6 | 2.2  | 15   | 33.6 | 1.4  | 40   | 15.6 | 0.6  |
| 15              | 20   | 45.8 | 2.1  |      |      |      | 20   | 20.8 | 0.9  |
| 20              | 20   | 65.0 | 3.4  | 10   | 60.2 | 2.8  | 40   | 23.8 | 1.0  |
| 30              | 20   | 91.6 | 3.8  | 16   | 94.9 | 3.3  | 40   | 35.5 | 1.3  |
| 40              | 20   | 123.5| 4.1  | 8    | 131.0| 4.5  | 20   | 45.1 | 1.6  |
| 50              | 20   | 154.6| 4.4  | 9    | 168.3| 4.0  | 21   | 57.0 | 2.3  |
| 60              |      |      |      |      |      |      |      | 15   | 60.9 |
| 70              | 10   | 197.5| 6.4  |      |      |      |      | 10   | 81.6 |
| 75              |      |      |      |      |      |      |      |      | 15   |
| 100             |      |      |      |      |      |      |      |      | 10   |
| 150             |      |      |      |      |      |      |      |      | 10   |
| 200             |      |      |      |      |      |      |      |      |      |

$^a$ All data for Cr are calculated in this study.
$^b$ All data for Fe are from [26].
$^c$ For Mo, data at 1, 2, 10, 20, 30 and 50 keV are from [40], the rests are calculated in this study.
$^d$ Data for W are from [31] except the one at 150 keV.

| $E_{\text{MD}}$ (keV) | Cr/W-mass | Cr/W-pka | W/Cr-mass | W/Cr-pka | W-björkas |
|-----------------|-----------|----------|------------|-----------|-----------|
|                | $N_r$ | $N_F$ | STE  | $N_r$ | $N_F$ | STE  | $N_r$ | $N_F$ | STE  |
| 0.1             | 40   | 1.4  | 0.1  | 40   | 1.8  | 0.1  | 40   | 1.0  | 0.1  |
| 0.2             | 40   | 2.5  | 0.2  | 40   | 2.9  | 0.2  |      |      |      |
| 0.3             | 40   | 3.2  | 0.2  | 40   | 4.0  | 0.2  |      |      |      |
| 0.5             | 40   | 3.6  | 0.2  | 40   | 4.7  | 0.3  | 40   | 1.3  | 0.1  |
| 0.75            |      |      |      | 40   | 1.7  | 0.1  | 15   | 1.5  | 0.1  |
| 1               | 20   | 6.7  | 0.5  | 7.1  | 0.6  | 40   | 2.0  | 0.2  |
| 1.5             |      |      |      | 40   | 2.5  | 0.2  | 2.6  | 0.2  |
| 2               | 15   | 11.7 | 0.6  | 10.1 | 0.7  | 20   | 3.2  | 0.2  |
| 3               | 15   | 13.4 | 0.7  | 12.2 | 0.9  | 20   | 4.2  | 0.3  |
| 5               | 15   | 19.9 | 1.3  | 14.8 | 1.1  | 15   | 5.8  | 0.4  |
| 7.5             | 20   | 26.8 | 1.7  | 21.5 | 1.4  | 15   | 9.7  | 0.5  |
| 10              | 20   | 33.6 | 1.9  | 29.4 | 1.9  | 15   | 11.0 | 0.6  |
| 15              | 20   | 50.1 | 2.0  | 39.4 | 2.1  | 15   | 14.4 | 0.8  |
| 20              | 15   | 65.1 | 3.6  | 55.7 | 2.8  | 20   | 18.5 | 1.1  |
| 25              |      |      |      |      |      |      | 20   | 23.0 | 1.3  |
| 30              | 15   | 96.4 | 3.4  | 77.5 | 5.5  | 20   | 25.2 | 1.4  |
| 40              | 15   | 119.9| 4.5  | 108.0| 4.6  | 20   | 35.0 | 1.7  |
| 50              | 15   | 157.2| 8.1  | 128.1| 4.4  | 15   | 47.7 | 3.4  |
| 60              |      |      |      | 15   | 59.7 | 2.3  | 58.9 | 3.6  |
| 75              |      |      |      | 15   | 90.5 | 8.7  | 75.5 | 5.1  |
| 100             |      |      |      | 15   | 141.3| 13.7 | 115.4| 13.1 |
| 150             |      |      |      | 10   | 216.8| 32.9 | 176.5| 17.7 |

Note: All data for the Cr/W-mass, Cr/W-pka, W/Cr-mass, W/Cr-pka and W-björkas simulations are calculated in this study. The list of $N_r$ for Cr/W-pka is the same as Cr/W-mass. The list of $N_r$ for W/Cr-pka is the same W/Cr-mass.

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