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Molecular Dynamics Studies of the Primary State of Radiation Damage

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Abstract

This paper summarizes recent progress in the understanding of energetic displacement cascades in metals achieved with the molecular-dynamics (MD) simulation technique. Recoil events with primary-knock-on-atom (PKA) energies up to 5 keV were simulated in Cu and Ni. The initial development of displacement cascades was similar in both metals, with replacement collision sequences providing the most efficient mechanism for the separation of interstitials and vacancies. The thermal-spike behavior in these metals, however, is quite different; Cu cascades are characterized by lower defect production and greater atomic disordering than those in Ni. The thermal spike significantly influences various other properties of cascades, such as total defect production and defect clustering.

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1. Introduction:

The primary state of damage resulting from energetic displacement cascades has been a focus of research for over forty years. Much of the work was motivated by the need to characterize the effects of radiation on materials in a nuclear reactor. Recently, interest in the application of ion beams for materials modification has provided additional incentive for understanding the primary state of damage. Since the lifetime of a cascade is short (≈ 10 ps) and its volume is small ($\approx 10^{-20}$ cm³), direct experimental observation is difficult. Few techniques provide the atomic resolution necessary to study the primary state of damage, and those that do monitor only the final state of damage. Moreover, the inhomogeneous, nonlinear and many-body character of cascades make theoretical modeling difficult, and most analytical work has been limited to highly idealized treatments (1). In recent years, however, molecular dynamics (MD) computer simulation has become a practical tool for the study of displacement cascades. The small size and short time scale of the cascade that hamper experimental investigation are actually advantageous from the standpoint of simulation. This paper highlights our recent studies using this technique. Simulations of cascades in Cu and Ni at energies up to 5 keV are presented. Comparison with experiment is made wherever possible to provide an indication of the reliability of the simulations.

2. Molecular Dynamics Simulations:

The molecular dynamics code employed in the present study was adapted from one developed by J.R. Beeler, Jr. A brief description is given in the references cited in (2). Interatomic forces were represented by pairwise central-force interactions. The Gibson II Born-Mayer potential (3), and the Johnson-Erginsoy potential (4,5) were used to model Cu and Ni, respectively. These

potentials yield reasonable values for elastic constants and point defect properties (3-6) and are convenient computationally because of their short range (cut off between the first and second nearest neighbors). Both potentials were constructed to yield the known minimum threshold displacement energies $\approx 25 - 30$ eV. Recently, more realistic potential models for d-electron materials have been developed (7,8). These potentials, however, are longer range and include non-pairwise contributions. The shorter-range pair potentials (3-5) were adopted for our first studies in the interest of numerical efficiency; simulations based on embedded-atom-model potentials (8) are now in progress and will be presented elsewhere.

The simulations employed cubic unit cells with length up to $36a_0$ on a side (a_0 is the lattice parameter). This corresponds to approximately 170,000 movable atoms.

Two types of simulations were performed: primary recoil events and heat spikes. Initial conditions in the primary recoil events are set such that a single atom has nonzero kinetic energy (the PKA energy) with the remaining atoms being at rest. This corresponds to a 0 K cascade. To initialize a heat spike event, 95 % of the cascade energy was distributed randomly to atoms within a central sphere according to a Maxwellian distribution. The remaining cascade energy was distributed to atoms in two thin concentric shells to smooth the temperature gradient. Heat spike simulations require a relatively small computational cell since replacement sequences and focusons are insignificant.

3. Cascade Dynamics:

Some characteristic features of cascade dynamics are illustrated by plotting the lattice sites on which atomic replacements have occurred. Fig. 1 shows results for a 5 keV event in Cu. Also shown in the figure are the final locations of vacancies and self-interstitial atoms (SIA's). The majority of replacements occur in the core of the cascade; a few of the replacements form linear

trails (RCS's) which lead to stable SIA's. Whereas the SIA's all lie outside the central core, the vacancies, shown in Fig. 1b (open circles), form a compact depleted zone. Similar features were observed in simulated Ni cascades. Although some qualitative features of these results are similar to those obtained in binary collision computer simulations (10,11), it will become clear that a detailed understanding of defect production, clustering, and atomic mixing is only possible with MD simulation.

Additional insight into the process of cascade evolution is obtained by taking "snapshots" of the atom positions at different times. Figs. 2 (a-f) show the configuration of atoms within a slab of thickness $a_0/2$ near the center of the cascade projected onto a (001) plane at various instants of time. The left- and right-hand panels refer to 5-keV cascades in Cu and Ni, respectively. Regions in which crystalline order is destroyed are clearly visible. The disordered region persists longer in the Cu than in the Ni cascades. Radial pair distribution functions, $g(r)$, for the atoms located within the disordered regions at two instants of time are shown in Figs. 3a-3b; a simulation for bulk liquid Cu (12) is shown for comparison in Fig. 3a. The results in Fig. 3a demonstrate that melting occurs in the cascade core. Most striking in these figures is the disappearance of the (200) peak in $g(r)$ at $3.6 \text{ \AA}$ (in crystalline Cu and Ni) at $t=1.1 \text{ ps}$. Note also that this peak is starting to reappear and the diffuse peaks are sharpening earlier in Ni than in Cu.

Further characterization of the thermal spike is provided in Figs. 4a and 4b, which show the atomic densities and temperatures, normalized to the melting temperature, as functions of distance from the center of the cascade at different times for Cu and Ni, respectively. The temperatures were obtained by equating the average kinetic energy in a spherical shell of radius r with $3/2 k_B T$. At early times, $t \approx 0.25 \text{ ps}$, the average temperature at the center of the cascade, $r < 13 \text{ \AA}$, is $\approx 4000 \text{ K}$ for both Cu and Ni, and the temperature gradient outside this central core is $\approx 140 \text{ K/\AA}$. The initial cooling rate is $\approx 10^{15} \text{ K/s}$ in the center of the cascade. At 1.4 ps , the temperature in Cu begins to fall below the melting temperature T_m at $r \approx 20 \text{ \AA}$. It can be seen in Fig. 2e that this

radius corresponds approximately to the radius of the disordered zone at 1.1 ps. For Ni, the temperature falls below the melting point much earlier in time, although the absolute temperature remains quite similar to that in Cu. Further analysis will be required to determine, e.g., the degree of undercooling at the melt front and the melt front velocity.

Figs. 4(a-b) show that the atomic densities reflect the T/T_m profiles. Expansion in the hot central core of the cascade gives rise to a much reduced density, as much as $\approx 15\text{-}20\%$ at 1.14 ps in Cu and $\approx 15\%$ in Ni at 0.8 ps. It can also be seen that a high-density ridge is formed outside the hot core, particularly for Cu. The high densities do not result from SIA's transported from the center of the cascade since too few RCS's occur to account for this effect. Moreover, as the high temperature zone cools, the compression at the cascade periphery relaxes, returning the density to its equilibrium value, leaving only the stable interstitial atoms.

4. Defect Production:

Careful analyses of various low-temperature radiation-damage rate experiments have demonstrated that the modified Kinchin-Pease expression overestimates the number of point defects produced in a cascade by a factor of about three in most metals (13,14). Above 5-10 keV, the defect production efficiency, ζ , i.e., defect production relative to that predicted by the modified Kinchin-Pease expression, becomes rather constant, apparently as a result of the formation of subcascades (15). In ref.(13) it was proposed that the decrease in defect production was a consequence of "residual agitation in the lattice" which stimulated recombination of close Frenkel pairs. Previous MD simulations of cascades in W provided support for this interpretation (16). The present simulations have given a more quantitative characterization of the "residual agitation" and its influence on defect production.

Figs. 2(a-f) show that the central core region assumes a highly disordered melt-like structure

for a certain time interval during the evolution of the cascade. "Interstitial" atoms and "vacancies" lose their precise identity within this region. When crystallinity is reestablished, this central region is free of interstitials as is illustrated in Figs. 5a and 5b for simulated events in Cu and Ni, respectively. Here the number of stable vacancies and interstitials are plotted as a function of distance from the center of the cascade. Little overlap is observed in the vacancy and interstitial-atom distributions, with no SIA's in the central core of the cascade, $r \leq 15 \text{ \AA}$. Thus cascade melting results in an "excluded-volume" for the interstitials, which reduces the defect-production efficiency. The defect production efficiency in a simulated Ni cascade, $\zeta = 0.4$, is somewhat higher than that obtained for Cu cascades, $\zeta = 0.2$. As only one 5 keV cascade event has been run to completion in Ni, this comparison must be considered preliminary.

The simulations demonstrate that the number of stable Frenkel pairs produced in a cascade is determined primarily by the number of SIA's transported beyond the boundary of the melt region. This transport occurs by replacement collision sequences, as shown in Fig. 1. In fcc crystals the replacement sequences are mostly in [100] and [110] directions, although some sequences along [111] directions are also observed. To further elucidate the role of replacement sequences, we have calculated the probability for an RCS to "escape" the core of the cascade as a function of RCS length. On the basis of the core volume obtained for a 5 keV event and assuming that the RCS's are initiated isotropically and homogeneously within this volume we find that the escape probability is 0.2, 0.3, 0.43 and 0.7 for a RCS length of three, four, six and ten atomic distances, respectively. As the PKA energy increases (but below the subcascade threshold), the size of the core region becomes larger and the escape probability decreases. As a consequence, the Frenkel-pair production efficiency decreases as a function of increasing PKA energy.

We note, incidentally, that field ion microscopy (FIM) observations of displacement cascades in W (17) indicate a somewhat larger defect production efficiency than is observed in most other metals (14). The FIM studies also show a correspondingly high average RCS range, $\approx 170 \text{ \AA}$

(16). Whether W is anomalous remains to be established. Nevertheless, the results for W suggest that the quantitative behavior exhibited in our simulations for Cu and Ni may not apply to all metals.

4. Atomic Mixing and Disordering

A convenient measure of atomic mixing is the mean-square displacement per atom,

$$\sum_i [r_i(t_0, r) - r_i(0, r)]^2 / n(r) = 6 \langle D_c(r) t_0 \rangle. \quad (1)$$

We denote the (perfect lattice) position of the i^{th} atom in a coordination shell at radial distance r from the origin as $r_i(t=0, r)$. At time t_0 during the development of a cascade, the instantaneous position of the atom is $r_i(t_0, r)$. $D_c(r)$ refers to the effective diffusion coefficient associated with the atomic motion in the cascade. Treating D_c as a function of r is, of course, correct only if the cascade is essentially spherically symmetric. The integral of eq. (1) over all space, however, is independent of symmetry. The sum of the mean square displacements for a 5 keV recoil event in Cu and Ni is $5.1 \times 10^4 \text{ \AA}^2$ and $1.4 \times 10^4 \text{ \AA}^2$, respectively.

A comparison between simulated and experimental results for atomic mixing in Cu and Ni is given on the ordinate axis in Fig. 6. The integrated values of $\langle D \rangle$ are normalized to damage energy per unit volume so that the simulations can be compared with experiments performed at much higher cascade energies, e.g., 1 MeV Kr irradiation (18). Comparison of such disparate irradiations is still meaningful in view of the formation of subcascades in high energy irradiations. Nevertheless, the close quantitative agreement between theory and experiment must be considered somewhat fortuitous. The qualitative differences between Cu and Ni, however, are clearly reproduced in the simulations, and these, we believe, are not fortuitous.

Cascade mixing was also studied using "heat spike" simulations, as mentioned in section 2. The results are shown in Fig. 6 for Cu and Ni plotted as a function of energy density in the cascade. For appropriate values of the energy density in a 5 keV Cu or Ni cascade, $\approx 1-2$ eV/atom, satisfactory agreement is found between the heat spike simulations, the primary recoil atom simulations and experiment. Since mixing in the heat spike simulation is due entirely to diffusive processes (ballistic effects do not occur), the difference in mixing between Cu and Ni in these simulations must arise from differences in their thermodynamic properties. Since Cu is at a higher homologous temperature than Ni during the thermal spike as shown in Figs. 4(a-b), more extensive diffusion is expected to occur in Cu. Indeed, Peak et al. have shown that the atomic mixing in Cu can be successfully modeled in terms of liquid-state diffusion (18). Possible alternative explanations for the different extent of mixing in Cu and Ni are (i) longer replacement sequences in Ni, which we do not observe in the PKA simulations and which would not account for the differences observed in the heat spike simulations, and (ii) a strong coupling between the phonon and electron systems in Ni that results in rapid quenching of the thermal spike in this material; this mechanism will be discussed in section 6 below.

5. Cascade Collapse and Clustering:

Not only the total defect production in cascades but also the degree of clustering of SIA's and vacancies is important for the kinetics of radiation effects at high temperatures. In the following, we discuss interstitial and vacancy clustering in cascades in the light of our simulation studies. Reference will also be made to some recent experimental work.

The SIA's that do not suffer recombination during the thermal spike can still undergo extensive diffusive motion. Owing to their strong elastic interactions, the SIA's tend to cluster during the thermal spike, as shown in Figs. 1(a-b). Clusters containing $\approx 3-5$ SIA's in nascent cascades

have been observed experimentally by diffuse x-ray scattering measurements on fast-neutron irradiated specimens at 6 K (19). The clusters observed in the present simulations are expected to be smaller since our PKA energies are lower than those typical of fast neutron recoil events in Cu or Ni, $\approx 25\text{-}50\text{ keV}$.

The removal of atoms from the core of the cascade by RCS's results in a depleted zone after the melt recrystallizes. Seidman and coworkers observed highly clustered configurations of vacancies in W and Pt cascades by Field-ion microscopy and concluded that the locations of vacancies within depleted zones had little correlation to the sites on which they were produced. In some cases, voids and dislocation loops were observed (20). In the past few years, detailed studies of the dynamic collapse of the depleted zones in cascades at low temperatures into dislocation loops and stacking-fault tetrahedra have provided additional insight into the local configuration of point defects in displacement cascades (21,22). These studies have involved transmission- electron-microscope observation of in situ ion-irradiated specimens at low temperature. Table 1 lists the vacancy dislocation-loop yield for a variety of ion-target combinations. Corresponding values of the ion beam mixing parameter, $Dt/\Phi F_D$ are shown to illustrate the correlation between mixing and cascade collapse. This correlation suggests that the thermal spike plays an important role in cascade collapse.

Seidman has suggested that the rearrangement of vacancies within the cascade derives from the precipitation of vacancy clusters in the highly supersaturated depleted zone and their growth during the thermal spike (20). Another suggested mechanism of collapse is the thermotransport of vacancies towards the center of the cascade and interstitial atoms towards the periphery, driven by the steep temperature gradients in cascades (23,24). Both of these mechanisms require high vacancy mobility during the thermal spike. The MD simulation result that a melt zone develops in the cascade suggests an alternative, although related, explanation. The melt zone is regarded not as a region with high vacancy density, but as a liquid with lower atomic density than

the surrounding matrix, as shown in Fig. 4. Since density fluctuations at the melt front are initially small, the crystal regrowth begins with few frozen-in vacancies. As the solidification process proceeds, the density fluctuations increase due to the increasing fraction of missing atoms in the melt, until vacancies finally begin to freeze out in the solid. By this mechanism, vacancies are driven to higher concentrations in the center of the cascade. Although the collapse of the depleted zone into a dislocation loop has not yet been observed in the simulations, the regrowth mechanism might establish the conditions necessary for collapse; actual collapse would require higher energy cascades. We note that no experimental evidence has been reported for vacancy collapse in Cu or Ni at energies less than 10 keV.

Heat-spike simulations provide some support for the above interpretation. In a simulated heat spike of 1.1 eV/atom with a doped-in concentration of 2 at.% vacancies, it was found that the radius of gyration of the vacancy distribution decreased from an initial value of 16.25 Å to 9.9 Å, demonstrating the inward motion of vacancies during a thermal spike. In another simulation, four vacancies were placed symmetrically on a (010) plane in a region heated to 1 eV per atom. The radius of gyration of the four defects decreased from 12.76 Å to 7.52 Å. Three of the vacancies had agglomerated by the end of the event into a cluster near the center of the heat spike. Initial and final coordinates of the vacancies are listed in table 2.

Finally, we mention some recent experimental studies of the dissolution of pre-existing vacancy-dislocation loops. Employing in situ ion irradiations at 30 and 300 K in an electron microscope, Robertson and co-workers found that some of the dislocation loops produced during the early part of irradiations of Cu and Ni disappear with continued irradiation (25). This phenomenon is illustrated in Figs. 7(a-b) where micrographs of the same area of the specimen after successive ion irradiations are shown; examples of dislocation loops that are present after the first irradiation, but absent after the second, are marked with arrows. This result suggests that the dislocation loop produced in a previous cascade dissolves when it overlaps spatially with the core

of a fresh cascade. The probability for loop reformation is certainly enhanced by the high local density of vacancies, however, in the case of Ni the probability for initial loop collapse is ≤ 0.1 , and thus there is a high probability that a loop will not reform after dissolution. Some initial attempts were made to simulate this phenomenon by forming a dislocation loop consisting of seven vacancies on a (111) plane in Cu (one vacancy and six nearest neighbors) and subsequently overlapping a heat spike. In the simulation, three vacancies were emitted from the loop. Although this calculation was rather crude, it does suggest that there is sufficient atomic motion in a cascade to dissolve vacancies from a nearby loop. More realistic simulations of this effect are being planned.

6. Concluding Remarks:

It has been shown in this paper that molecular dynamics computer simulations can help elucidate the dynamics and structure of energetic displacement cascades. Moreover, the value and accuracy of these simulations should improve as more realistic interatomic potentials currently available are implemented into the simulation codes.

One of the underlying assumptions in the simulations is that the electronic system does not couple significantly to the lattice during the lifetime of the cascade, an assumption invoked in nearly all theoretical treatments of cascades. Rapid coupling, however, might cause the thermal spike to quench by (i) transfer of energy from the ionic to the electronic system, and (ii) transport of energy from the cascade region by electronic thermal conduction. The assumption of weak coupling is correct if the electronic mean free path is greater than the cascade dimensions; in that case the electrons do not equilibrate (26), although some damping of the thermal spike would still occur due to electronic excitations. The electronic mean free path in liquid Cu at its melting point is $\approx 45 \text{ \AA}$ (27) which is slightly larger than the dimensions of a typical cascade. However, in

transition metals with high electron density of states at the Fermi level, such as Ni, Pd and Pt, electron mean free paths will be smaller and coupling between the phonon and electron systems will be more significant. Thus, phonon-electron interactions may contribute to the experimentally observed differences between Cu and Ni noted in this article. We believe, therefore, that phonon-electron damping of the cascade thermal spike deserves further study.

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Figure Captions

1. a) Stable SIA defects (●) and atomic replacements sites (x) for a simulated 5 keV cascade in Cu. Polar and azimuthal angles of the primary recoil direction were 39.1° and 22.5° , respectively. The cell is tilted 15° about the (110) axis to aid viewing.
b) Vacancies and SIA's for the event illustrated in (a).
2. (100) projection of instantaneous atomic configuration within cross sectional slabs of thickness $a_0/2$ near the center of 5 keV cascades in Ni (a-c) and Cu (d-f) at various times.
3. Radial pair distribution functions, $g(r)$, corresponding to the disordered zones at $t = 1.10$ and 3.84 ps for Cu (a) and at $t = 1.1$ and 2.8 ps for Ni (b). simulated pair distribution function for liquid Cu is included for comparison. (Ref. 12)
4. Temperature, T/T_m , and density profiles at three times for MD simulations of 5 keV cascades in Cu (a) and Ni (b).
5. Fraction of vacancies and interstitial atoms as a function of distance from the center of 5 keV cascades in Cu (a) and Ni (b).
6. Atomic mixing obtained in "heat spike" simulations for Cu and Ni as a function of energy density. Also shown are values obtained for a 5 keV primary recoil events in these metals and from experiment.
7. Micrographs showing the dissolution of a vacancy dislocation loop (marked by arrows) in Ni during irradiation with 100 keV Ni^+ at 300 K. (a) $1.1 \times 10^{12}/cm^2$; (b) $3.3 \times 10^{12}/cm^2$ (ref. 25).

Table 1. Yields for Cascade Collapse

Metal	Ion	Temp(K)	Yield	Ref.	$D_t/\Phi F_D^a$
Ag	100-keV Kr	10	1.0	28	60-90
Au	140-keV Kr	10	1.0	29	80-140
Cu ₃ Au	50-keV Kr	30	0.5	30	20-40 ^b
Fe	50 keV Fe	30	0.0	31	6-7
Mo	60 keV Mo	300 ^c	0.16	32	6-10
Ni	50-keV Ni	30	0.08	22	8-10

^a Data of Kim et al (18)

^b Value for Cu

^c Below annealing stage III

Table 2. Relocation of vacancies during a heat spike

Initial	(25,20,25)	(25,20,15)	(15,20,25)	(15,20,15)
Final	(18,17,23)	(17,17,22)	(18,18,22)	(24,24,20)

Fig 16