

Primary defect production from molecular dynamics simulations of high-energy displacement cascades in NbMoTaW alloys

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In this work, we report on large-scale molecular-dynamics (MD) simulations of displacement cascades in equiatomic NbMoTaW alloys at PKA energies ranging from 0.15 to 150 keV. We find defect production to be strongly dependent on recoil energy, scaling sublinearly up to 10 keV, and linearly thereafter. We find the sublinear regime to be defined by low values of surviving Frenkel pairs, typically found as isolated point defects or small defect clusters, while at higher recoil energies dense cascades become more frequent, leading to splitting into subcascades and the production of relatively large prismatic-dislocation loops with $\langle 111 \rangle$ and $\langle 001 \rangle$ Burgers vectors. These loops immobilize large fractions of defects, leading to a rapid growth of the number of surviving defects in the linear regime. We also anneal post-cascade defect configurations using object-kinetic Monte Carlo (OKMC) simulations to account for intracascade recombination on time scales not accessible to MD simulations. Cascade annealing is strongly temperature dependent, with the OKMC simulations only showing significant recovery at 1000 K but not below. Our results are in general agreement with existing published data for refractory concentrated alloys.

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I. INTRODUCTION

Refractory multielement alloys (RMEA) are a special class of materials typically composed of four or more refractory metal elements, such as Nb, Mo, Ta, V, W, Cr, Hf, or Zr, mixed in near-equal proportions. These alloys generally crystallize into a single phase with body-centered cubic (BCC) crystal structure, and their superior high temperature properties make them attractive candidates as structural materials in the power, aerospace, or nuclear sectors [1–5]. In particular, RMEA are being actively considered as irradiation-tolerant materials in nuclear environments [1,6–11] due to promising features such as high defect-formation energies and threshold displacement energies [12–16].

Microstructural evolution under irradiation starts with the introduction of point defects and small point-defect clusters resulting from the collapse of displacement cascades created by primary knock-on atoms (PKA) [17–21]. This so-called “primary damage” is thus composed of defect clusters containing vacancies and self-interstitial atoms (SIA) in different amounts and with different morphologies. Thus, in evaluating how RMEA respond to irradiation damage, it is crucial to

characterize the production of defects in high-energy displacement cascades as a function of PKA energy. Cascades are simulated using large-scale molecular-dynamics (MD) simulations using state-of-the-art interatomic potentials. One key limitation to perform these MD simulations in RMEA has been the limited number of potentials available to model concentrated BCC alloys [13,22–24].

Recent progress includes various alloys containing V and Ta [25–27], tungsten-containing systems [27–29], and several iterations of materials containing Zr, Hf, and Nb, including the ternary ZrHfNb system [30] and the quinary HfNbTa-TiZr [31]. In general, these studies find significantly lower surviving-defect counts after displacement cascades compared to pure metals such as W, Ta, or Nb. In addition, large cluster formation has been shown to be inhibited in concentrated alloys relative to pure metals [11,25,32]. This, coupled to exceedingly low defect mobilities [14–16,25,32–35] has been used to invoke an intrinsic RMEA radiation resistance. It is thus of importance to continue to investigate how primary damage production might set the stage for this resistance. As one of the “flagship” alloys of the BCC RMEA family, the NbMoTaW system presents an important and interesting study case for primary-damage calculations.

In this paper, we report on large-scale MD simulations of displacement cascades in equiatomic NbMoTaW alloys using molecular-dynamics (MD) simulations with PKA energies ranging from 0.15 to 150 keV. The paper is organized as follows. In Sec. II we provide all the simulation details. Section III A contains all the results pertaining to the MD simulations alone, while the effect of thermal annealing is quantified in

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TABLE I. Details of the MD simulations carried out for each cascade energy. L is the side in nm of the cubic cell employed in the simulations. N_{sim} is the number of independent simulations for each PKA energy.

E_{PKA} [keV]	L [nm]	N	N_{sim}
0.15	1.0	54 000	5
0.5	1.0	54 000	10
1	1.0	54 000	8
2	1.6	250 000	6
5	2.3	690 000	12
10	2.6	1 024 000	16
20	2.6	1 024 000	7
50	2.6	1 024 000	10
100	6.5	16 000 000	5
150	9.7	54 000 000	3

Sec. III C. We discuss the main implications of our study in Sec. IV and finish the paper with our main conclusions in Sec. V.

II. METHODS

A. Molecular-dynamics simulations

All the atomistic calculations were performed using the LAMMPS code [36] with the interatomic potential developed by Byggmästar *et al.* [15,23] for the NbMoTaW system connected to the universal Ziegler-Biersack-Littmark (ZBL) potential implemented for short-range interactions [37,38]. This potential represents the current state of the art for the NbMoTaW system as it has been fitted to density-functional theory (DFT) calculations of key defect properties relevant to irradiation damage, including vacancy formation and migration energetics, self-interstitial atom formation energies and morphologies, as well as elemental segregation and ordering energetics around voids and dislocation loops.

Cubic cells with a BCC lattice structure and a random distribution of Nb, Mo, Ta, and W in equal proportions were generated for each cascade simulation. All cells were oriented along $x = [100]$, $y = [010]$, $z = [001]$, with periodic boundary conditions enforced in all three dimensions. The size of the cells L , scaled with the PKA energy E_{PKA} , and all simulation cells were initially equilibrated at 300 K and zero pressure in the NpT ensemble (where N is the total number of atoms, p the pressure, and T the temperature). Subsequently, the cascade simulations were run in the NVE ensemble (with $V = L^3$ being the total simulation volume and E the total system energy) to a total time of 50 ps using an adaptive time step to ensure that all atom trajectories were properly resolved in time. A thin “skin” region enveloping the total simulation volume was kept at constant temperature and pressure using a Nosé-Hoover barostat to remove heat from the simulations and absorb elastic shock waves generated by high-energy PKA and thus avoid unphysical boundary effects. Details for each value of E_{PKA} are given in Table I, including the number of independent simulations carried out with each PKA energy.

The relaxed cascade configurations were visualized using OVITO [39] for extraction of defects and dislocation loops.

TABLE II. Diffusion parameters used in the OKMC simulations (from Refs. [33] and [34]).

Defect	D_0 [m^2s^{-1}]	E_m [eV]	f	Dim.
I_1 ($T \leq 600$ K)	4.4×10^{-11}	0.25	1.0	1D
I_1 ($T > 600$ K)	1.2×10^{-8}	0.57	1.0	3D
V_1	3.0×10^{-6}	1.71	0.6	3D
I_m ($m > 1$)	0	0	—	—
V_n ($n > 1$)	0	0	—	—

Specifically, individual Frenkel pairs were identified using the Wigner-Seitz method, while defect clusters were extracted using the cluster-analysis algorithm with a connectivity cutoff radius equal to the first nearest-neighbor distance [40,41]. Regarding the classification of defect morphologies, we utilized the dislocation extraction algorithm (DXA) as the distinguishing criterion: defect structures successfully identified by DXA were classified as planar prismatic loops, while the remaining clusters not captured by DXA were categorized as compact clusters.

B. Cascade-aging simulations

It has long been recognized that the defect configurations resulting from MD simulations of high-energy displacement cascades overestimate the total number of defects that realistically survive the cascade quench [42,43]. Correlated recombination and defect rearrangements within the cascade region are stopped short due to time-scale limitations in MD simulations. A common approach to resolve that limitation has been to perform a “cascade aging,” typically using *object-* or *lattice-*kinetic Monte Carlo to advance the time scale of the cascades from a few picoseconds to several nanoseconds [44–51].

Here we use object-kinetic Monte Carlo simulations [52] to anneal the post-cascade defect configurations for 500 ns at 300, 600, and 1000 K. Following standard practice [46,53,54], we assign vacancy clusters with less than 25 vacancies in them a spherical shape with a radius given by

$$r_m = \left(\frac{3n\Omega_a}{4\pi} \right)^{\frac{1}{3}} \quad (1)$$

and lenticular shape for all SIA clusters and vacancy clusters larger than $m = 50$, i.e., with their radius defined as

$$r_n = \left(\frac{m\Omega_a}{\pi b} \right)^{\frac{1}{2}}, \quad (2)$$

where m and n are the numbers of point defects in the respective clusters, $b = a_0\sqrt{3}/2$ is the first-nearest-neighbor distance (with $a_0 = 0.32$ nm being the lattice parameter), and $\Omega_a = a_0^3/2$ is the atomic volume. In NbMoTaW, only single SIA and monovacancies are mobile [33,34], with diffusivity parameters given in Table II. An important factor in these cascade-annealing simulations is the dimensionality of defect diffusion, which can be one-dimensional (1D) or three-dimensional (3D), depending on temperature and defect type. Here, we ascribe 3D dimensionality to monovacancies

at all temperatures [33], while SIA were seen to move in 1D below 600 K, and in 3D above that temperature [34].

The OKMC approach samples from among the set of diffusion rates of all mobile defects in the system, calculated as

$$q_i(T) = \frac{D(T)}{z f_i b^2} = \frac{D_0^i}{z f_i b^2} \exp\left(-\frac{E_m^i}{kT}\right), \quad (3)$$

where D_0^i and E_m^i are, respectively, the diffusion prefactor and migration energy of species i , z is the number of possible jump directions (and crystallographically equivalent), f_i is the diffusion-correlation factor and k is Boltzmann's constant. The subindex i runs through all mobile-defect species present in the simulation box at any given time. In the case of three-dimensional diffusers, $z = 8$, while for 1D diffusers, $z = 2$. We use $f_{\text{SIA}} = 0.4$ [55,56], while for monovacancies, a value of $f_V = 0.6$ is used [57]. The time step is sampled from a Poisson distribution as

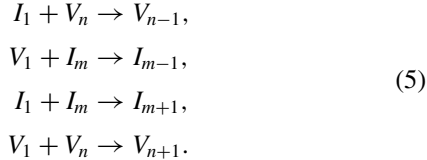
$$\delta t = -\frac{\log \xi_1}{\sum_i q_i}. \quad (4)$$

In each iteration, an event j is selected such that

$$q_j < \xi_2 \sum_i q_i < q_{j+1},$$

where $\xi_1, \xi_2 \in (0 : 1]$ are a pair of uniform random numbers. Finally, a random orientation in the entire solid angle is chosen for three-dimensionally migrating species, whereas a fixed direction is maintained for 1D diffusers for the entire duration of the simulation.

Mobile defects are tracked until (i) they exit the simulation domain, (ii) the simulation ends, or (iii) they collide with another object according to the following interaction rules:



In all cases $m, n \geq 1$. The first two reactions represent annihilation of monomers and shrinkage of clusters when $m > 1$ and $n > 1$. When $m = 1$ or $n = 1$, these reactions represent recombination. The two bottom reactions represent annihilation of monomers and growth of clusters. A reaction is assumed to take place when the following condition is met:

$$|\vec{r}_k - \vec{r}_l| < r_\alpha + r_\beta,$$

where $\vec{r}_k$ and $\vec{r}_l$ are the positions of defects k and l , and r_α and r_β are their respective sizes obtained according to Eqs. (1) and (2), i.e., depending on whether $\alpha, \beta \equiv m, n$. More details about the implementation of the OKMC model are given in Ref. [58].

III. RESULTS

A. Defect production from direct MD simulations

Figure 1 shows all the MD-simulation data points as a function of PKA energy. The average numbers of Frenkel pairs $\bar{N}_{\text{FP}}$ for each energy are shown as blue crosses. As the plot

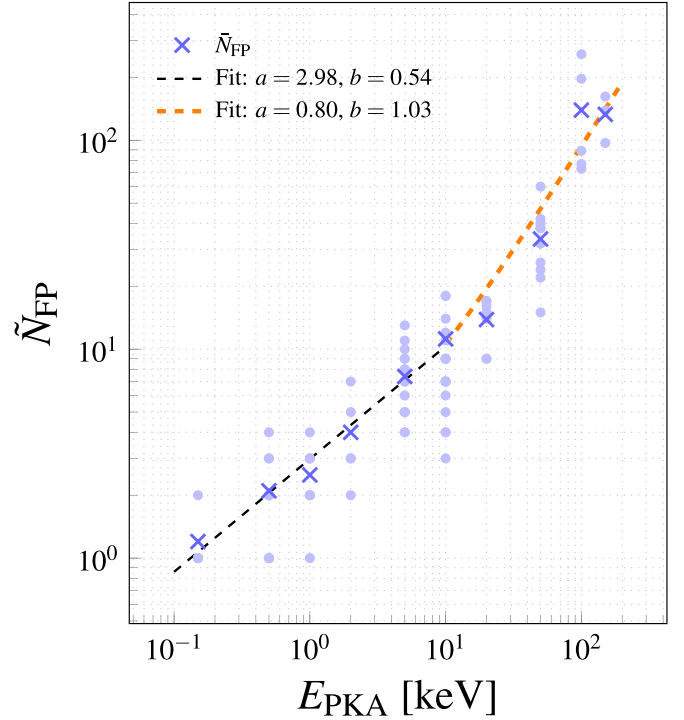


FIG. 1. Number of stable Frenkel pairs as a function of PKA energy. The round dots in the background represent the actual simulation counts, while the “x” symbols represent the average value $\bar{N}_{\text{FP}}$. Power-law fits to the data are split into two PKA energy regimes.

shows, the data points can be broadly separated into two distinct regimes, with a transition taking place at PKA energies between 10 and 20 keV. Below the transition, N_{FP} grows sub-linearly with E_{PKA} , while above it, the dependence is linear. Power-law fits to the data of the form $\bar{N}_{\text{FP}} = aE_{\text{PKA}}^b$ yielding values for the coefficients a and b are given in Table III.

While N_{FP} is a useful value linking the PKA energy with defect production, it does not provide information about the nature of the actual defects produced. We analyze this aspect of the results in Figs. 2 and 3. Figure 2 shows the fraction of vacancies and SIA found in defect clusters at the end of the cascade cooling phase. In general, a rising trend is found for both vacancies and SIA as the PKA energy increases, ranging from zero at $E_{\text{PKA}} = 0.15$ eV to 40~50% at 100 and 150 keV. However, no SIA clustering was observed in any of the cascade simulations with $E_{\text{PKA}} = 1, 2$, or 10 keV, while no vacancy clustering was seen at 1 keV (see Table I for the number of simulations at each PKA energy).

In terms of the size of these clusters, Fig. 3 shows the occurrence probability of clusters of different sizes (m for vacancies, and n for self-interstitials) for all cascades regard-

TABLE III. Coefficients of the fits to the power law $\bar{N}_{\text{FP}} = aE_{\text{PKA}}^b$ below and above PKA energies of 10 keV.

E_{PKA} regime	a	b
≤ 10 keV	2.98	0.54
> 10 keV	0.80	1.03

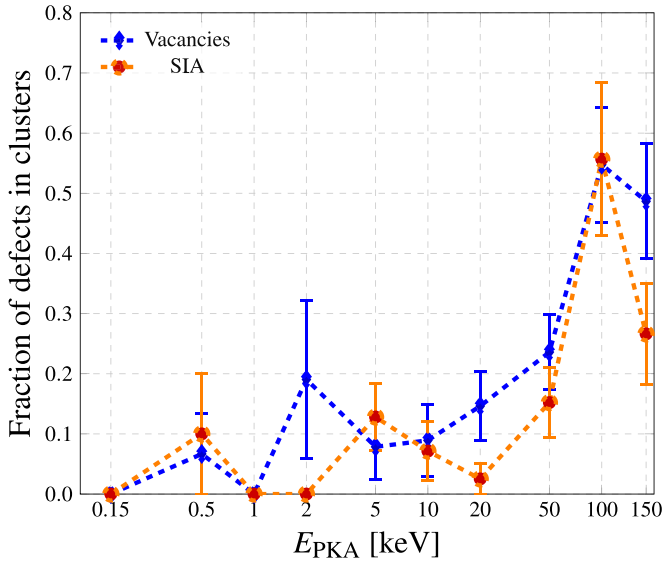


FIG. 2. Fraction of defects found forming part of clusters at the end of the cascade simulation.

less of their PKA energy. Clearly, $m = 2, 3$ and $n = 2, 3, 4$ are the most likely configurations. However, as the PKA energy increases above 50 keV, dense cascades are produced which collapse into planar clusters with sizes above $m, n > 20$. This is the “subcascade” regime where dislocation loops are produced, both of SIA and vacancy character. These loops immobilize a large number of point defects, reducing the probability of recombination, and are responsible for the sharp increase in the number of Frenkel pairs with PKA energy observed in Fig. 1.

B. Production of prismatic dislocation loops

As mentioned above, with increasing PKA energy comes a substantially higher probability of producing prismatic dis-

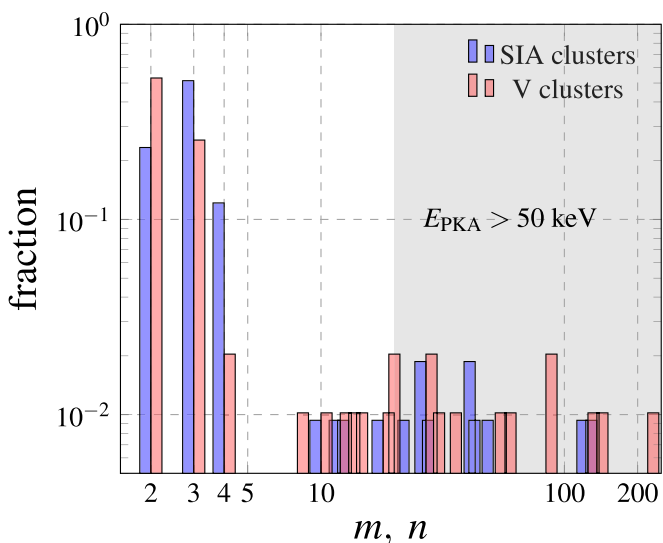


FIG. 3. Occurrence probability of all clusters with $m, n > 1$ for all PKA energies combined. The shaded region for $m, n > 20$ represents dislocation loops produced only in cascades of 100 or 150 keV.

TABLE IV. Characterization of all the prismatic dislocation loops observed in our simulations.

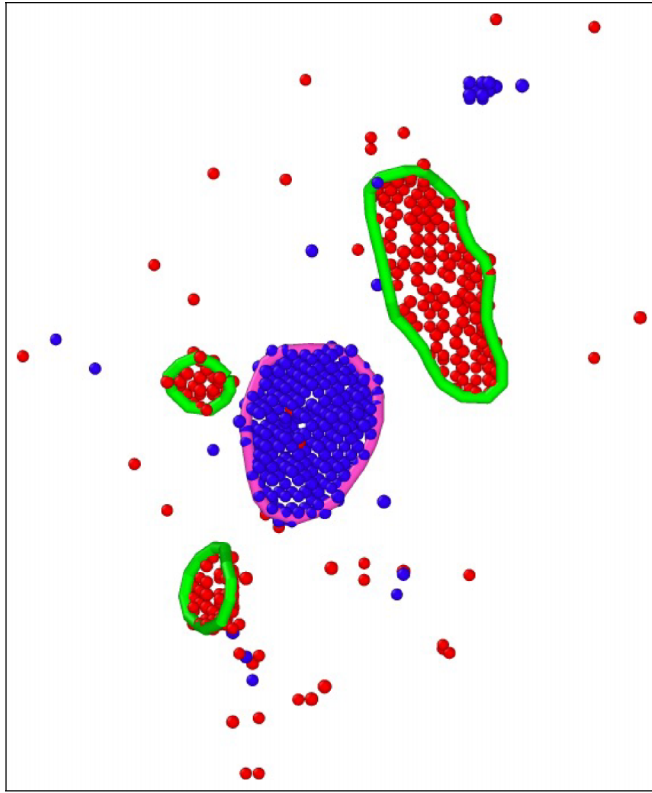
E_{PKA} [keV]	Simulation ID	Type	Size [m, n]	Burgers vector
50	1	SIA	13	$\frac{1}{2}[111]$
50	2	SIA	29	$\frac{1}{2}[\bar{1}1\bar{1}]$
100	3	V	27	$\frac{1}{2}[\bar{1}1\bar{1}]$
100	4	V	52	$\frac{1}{2}[\bar{1}11]$
100	5	V	85	$[001]$
100	6	V	220	$[00\bar{1}]$
100	5	SIA	10	$\frac{1}{2}[11\bar{1}]$
100	3	SIA	12	$\frac{1}{2}[\bar{1}1\bar{1}]$
100	7	SIA	18	$\frac{1}{2}[11\bar{1}]$
100	4	SIA	27	$\frac{1}{2}[\bar{1}11]$
100	6	SIA	27	$\frac{1}{2}[\bar{1}11]$
100	6	SIA	51	$\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$
100	5	SIA	125	$\frac{1}{2}[\bar{1}\bar{1}1]$
100	6	SIA	136	$\frac{1}{2}[\bar{1}11]$
150	8	V	8	$\frac{1}{2}[\bar{1}11]$
150	8	V	57	$\frac{1}{2}[\bar{1}\bar{1}1]$
150	9	SIA	14	$\frac{1}{2}[111]$
150	8	SIA	19	$[0\bar{1}0]$
150	10	SIA	34	$\frac{1}{2}[\bar{1}\bar{1}1]$
150	8	SIA	84	$\frac{1}{2}[\bar{1}1\bar{1}]$

location loops within the cascades. In our simulations, small loops are seen to form at energies of $E_{\text{PKA}} = 50$ keV and above, first as small SIA clusters, and then as both SIA and vacancy loops of increasing size and number. In addition, while most loops belong to the $\frac{1}{2}\langle 111 \rangle$ family, $\langle 100 \rangle$ loops are occasionally seen to form as vacancy clusters (for 100 keV PKA) or SIA (at 150 keV). Table IV lists all the instances in which prismatic dislocation loops were observed, indicating the type, size, and Burgers vector in each case. The table also contains an identifier that is unique to each simulation, such that the reader can see to which cascade each loop belongs. This information helps identify which cascades were more prolific in terms of damage production, e.g., number 6 ($E_{\text{PKA}} = 100$ keV) or number 8 (150 keV).

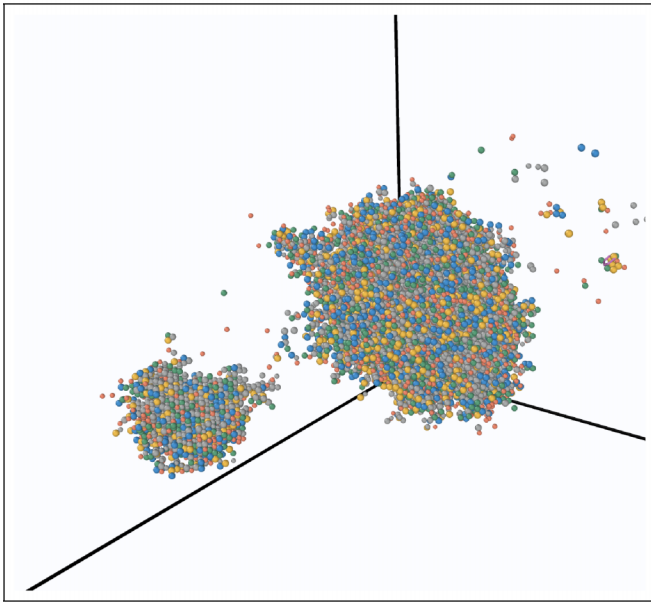
Figure 4(a) displays the surviving defect configuration for one of the 100-keV cascades, where three $\frac{1}{2}\langle 111 \rangle$ SIA loops (with $n = 27, 51$, and 136) and a large $\langle 100 \rangle$ vacancy loop ($m = 220$) can be observed. The production of loops is directly connected to the transition into the subcascade regime at PKA energies above approximately 10 keV. Figure 4(b) shows a snapshot of a 50-keV cascade during the thermal spike (maximum cascade extension), clearly showing the splitting into two subcascades. This is a general trend observed in all cascades with PKA energies of 50 keV or higher.

C. Annealed cascade-defect configurations

As indicated earlier, all cascade configurations were annealed for 500 ns at several temperatures using the OKMC model described in Sec. II B. Figure 5 shows the total number of Frenkel pairs remaining after annealing at 300 (the temperature of the MD simulations), 600, and 1000 K. The



(a)



(b)

FIG. 4. (a) Defect configuration at the end of a 100-keV cascade. Red spheres (●) represent self-interstitial atoms, while blue spheres (●) represent vacancies. Green segments (—) indicate a $\frac{1}{2}\langle 111 \rangle$ Burgers vector, while purple ones (—) correspond to $\langle 100 \rangle$ segments. The image shows three SIA loops (with $n = 27, 51$, and 136) and a large vacancy loop ($m = 220$). (b) Snapshot of a 50-keV cascade during the thermal spike, clearly showing the splitting into two sub-cascades. Atoms are colored by their chemical identity (Nb, Mo, Ta, or W).

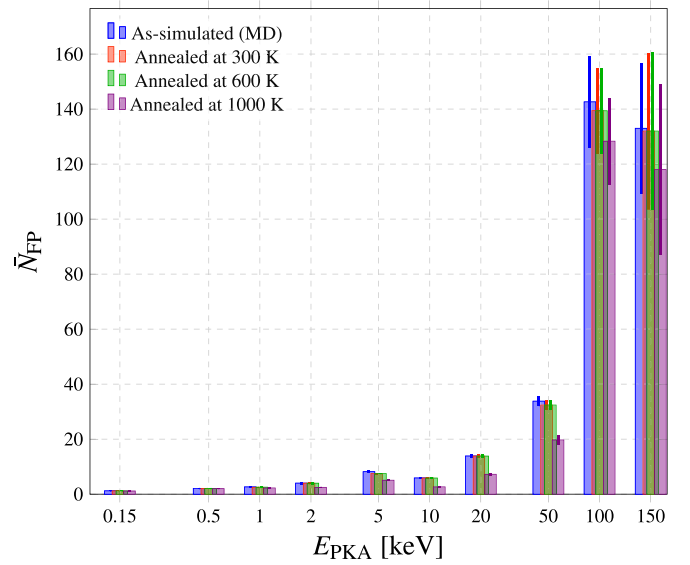


FIG. 5. Effect of cascade aging at different temperatures as a function of PKA energy.

figure shows very modest defect recovery at 300 and 600 K, while reductions between 20 and 30% are observed at 1000 K. This is not an unexpected result in view of the monovacancy and SIA diffusivities calculated at each temperature [33,34], which essentially keep vacancies immobile at all temperatures while allowing for null (at 300 K), modest (at 600 K), and significant (1000 K) SIA mobility depending on temperature. SIA mobility thus controls recombination during the OKMC simulations, which is set by temperature. Overall, sluggish point-defect mobility points to relatively low post-cascade recombination rates and thermally stable cascade-defect distributions.

Annealing has a secondary effect on post-cascade defect evolution besides SIA-vacancy recombination. Some of the mobile SIA can also migrate to existing dislocation loops, contributing to loop growth and competing with recombination for point-defect survival. Figures 6(a) and 6(b) provide the evolution with temperature of the defect-clustering fractions in reference to the as-simulated cases. While the vacancy-clustering fractions are seen to change little, a clear uptick is observed in the SIA subpopulation at 1000 K. Clustering fractions above 70% are measured for PKA energies larger than 10 keV, and of 80% or higher for energies of 100 and 150 keV. This is strong evidence that, when loops are present, they act as strong attraction poles for SIA, depleting the populations to very low values.

IV. DISCUSSION

A. Defect production in refractory alloys

Studies of defect production in high-energy displacement cascades in RMEA are scarce in the literature. In general, there is consensus in the observation that chemical complexity both reduces the threshold-displacement energy relative to pure metals and limits its dependence on crystal orientation [15,26,27,29]. This leads to an enhanced defect production in the cascades, aided by the typically low mobilities of defects

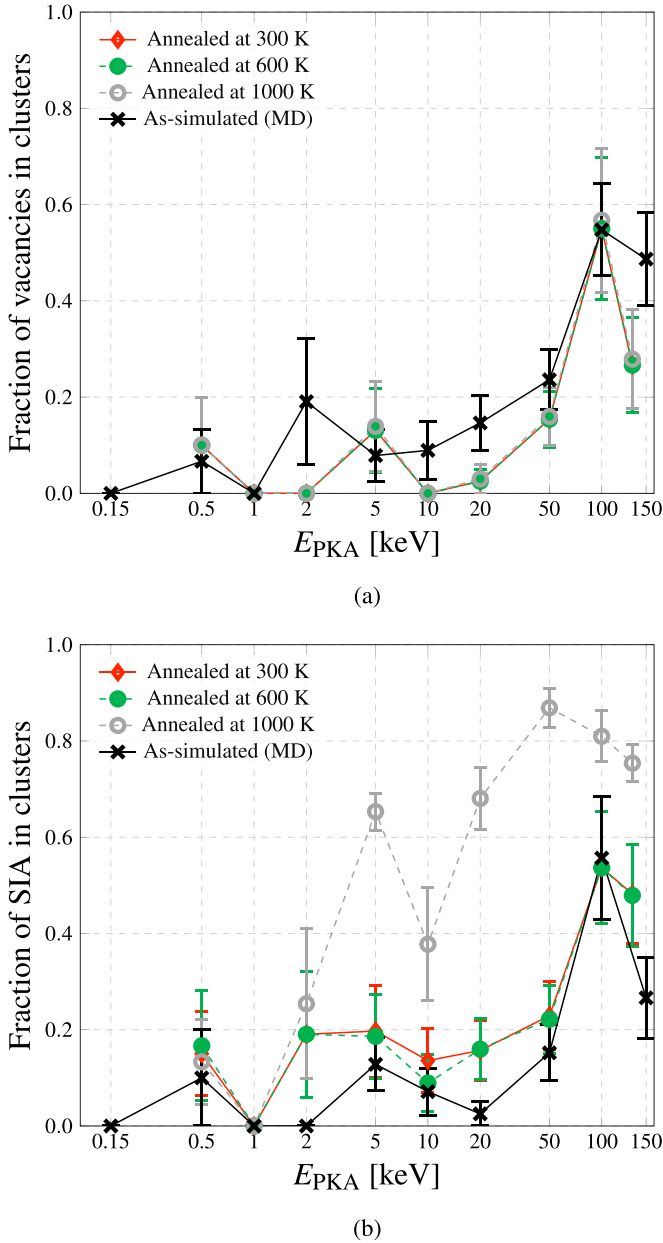


FIG. 6. Clustering fractions of (a) vacancies and (b) SIA as a function of PKA energy and annealing temperature. Vertical segments at the top of each bar represent the amplitude of the standard deviation in each case.

in RMEA, which result in decreased correlated recombination immediately after the cascade collapse phase. Chen *et al.* [27] studied the $\text{W}_{38}\text{Ta}_{36}\text{Cr}_{15}\text{V}_{11}$ alloy and found values of N_{FP} twice as high as in pure W. Qiu *et al.* [26] found defect production in equiatomic VTiTaNb to be 30% higher than in pure V, coupled with lower clustering fractions. Studies in MoNbTaWV [15,29] also found evidence of lower point-defect clustering fractions than in pure W. Figure 7 shows the surviving number of Frenkel pairs as a function of E_{PKA} after the cascade phase in several refractory systems published in the literature. The graph shows results for several RMEA, including the one studied here, as well as for Ta and W for comparison with pure metals. The scaling of defect production

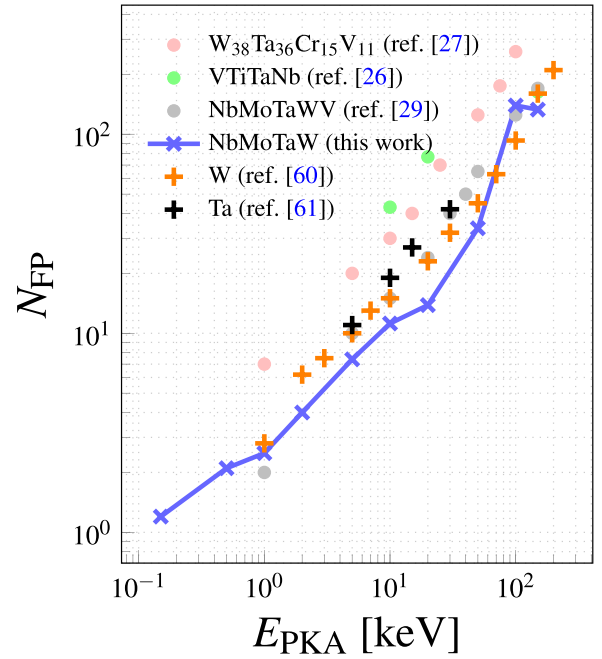


FIG. 7. Frenkel-pair production after displacement cascades simulated using molecular dynamics for several PKA energies. The graph shows results for several RMEA, including the one studied here, and also for pure Ta and W.

with PKA energy is similar in all systems and, while the values of N_{FP} are generally higher in the RMEA, our results lie just below those of pure W published in a recent study [59]. It is worth noting that, despite differences in the interatomic potentials employed and whether electronic stopping was considered or not, defect production in these alloys is relatively similar, pointing to qualitative commonalities across BCC refractory metal alloys and pure systems that go beyond compositional differences.

One such common feature is the production of large prismatic loops at high PKA energies. In BCC metals these loops are overwhelmingly $\frac{1}{2}\langle 111 \rangle$ [60–62], although the observation of $\langle 100 \rangle$ loops is not uncommon [61,63,64]. As well, while most of these loops are self-interstitial in character, vacancy loops can also be observed in dense cascades.

B. Compositional complexity and damage production

To first order, for a given PKA energy, defect production can be assessed in terms of the value of the threshold-displacement energy (TDE), which is defined as the minimum PKA energy to produce a stable Frenkel pair. The TDE is mainly a function of material type and crystal orientation, and it scales roughly with atomic number. In chemically complex alloys (CCA), chemical fluctuations turn these dependencies into statistical distributions, rather than single-valued functions. Studies in the literature have shown that, everything else being the same, damage production in CCA is higher than in their pure or dilute counterparts because the low-energy tail of the TDE distributions disproportionately contributes many Frenkel pairs to the total tally [27,65]. This effect weakens as damage starts to be produced as dislocation loops. Inter-

estingly, as shown in Fig. 7, the alloy studied here displays a reduced defect production compared to pure W and Ta at low PKA energies, gradually converging—and even surpassing—the other materials analyzed at the highest PKA energies of 100 and 150 keV.

In terms of chemical short-range order, which has been much heralded as a unique feature of CCA with implications on physical and mechanical properties, the evidence in the literature thus far is inconclusive [31,66]. In dense cascades, the material melts during the thermal spike, randomizing the alloy configuration and destroying the chemical order (and thus negating its effects) [67,68]. Conversely, recent studies have shown that short-range order enhances the irradiation resistance of certain alloys by lowering the transition energy to the subcascade regime [31]. Chemical short-range order is also known to increase threshold displacement energies, potentially leading to lower defect production [65]. However, this effect quickly decays as damage accumulates with irradiation at high doses [69].

C. Power-laws fits for Frenkel-pair production as a function of PKA energy

In most damage-production studies it is customary to relate N_{FP} and E_{PKA} through power laws of the type $N_{FP} = aE_{PKA}^b$. The exponent b is of particular interest, as it has been shown that, in metals, a transition is observed at a certain PKA energy from a “single-cascade” regime to the subcascade regime. Generally, the latter is characterized by $b < 1$ (sublinear), while the subcascade regime is defined by $b \approx 1$ (quasilinear).

There is strong consensus in the literature about the sublinear regime, which has been observed independently in many metallic materials [21,46,59,70,71]. There are fewer data regarding the linear regime. Recent simulations in pure metals have found values of 1.01 in Fe, 1.15 in W, and 0.94 in V [59]. This is consistent with the value obtained by Liu *et al.* [29] of $b = 0.94$ above 30 keV in MoNbTaVW. Thus, our data, with $b = 1.03$, are in agreement with this partition between sublinear and linear defect-production regimes. Indeed, starting at 50 keV, we see evidence of subcascade formation in our simulations (understood as a heterogeneous, spatially disjoint mode of defect production). However, this is also when we observe the formation of large prismatic loops. In our simulations, the transition from defect production dominated by point defects to being produced as large loops takes place between 10 and 20 keV. This energy is similar to that in BCC Fe and V [59].

The choice to locate the transition from sublinear to quasilinear scaling at a specific PKA energy, however, has to do more with mathematical convenience for fitting the respective power laws than with concrete physical reasons. Indeed, the transition is better represented by a range of energy values where both cascade modes likely coexist, rather than by a single energy value.

D. Implications of damage production and annealing on defect-structure evolution

At low PKA energies, defect production is low and characterized by single, di-, and tri-interstitials and vacancies (see

Fig. 3). Of these, only single SIA have sufficient mobility to undergo further evolution. However, as demonstrated by Zhou *et al.* [34], most of the SIA motion takes place one dimensionally (it is not until temperatures above 1000 K that the diffusion mode switches to 3D), which means that there will be limited SIA-vacancy recombination. Indeed, as revealed by Fig. 6, vacancy clustering remains essentially unchanged even at 1000 K and one can simply see low-energy, low-temperature irradiation as a spatially frozen collection of mainly point defects.

At high PKA energies ($E_{PKA} > 50$ keV), large, stable loops appear consistently within the cascades. The loops are both of interstitial and vacancy nature, with Burgers vectors of $\frac{1}{2}\langle 111 \rangle$ (mostly) and $\langle 100 \rangle$ (occasionally). These loops are predicted to be essentially immobile, but can grow at the expense of three-dimensionally migrating SIA at high temperatures. As shown in Fig. 6(b), this is precisely what happens at 1000 K, with the fraction of clustered SIA significantly increasing relative to the as-simulated case. This scenario, defined by the sporadic generation of few but large and very stable prismatic loops, and limited single SIA mobility, is potentially conducive to the formation of (first) loop rafts and then loop networks. The only necessary ingredients are cascades of sufficient energy, which can be attained with ions or neutrons with high-incident energy, and temperatures above the mobility limit of SIA ($T > 600$ K). The formation of such structures can also be simulated using more coarse-grained models that combine linear elasticity with kinetic-rate theory [72–74]. In these models, cascade defects are generated on the fly at prescribed temperatures and dose rates using correlations based on the results shown in Figs. 1, 3, and 6.

V. CONCLUSIONS

We finish the paper with our most important conclusions. We have conducted an MD study of displacement cascades in NbMoTaW from PKA energies in the 0.15 to 150-keV range. These simulations have been followed by OKMC simulations of cascade annealing at 300, 600, 900, and 1000 K.

Our results point to the existence of two irradiation-damage regimes, one at low PKA energies (< 10 keV) characterized by production of Frenkel pairs and small point-defect clusters, and a second one defined by large prismatic loops emerging from the collapse of high energy-displacement cascades.

Both damage-production regimes are captured by power laws of the type $N_{FP} = aE_{PKA}^b$, one sublinear with $a = 2.98$ and $b = 0.54$, and a linear one with $a = 0.80$ and $b = 1.03$.

Prismatic dislocation loops are observed as being of vacancy type (30%) and SIA type (70%), and with Burgers vectors of $\frac{1}{2}\langle 111 \rangle$ (85%) and $\langle 100 \rangle$ (15%).

Cascade aging remains largely ineffective below 1000 K due to the very low mobility of vacancies and the limited mobility of self-interstitials. Noticeable recombination and the transfer of individual SIA to larger loops is seen to only begin at 1000 K.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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