

## MOLECULAR DYNAMICS STUDIES OF DISPLACEMENT CASCADES\*

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**MASTER**

# Molecular Dynamics Studies of Displacement Cascades

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## Abstract

Molecular-dynamics simulations of cascades in Cu and Ni with primary-knock-on energies up to 5 keV and lattice temperatures in the range 0 K - 700 K are described. Interatomic forces were represented by either the Gibson II (Cu) or Johnson-Erginsoy (Ni) potentials in most of this work, although some simulations using "Embedded Atom Method" potentials, e.g., for threshold events in Ni<sub>3</sub>Al, are also presented. The results indicate that the primary state of damage produced by displacement cascades is controlled by two phenomena, replacement collision sequences during the collisional phase of the cascade and local melting during the thermal spike. As expected, the collisional phase is rather similar in Cu and Ni, however, the thermal spike is of longer duration and has a more pronounced influence in Cu than Ni. When the ambient temperature of the lattice is increased, the melt zones are observed to both increase in size and cool more slowly. This has the effect of reducing defect production and enhancing atomic mixing and disordering. The implications of these results for defect production, cascade collapse, atomic disordering will be discussed.

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## 1. Introduction:

The phenomenon of energetic displacement cascades has been a focus of research ever since the birth of nuclear energy [1]. Moreover, new materials requirements in advanced fusion reactors and applications of ion beams for materials modification have provided added impetus for understanding the physics of cascades. The elucidation of the dynamics and structure of displacement cascades by experimental means has been hampered by the small time scale ( $\approx 10$  ps) and volume ( $\approx 10^{-20}$  cm<sup>3</sup>) that characterize individual cascade events. These features, however, although disadvantageous from the standpoint of experiment, are highly beneficial from the standpoint molecular dynamics (MD) computer simulation. This paper highlights our recent work using this technique. In particular, we discuss: the dynamics and structures of 5 keV cascades in Cu and Ni; the influence of temperature on 3 keV events in Cu; preliminary results on cascades in Cu using "embedded atom potentials"; and finally, initial studies of defect production in the intermetallic, Ni<sub>3</sub>Al.

The molecular dynamics code employed in most of this work was tailored after the SUPERGLOB code originally developed by J.R. Beeler, Jr. [2]. Pair potentials have been employed in the majority of our work, although EAM potentials are now also being used. The Gibson II form of the Born-Mayer potential was selected to represent Cu [3], and the Johnson-Vineyard Erginsoy potential for Ni [4,5]. These potentials are short range, cutting off between the first and second nearest neighbor distance and they yield reasonable values for elastic constants and point-defect properties [3-6]. Both potentials were constructed to yield approximately correct threshold displacement energies along close-packed directions [7]. More realistic potentials are now available for d-electron metals, [8,9], however, because of their longer range and the many-body terms, they require more numerical computation. Our first results with EAM potentials will be described. Cascades at elevated temperatures were simulated by controlling the temperature of the cell interior by adding random forces to the two damped layers of atoms at the boundaries in accordance with Langevin dynamics [10]

## 2. Cascade Dynamics:

Some key features of cascade dynamics are illustrated in Fig. 1, where atomic replacements for a simulated 5-keV cascade in Cu are marked. Also shown in the figure are the final locations of self-interstitial atoms (SIA's). Most replacements occur in the central core of the cascade, but some replacement collision sequences (RCS's), which lead to stable SIA's, are observed. Whereas the SIA's all lie outside the central core, the vacancies, open circles in Fig. 1b, form a compact depleted zone. Similar features were observed in simulated Ni cascades [11].

Instantaneous atomic configurations at a particular instant of time during the evolution of a 5 keV cascade in Cu is shown in Fig. 2 [based on atoms within a cross sectional slab of thickness,  $a_0/2$ , through the center of the cascade]. Disordered, liquid-like zones, similar to that seen in Fig. 2 for Cu at 1.1 ps, were found at other times during the evolution and also for Ni [11]. Although the qualitative features of disorder in Cu and Ni are similar, the disordered regions in Cu persist over a longer time. The radial pair distribution functions,  $g(r)$ , of the atoms located within the cascade core, along with that for equilibrium liquid Cu (12), are shown in Fig. 3. The similarity between these curves provides a clear indication of melting in the cascade core. Again, similar results are found for Ni [11].

Local temperature distributions in 5 keV cascades were estimated by equating  $3/2 k_B T$  with the average kinetic energy of the atoms in a spherical shell at radius  $r$  with respect to an approximate cascade center. At early times,  $\approx 0.25$  ps, the average temperature in the center of a 5 keV cascade,  $r < 13 \text{ \AA}$ , is  $\approx 4000$  K for both Cu and Ni, and the temperature gradient outside this central core is  $\approx 140 \text{ K/\AA}$ . The initial cooling rate in the cascade is  $\approx 10^{15} \text{ K/s}$ . At  $\approx 1.0$  ps, for example, the temperature in Cu begins to fall below  $T_m$  at a position  $r \approx 25 \text{ \AA}$ , which from Fig. 2, can be seen to correspond rather closely to the radius of the disordered zone at 1.1 ps, thus illustrating the local temperature of the disordered zone is above  $T_m$ . For Ni, the temperature falls below the melting temperature much earlier in time, although the absolute temperature remains quite similar to that in Cu [11].

### 3. Defect Production:

It has been recognized for several years 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, i.e., defect production relative to that predicted by the modified Kinchin-Pease expression, becomes fairly constant, probably due to the formation of subcascades (15). MD simulations provide a simple explanation for reduced defect production in cascades.

In the Kinchin-Pease model for defect production, an interstitial atom that lies outside the spontaneous recombination volume of its own vacancy is considered stable. Binary collision simulation models have shown that spontaneous recombination of an interstitial with a vacancy other than its own is an unlikely event, even for dense cascades, like those in Au (16, 17). Our picture of local melting suggests that the stability of a Frenkel pair depends on whether the RCS producing the interstitial atom extends beyond the boundary of the melt zone, rather than beyond the recombination radius of the vacancy. Interstitials deposited within the melt zone are absorbed in the liquid and annihilated upon resolidification. The effectiveness of this mechanism can be seen by plotting the fraction of vacancies and interstitial atoms as a function of distance from the center of the cascade, as shown in Fig. 4 for a 5 keV cascade in Cu. The behavior in Ni is similar [11]. Little overlap is observed in the vacancy and interstitial-atom distributions, with no SIA's in the central core of the cascade,  $r \leq 15 \text{ \AA}$ . The defect production efficiency,  $\zeta_{FP}$ , in simulated Ni cascades,  $\zeta_{FP} = 0.4$ , is somewhat higher than, although similar to, that in Cu cascades,  $\zeta_{FP} = .2$ . The efficiency in Ni, however, derives from a single event so that its higher value should not be considered overly significant. The important point here is that the critical parameter for defect production in cascades is the ratio of RCS length to the radius of the cascade melt.

#### 4. Atomic Mixing and Disordering

Atomic mixing can be represented by the mean square displacement per atom as given by the relation,

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

The index  $i$  refers to the  $i^{\text{th}}$  atom initially in a coordination shell containing  $n(r)$  atoms at a distance  $r$  with respect to the center of the cascade.  $D_c(r)$  refers to the

average "diffusion coefficient" at a position  $r$  and time interval between the initiation of the event and  $t_0$ . The sum of the mean square displacements per atom at the end of a 5 keV recoil event in Cu and Ni is  $51,261 \text{ \AA}^2$  and  $14,290 \text{ \AA}^2$ , respectively. Although experimental data for mixing in 5 keV cascades are not available, a reasonable comparison can be made by considering the normalized quantity,  $\zeta_{\text{mix}} = \langle D_c(r)t_0 \rangle / n_0 E'_D$  where  $E'_D$  is the damage energy per atom and  $n_0$  is the atomic density. Values of  $\zeta_{\text{mix}}$  for 1 MeV Kr irradiation of Cu and Ni are 20 and  $8 \text{ \AA}^5/\text{eV}$  [18] which compare rather closely with those derived by the simulations, 16 and  $5 \text{ \AA}^5/\text{eV}$  in Cu and Ni respectively [11]. Similar values of mixing are deduced from disordering experiments of neutron irradiated  $\text{Cu}_3\text{Au}$  [19]. The excellent agreement must be considered somewhat fortuitous since 5 keV cascades can not accurately represent the entire primary recoil spectrum of 1 MeV Kr irradiation. Formation of subcascades during 1 MeV Kr irradiation and the normalization procedure employed here, however, make this comparison at least reasonable. Note, however, that mixing in Cu is far greater than that in Ni, and this is a consequence, we believe, of mixing takes place primarily in the local melt of the cascade. Since Cu has a lower melting temperature than Ni, the melt zone in Cu will last longer and it will occupy a greater volume. Moreover, the homologous temperature in Cu cascade will be higher than one in Ni, and this causes a higher diffusion coefficient in the melt.

## 5. Cascade Collapse and Clustering:

An important consideration in calculations of various radiation effects at high temperatures is not only total defect production but also the local distribution of SIA's and vacancies in their nascent cascades prior to migration. Figs.1b and 4 show that nearly the entire SIA distribution lies outside the vacancy rich core of the cascade but within the approximate boundaries of the thermal spike. Owing to their high concentration on the periphery of the cascade and their strong elastic interactions, the SIA's tend to cluster during the thermal spike as is seen for a 5 keV event in Fig. 1. Clusters containing  $\approx 3\text{-}5$  SIA's in nascent cascades have also been observed experimentally by diffuse x-ray scattering measurements on a number of pure metals following fast neutron irradiation at 6 K (20).

The loss of atoms from the core of the cascade by RCS's results in a depleted zone

after the melt resolidifies. In the past few years, detailed studies of the dynamic collapse of the depleted zones into dislocation loops and stacking-fault tetrahedra have greatly contributed to the understanding of the primary state of damage (i.e., the local configuration of point defects in displacement cascades) (21,22). These studies have employed ion irradiations of thin film specimens, some of which were performed in situ at low temperatures in a transmission electron microscope. The results of some of these studies are summarized in Table 1, which lists the dislocation loop yield, for a variety of ion-target combinations. Corresponding values of the ion beam mixing parameter,  $Dt/n_0 E_D'$  are listed to illustrate the correlation between mixing and cascade collapse. This correlation suggests that thermal spikes play an important role in cascade collapse.

The MD simulation result that a melt zone develops in the cascade suggests a simple model of cascade collapse which is akin to zone refining. We assume that vacancies can delocalize in the disordered (molten) cascade zone within the lifetime of the melt. Since density fluctuations in the cascade are initially small, especially in the cooler periphery of the cascade, the melt begins to regrow without defects. As the solidification process proceeds, the density fluctuations increase due to the increasing fraction of missing atoms, until vacancies begin to freeze out in the solid. In this way vacancies are driven to higher concentrations in the center of the cascade. The effectiveness of the "zone refining" depends, of course, on the velocity of the melt-solid interface and this will be strongly influenced by the size of the cascade and its initial temperature relative to the melting temperature. Thus, high energy densities, low melting temperatures and large (high energy) cascades are conducive to collapse; these predictions are experimentally verified (see Table 1).

## 6. Cascades at Elevated Temperatures:

The importance of thermal spikes in cascade dynamics suggests that the ambient lattice temperature should play a role in cascade dynamics as: (i) it increases the maximum temperature, (ii) it increases the size of the melt zone, and (iii) it reduces the cooling rate. We have simulated 3 keV events in Cu using various ambient temperatures [28]. In Fig. 5 are plotted the effective temperature vs. time at the center of the simulated cascades. This temperature is defined by the relation,  $K.E. = 3/2 k_B T$ , where K.E. is the average kinetic energy inside a sphere of radius  $3.5a$  ( $\sim 200$

atoms). By  $t \sim 0.5$  ps., equipartition of energy between kinetic and potential modes is nearly complete and considerable equilibration has occurred. The cooling rate of the cascade is given by  $(T(t) - T_0) \sim t^{-1.35}$ , where  $T_0$  is the ambient lattice temperature. This behavior corresponds rather closely to analytical thermal spike models [29,30]; Seitz and Koehler [29], for example, find an exponent of -1.5, based on the assumption of a temperature independent thermal diffusivity.

To further test the usefulness of temperature in characterizing the instantaneous state of a cascade, we have evaluated effective self-diffusion coefficients in simulated events as a function of time, using eq. (1). The sampled region is the same as that used in the temperature determination discussed above, and the time intervals  $\Delta t$  are of the order of 2 ps. Diffusion coefficients for the simulated cascades at four ambient temperatures are plotted in Fig. 6 as a function of reduced cascade temperature,  $T/T_m$ , ( $T_m = 1000$  K for the Gibson II potential [10]). Simulated self-diffusion coefficients for equilibrium liquid Cu using the Gibson II potential are shown for comparison, as are experimental values for Au tracer impurity diffusion in liquid Cu [31]. The cascade diffusion coefficients in the reduced temperature range 1 to 1.2 agree closely with liquid-state diffusion coefficients and confirm the local-melt interpretation of the cascade thermal spike. The deviations at  $T/T_m > 1.5$  occur at early times in the cascade evolution and most likely arise from insufficient equilibration. After resolidification occurs ( $T < T_m$ ), the diffusion coefficient is drastically reduced. The total amount of mixing in the cascades,

$$\langle R^2(t) \rangle = \sum_i \{ r_i(t) - r_i(0) \}^2 \quad (2)$$

has also been calculated as a function of time.  $\langle R^2(t) \rangle$  is found to increase rapidly at short times and saturate as the cascade region comes to equilibrium with the surrounding crystal (thermal diffusion of the vacancies and interstitials occurs on a much longer time scale). In fact,  $\langle R^2(t) \rangle$  reaches its asymptotic value when  $T$  crosses  $T_m$ . This indicates that mixing virtually ceases when resolidification is complete. The total atomic mixing is a factor of four greater at 700 K ( $\approx 0.7 T_m$ ) than at 0 K. This behavior follows from the longer lifetime of the local melt, i.e., the time interval over which  $T > T_m$  (cf. Fig 1), and also from the larger size of the locally melted region in the higher temperature events. The maximum effective radius of the melt regions was  $r_{\max} = (16, 20, 25, \text{ and } 29 \text{ \AA})$  for cascades at ambient

temperatures  $T = (0, 300, 500, 700 \text{ K})$ , respectively [28].

Finally we note that the number of Frenkel pairs produced in the simulated cascades at temperatures  $(0, 300, 500, 700 \text{ K})$  was  $(8, 3, 2, 3)$ . With only a single event at each temperature, however, it is not certain whether these numbers are representative. Nevertheless, a trend toward reduced defect production above  $0 \text{ K}$  is suggested by the results. The lower Frenkel pair production may result from shorter replacement sequences and larger droplet sizes; for as discussed above, an interstitial must be transported beyond the melt boundaries to survive recombination during the thermal spike. It is noteworthy that the defect production efficiency at elevated temperatures found in these simulations relative to the Kinchin-Pease formula, i.e.,  $\approx 10\%$ , is comparable to that deduced from macroscopic measurements of RED, radiation-induced segregation and radiation induced embrittlement [32].

## 7. Preliminary Studies With EAM Potentials:

Cascades in Cu: We have begun cascade simulations with embedded atom potentials for Cu [2,33]. Our first studies have employed a simple hybrid model where pair potentials are employed for the first 0.1 ps and EAM potentials thereafter. Since this work is at a rather preliminary stage, we summarize here only the thermal spike behavior since it provides perspective for the results discussed above. Cooling curves for the two potentials are plotted in Fig. 7. Little difference is observed between the two until  $t = 3 \text{ ps.}$ ; at that time, differences in the damping at the boundaries may play a role. We also find a decrease by nearly a factor of three in the total mixing when the EAM potential is employed. A part of this difference derives from the melting temperatures of the potentials. For the EAM,  $T_m$  is close to its true value in Cu, whereas for the Gibson II, it is  $\approx 1000 \text{ K} \pm 100 \text{ K}$ . Since mixing takes place mostly in the cascade melt, as discussed above, the lower value of  $T_m$  for the Gibson II potential can be significant. Since cascade collapse is also sensitive to  $T_m$ , predictions of collapse will require accurate potentials. Nevertheless, we find from this initial study that the qualitative predictions derived from using the Gibson II potential are born out by use of EAM potentials. The quantitative deficiencies of the Gibson II potential appear to derive from its too low value of  $T_m$ .

Threshold Energies in  $\text{Ni}_3\text{Al}$ : Threshold energies were studied in the intermetallic

compound, Ni<sub>3</sub>Al using EAM potentials [34]. Ni<sub>3</sub>Al has a L1<sub>2</sub> structure comprised of "A" and "B" alternating (100) planes with spacing  $a_0/2$ . "A" planes contain equal numbers of Ni and Al atoms and "B" planes contain only Ni atoms. The results for a several different PKA directions are tabulated in Table 2; they can be summarized as follows. (i) The threshold energy and number of replacements along  $\langle 110 \rangle$  directions is not strongly influenced by whether the chain is comprised of alternating Ni and Al atoms, or all Ni atoms, i.e., the mass mismatch does not strongly influence replacement sequences; (ii) The defect produced in the "A" planes is a crowd-ion, but it is a (100) dumbbell in the "B" planes. A brief annealing (1.0 ps) of the crystallite at 600 K caused the crowd-ion to convert to a dumbbell without crowd-ion migration. (iii) An octahedral interstitial is produced by a  $\langle 100 \rangle$  sequence on an all Al chain; it is located at the next nearest neighbor distance from its vacancy. The close separation of the vacancy and interstitial indicates that the spontaneous recombination volume in this material can be very small for some defect configurations. (iv) The  $\langle 111 \rangle$  direction is extremely hard to displacements,  $\approx 200$  eV for Al primary knock-on atoms (PKA's); for a 50 eV Ni PKA, anti-site defects were formed by a ring exchange mechanism, but without the creation of a Frenkel pair. These initial studies of defect production in intermetallic compounds illustrate that defect production in rather simple alloys is complex and that an understanding of radiation effects in these materials can be greatly assisted by simulation studies. For example, the small recombination volume in this ordered material may have important implication for the amorphization process in irradiated intermetallic compounds.

## 8. Conclusions:

It has been shown in this paper that molecular dynamics computer simulations can be a powerful aid in elucidating the defect production mechanisms and the dynamics and structure of energetic displacement cascades. The remarkable result of this work is that defect production and the primary state of damage in metals are controlled by two fundamental processes, replacement collision sequences and local melting in the cascade core. We have shown how these mechanisms affect the number of Frenkel pairs, atomic mixing and cascade collapse. We have also shown

that lattice temperatures superposes onto the local heating in a cascade to produce larger melt zones which persist for longer times. This has the effect of reducing defect production and enhancing mixing. Our preliminary investigations using embedded atom potentials for 5 keV cascades in Cu and for threshold events in Ni<sub>3</sub>Al illustrate that the simulations can now be performed reliably for specific pure metals and for alloys. It appears that with the rapid development of reliable, yet efficient, interatomic potentials, the continued expansion of supercomputing capabilities, and the development of new, more efficient molecular dynamics codes, the longtime goal of reliably simulating the defect production process in metals for recoil energies ranging from threshold to those characteristic of subcascade formation, will soon be realized.

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## Figure Captions

1. a) View of the locations of stable SLA defects (o) produced in a 5 keV cascade event in Cu, and the sites on which replacements have occurred (x). The primary recoil direction corresponded polar and azimuthal angles of  $39.1^\circ$  and  $22.5^\circ$ , respectively.  
b) Locations of stable Frenkel pairs.  
The computational cell is tilted  $15^\circ$  about the (110) axis to aid viewing (Ref [11]).
2. Locations of atoms in (100) cross sectional slabs of thickness  $a_0/2$  through the center of a 5 keV cascade in Cu at  $t = 1.10$  ps.(Ref. 11).
3. Radial pair distribution functions,  $g(r)$ , corresponding to the disordered zones at  $t = 1.10$  and  $3.84$  ps for Cu (Ref. 11).
4. Fraction of vacancies and interstitial atoms as a function of distance from the center of 5 keV cascades in Cu (Ref. 11).
5. Temperature in the center of a 3 keV cascade versus time (Ref. 28).
6. Self-diffusion coefficients in the center of a 3 keV cascade plotted versus reduced temperature,  $T/T_m$ . Also shown (dashed line) are Au tracer diffusion coefficients in liquid Cu [37] and simulated values of self-diffusion in liquid Cu (Ref. 28).
7. Cooling curves for the centers of 5 keV cascades in Cu, comparing EAM and Gibson II potentials (33).

**Table 1. Yields for Cascade Collapse**

Metal	Ion	Temp(K)	Yield	Ref.	Dt/n <sub>0</sub> E' <sub>D</sub> <sup>a</sup>
Ag	100-keV Kr	10	1.0	23	60-90
Au	140-keV Kr	10	1.0	24	80-140
Cu <sub>3</sub> Au	50-keV Kr	30	0.5	25	20-40 <sup>b</sup>
Fe	50 keV Fe	30	0.0	26	6-7
Mo	60 keV Mo	300 <sup>c</sup>	0.16	27	6-10
Ni	50-keV Ni	30	0.08	22	8-10

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<sup>a</sup> Data of Kim et al (18)

<sup>b</sup> Value for Cu

<sup>c</sup> Below annealing stage III

**Table 2. Threshold Displacement Energies in Ni<sub>3</sub>Al [34]**

PKA	Direction	Energy [eV]	Type of Defect	R.C.S.
Al	$\langle 110 \rangle^i$ (A)	50	crowd-ion	15
Ni	$\langle 110 \rangle^i$ (A)	50	crowd-ion	15
Al	$\langle 110 \rangle^i$ (A)	30	crowd-ion	5
Ni	$\langle 110 \rangle^i$ (A)	30	crowd-ion	5
Al	$\langle 110 \rangle^i$ (A)	20	no defect	0
Ni	$\langle 110 \rangle^i$ (A)	20	no defect	0
Ni	$\langle 110 \rangle$ (A)	35	no defect	0
Ni	$\langle 110 \rangle$ (A)	50	crowd-ion	13
Ni	$\langle 110 \rangle$ (B)	20	no defect	0
Ni	$\langle 110 \rangle$ (B)	25	no defect	0
Ni	$\langle 110 \rangle$ (B)	30	dumbbell Ni-Ni (B)	6
Al	$\langle 100 \rangle$ (A)	50	octahedral Al (B)	1
Ni	$\langle 100 \rangle$ (B)	50	dumbbell Ni-Ni (B)	3
Ni	$\langle 100 \rangle$ (A)	50	crowd-ion Ni(A)	2
Al	$\langle 111 \rangle$	200	octahedral Al (B)	1
Al	$\langle 111 \rangle$	100	no defect	0
Ni	$\langle 111 \rangle$	50	2-ring exchange	0

(2-anti-site defects)

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<sup>(i)</sup> denotes PKA in a (100) plane but 2° away from  $\langle 110 \rangle$  direction. All other PKA's are not exactly in a low index plane.















