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Thermal excitation of electrons in energetic displacement cascades

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A thermal description of the electron-ion interaction in the cooling phase of the displacement cascade in metals is given. Differential equations governing the transfer of heat between the two systems are derived and solved numerically using physically reasonable parameters for cascades in Cu and Ni. Large differences are found in the cooling rates of cascades in these two metals and the differences are shown to depend on the ratio of a parameter T_0, the temperature at which the electron-phonon mean free path reduces to the radius of the Wigner-Seitz sphere and γ_e, the coefficient of the electronic heat capacity. Simplified versions of the heat-transfer equations have been incorporated into a molecular-dynamics code in order to include the interaction in simulations of cascades in Cu. The net effect of including the interaction is to actually inhibit defect production in low-energy cascades (~ 500 eV) by damping the ionic motion.

INTRODUCTION

It has been realized for some time now that an accurate description of point-defect production in energetic displacement cascades requires a good understanding of recombination efficiency as well as the initial displacement damage efficiency. Traditionally the formation and lifetime of an energetic cascade is divided into three stages: the displacement phase, the relaxation phase during which approximate equipartition of energy is established, and the cooling phase as the cascade energy dissipates into the surrounding lattice. Molecular-dynamics (MD) studies[1] and experimental low-energy ion irradiation studies[2] indicate that the traditional approaches to calculating the number of point defects, typified by the modified Kinchin-Pease formulas,[3] are largely correct at the end of the displacement phase. However, enhanced thermal motion during the cooling phase leads to a significant reduction in the number of point defects as Frenkel pairs recombine. A good description of the cooling phase is clearly important but not straightforward. A simple calculation using the bulk value of thermal conductivity shows the cascade quenching after several tens of fs, in conflict with experimental evidence for the collapse of cascades into dislocation loops, which requires times of the order of ps for the necessary atomic rearrangements. Further problems with simple thermal conductivity arguments are encountered when one considers the behavior of the apparently similar metals, copper and nickel, under heavy-in bombardment. Significant differences are observed in the cascade collapse behavior of these two metals, e.g., Ref. 4, where loop production is found to be much more efficient in Cu than Ni. One also finds that the fraction of vacancies produced which are contained within loops is higher in Cu than Ni.[5] This phenomenon is usually attributed to differences in the melting point of the two metals.

Flynn and Averback[6] have pointed out the reason for the inapplicability of the bulk value of thermal conductivity: in pure metals the conductivity is dominated by electronic rather than phonon conduction, but at the end of the displacement phase the majority of the energy is associated with the ion cores rather than the conduction electrons. If this energy is to be conducted away efficiently, it is necessary to have strong coupling between the electrons and phonons. Since the spatial size of the cascade is of the order of the electron-phonon mean free path, transfer of energy from the hot lattice to the electron gas may be dramatically reduced in the early stages of the cooling phase and in this case the effective thermal conductivity is just that of the lattice, which is many times lower than that of the electron gas. With these complications then, heat flow from the cascade cannot be described with a simple thermal conductivity. A detailed description of the cascade evolution from the displacement phase to the cooling phase requires a MD approach (see, for example, Refs. 7–9); however, in the standard MD approach, no coupling of the ionic motion to the electron system is considered, hence the heat-transfer rate is underestimated because it only includes the lattice thermal conductivity. The atoms are treated as rigid classical particles, interacting via simple pairwise or many-body potentials and although the validity of this classical model has been in question for many years, until recently there has been no physical model of the energy transfer from the hot ions to the conduction electrons (see the recent review by Stoneham[10]). The aim of the present paper is to provide such a model, based on a very simplified physical description of the energy transfer which closely follows the discussion of Flynn and Averback (FA).

FA describe a model of electrons diffusing randomly through the hot cascade and gathering energy $k\Theta_D$ at each encounter with a phonon, where Θ_D is the Debye temperature. They conclude that efficient transfer of energy from electrons to phonons is possible only if the cascade has a temperature higher than a critical value T_c.

From estimates of the values of T_c for copper and nickel, they conclude that cascades in nickel should quench much faster than those in copper.

In the analysis which follows, we derive expressions for the flow of heat in both electronic and ionic systems in the form of two coupled partial differential equations for T_e and T_i, the local temperatures of electrons and ions. We solve these equations numerically for simple initial conditions corresponding to a spherical cascade of uniform initial temperature, using the material parameters appropriate to Cu and Ni and for cascade energies of 2 and 5 keV. The results confirm Flynn and Averback's conclusion that quenching is much faster in Ni due to its higher electronic specific heat and smaller mean free path for electron-phonon scattering. Although the electronic conduction is more significant in Ni, in both metals we found that the lattice conductivity alone is insufficient to describe the quenching. For MD simulations of cascade quenching, we conclude that the electronic system must be included and we show how our partial differential equations can be discretized for this purpose. Simplified forms of these equations (which are valid when the electron temperature does not rise significantly), representing the flow of heat from ions to electrons during the thermal phase of the cascade, have been used to include the interaction in a MD simulation of cascades in Cu. The effect on the equations of motion proves to be numerically similar to that obtained by the quite different viewpoint of Caro and Victoria[11] who have proposed an interpolation formula linking the electron-ion interaction in the low-energy regime (electron-phonon scattering) to the high-energy regime (electronic stopping power).

ANALYSIS

We assume that the electronic system can be described as a uniform perfect gas obeying Fermi-Dirac statistics and that the cascade is sufficiently hot that only phonons at the Debye frequency need be considered. We further assume the validity of the harmonic approximation in describing the lattice vibrations by writing the electron-phonon mean free path as $\lambda = r_0 T_0 / T_i$, where r_0 is the radius of the Wigner-Seitz cell and T_i is the local ionic temperature, e.g., Ref. 6. T_e is the local electronic temperature and we assume that $kT_e N(E_F)$ electrons participate in scattering with phonons, where k is Boltzmann's constant and $N(E_F)$ is the density of states at the Fermi energy. τ is the mean free flight time for electron-phonon scattering, which we can replace by λ / v_F, where v_F is the Fermi velocity. We assume that energy $k\Theta_D$ is exchanged in each collision to obtain an expression for the rate of transfer of energy from ions to electrons:

$$R_t = \frac{k^2 \Theta_D N(E_F) v_F T_i T_e}{r_0 T_0} . \tag{1}$$

A net rate may be established by replacing T_i with $(T_i - T_e)$.

Now the standard expressions for the thermal conductivity and heat capacity of the electron gas[12] may be written in the form

$$\kappa = (\pi^2/9) k^2 T_e N(E_F) v_F \left[\frac{r_0 T_0}{T_i} \right] , \tag{2}$$

$$C_e = (\pi^2/3) k^2 N(E_F) T_e . \tag{3}$$

These expressions may be used in the energy balance equation for the electronic system

$$C_e \frac{\partial T_e}{\partial t} = \kappa \nabla^2 T_e + R_t \tag{4}$$

to derive an expression for the changing electronic temperature,

$$\frac{\partial T_e}{\partial t} = \left[\frac{3\Theta_D v_F}{\pi^2 r_0 T_0} \right] \left[\frac{T_i - T_e}{T_0} \right] + \frac{v_F r_0 T_0}{3 T_i} \nabla^2 T_e . \tag{5}$$

A similar expression may be obtained for the ionic system

$$\frac{\partial T_i}{\partial t} = \left[\frac{\kappa_i}{\sigma \rho} \right] \nabla^2 T_i - \left[\frac{3\Theta_D v_F \gamma_e}{\pi^2 r_0 \sigma \rho} \right] T_e \left[\frac{T_i - T_e}{T_0} \right] . \tag{6}$$

Here κ_i is the ionic thermal conductivity, σ is the specific-heat capacity, ρ is the density, and γ_e is the coefficient of the electronic heat capacity per unit volume.

The relationship of these formulas to the inequalities of FA may be noted if we consider characteristic time scales for the heating up and dissipation of energy in the electronic system. Returning to (5), let us rewrite this equation as

$$\frac{\partial T_e}{\partial t} = \frac{T_i - T_e}{\tau_h} + \frac{1}{\tau_c} (r^2 \nabla^2 T_e) , \tag{7}$$

where

$$\tau_h = \frac{\pi^2 r_0 T_0}{3\Theta_D v_F}$$

and

$$\tau_c = \frac{3 T_i r^2}{v_F r_0 T_0} . \tag{8}$$

τ_h is a characteristic heating time and τ_c is a characteristic cooling time. The temperature of the cascade is related to the initial energy input Q and its radius r. Supposing each atom of the cascade to have energy $3kT_i$; the number of atoms involved is r^3/r_0^3, where r_0 is the radius of the Wigner-Seitz cell. Hence, by energy conservation,

$$T_i = \frac{r_0^3 Q}{3kr^3} \tag{9}$$

and we obtain the following expression for τ_c:

$$\tau_c = \frac{Q r_0^2}{k v_F T_0 r} . \tag{10}$$

The factor r in the denominator explains why, for large times (corresponding to large r), the electrons have no time to equilibrate with the hot lattice. In fact, the critical radius for equilibration is when $\tau_h = \tau_c$. This equality recovers Eq. (5) of FA (with a slightly different numerical coefficient),

$$T_c = \frac{\pi^6}{81}\frac{T_0^6 k^2}{\Theta_D^3 Q^2} . \tag{11}$$

It is useful to consider a simplification of the above equations which occurs when we ignore phonon diffusion (which is much slower than diffusion in the electronic system) and assume T_e to be constant. Then Eq. (6) reduces to the following ordinary differential equation:

$$\frac{dT_i}{dt} = -\alpha(T_i - T_e) , \tag{12}$$

where $\alpha = (3\Theta_D \gamma_e T_e v_F)/(\pi^2 r_0 \sigma \rho T_0)$. In this approximation, the time constant for the cooling of the lattice by electrons is given by $\tau = \alpha^{-1}$, implying that rapid quenching of cascades is favored by small values of T_0 and large γ_e. Values of τ for Cu and Ni are 4.3 ps and 0.12 ps, respectively, for an electron temperature of 300 K. The value for Ni is of the order of 1 lattice vibration and so clearly some caution is needed in the sense of which the term "cooling" is applied; however, this approach does enable one to predict, from elementary considerations, whether cascades in otherwise similar metals will have different cooling characteristics—it is only necessary to compare values of $T_0/\gamma_e = \zeta$. Comparing Ni and Cu in this way, we find a ζ ratio of around 30, suggesting that the cooling characteristics of cascades in these two materials should differ significantly, with Ni cooling faster than Cu.

NUMERICAL SOLUTIONS

To substantiate this claim, numerical solutions of the coupled equations (5) and (6) were sought using realistic cascade parameters. For numerical work the equations were put in dimensionless form by choosing the unit of length as r_0, time as $3r_0/v_F$, and temperature as $9\Theta_D/\pi^2$. Then (5) and (6) take the following simple form:

$$\frac{\partial T_e}{\partial t} = \frac{T_0}{T_i}\nabla^2 T_e + \frac{T_i - T_e}{T_0} , \tag{13}$$

$$\frac{\partial T_i}{\partial t} = \left[\frac{3\kappa_i}{\sigma \rho r_0 v_F}\right]\nabla^2 T_i - \left[\frac{9\Theta_D \gamma_e}{\pi^2 \sigma \rho}\right] T_e \left[\frac{T_i - T_e}{T_0}\right] . \tag{14}$$

Discretized versions of the continuous equations were set up for a spherically symmetric cascade and solved using FACSIMILE—a commercially available numerical package.[13] The initial temperature distribution was

$$T_i = \begin{cases} T_1, & 0 < r < r_1, \\ T_{\text{am}}, & r_1 < r < 2r_1 , \end{cases} \tag{15}$$

$$T_e = T_{\text{am}}, \quad 0 < r < 2r_1 , \tag{16}$$

where T_1 is the initial cascade temperature, calculated from Eq. (9), and r_1 is the size of the cascade radius. This was estimated from MD studies of a 2-keV cascade in Cu (Ref. 14) to be about 2.5 nm. T_{am} denotes the ambient temperature, which was taken to be 300 K in all calculations. The boundary conditions imposed were (i) no heat flow at $r = 0$ and (ii) no temperature change in either system at $r = 2r_1$. Care was taken that this second condition did not significantly influence the cascade region. The values of parameters used in the calculation for Cu and Ni are shown in Table I. Values of T_0 were taken from FA for consistency to be 4.5×10^4 and 1.5×10^4 K for Cu and Ni, respectively. The lattice thermal conductivity κ_i is difficult to measure because it is dominated by the electronic thermal conductivity in pure metals. A value of 1.0 W/m/K was estimated from the aforementioned MD study of Cu and this value was also used for Ni. In practice, these calculations are rather insensitive to the value of κ_i since this is so much smaller than the electronic thermal conductivity.

The results of these calculations are shown in Fig. 1, where we plot the temperature at the center of the cascade as a function of time on a logarithmic scale. It is clearly seen that the Ni cascade quenches much faster than the Cu.

We can now go a step further and use our equations to assess the importance of terms omitted in conventional MD. MD studies of cascades in Cu are currently being carried out by several groups, but these do not take into account the potential cooling effect of electrons. In Fig. 2 we show how the temperature at the center of the 2-keV cascade in Cu changes with time when the electron-phonon interaction is both included and neglected. The effect clearly makes a significant difference in the cooling phase of the cascade. In Fig. 3 we present a similar graph for a 5-keV cascade in Cu showing that the effect is more pronounced at higher energies. The Ni cooling

TABLE I. Parameters used in numerical solution of heat-flow equations.

	Cu	Ni
v_F/ms^{-1}	1.57×10^6	1.57×10^6
Θ_D/K	343	440
r_0/nm	0.142	0.138
γ_e/J K^{-2} m^{-3}	104	1104
ρ/kg m^{-3}	8920	8900
σ/J K^{-1} kg^{-1}	385	460
T_0/K	4.5×10^4	1.5×10^4

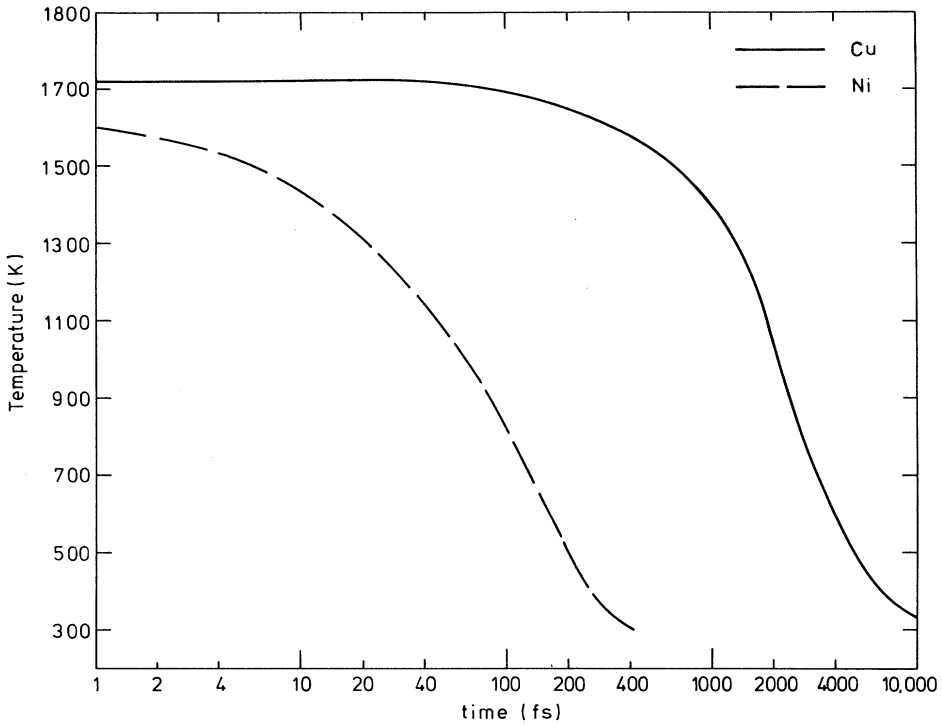

FIG. 1. Temperature variation at the center of a 2-keV cascade in copper and nickel. The stronger electron-phonon interaction causes much faster cooling in nickel.

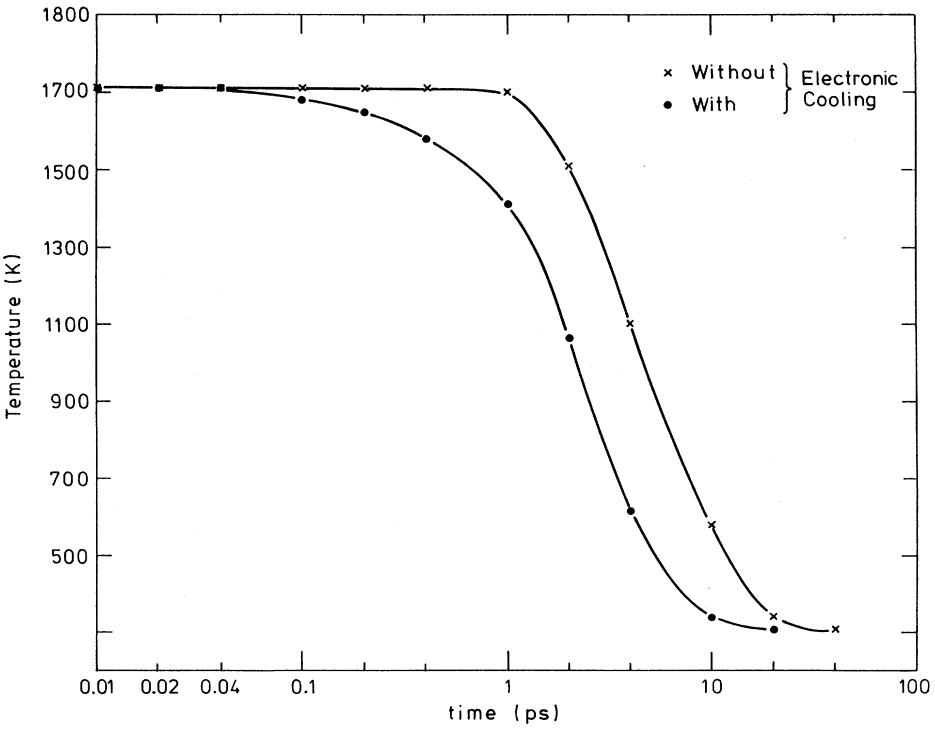

FIG. 2. Cooling rate of a 2-keV cascade in copper, calculated with and without electronic cooling.

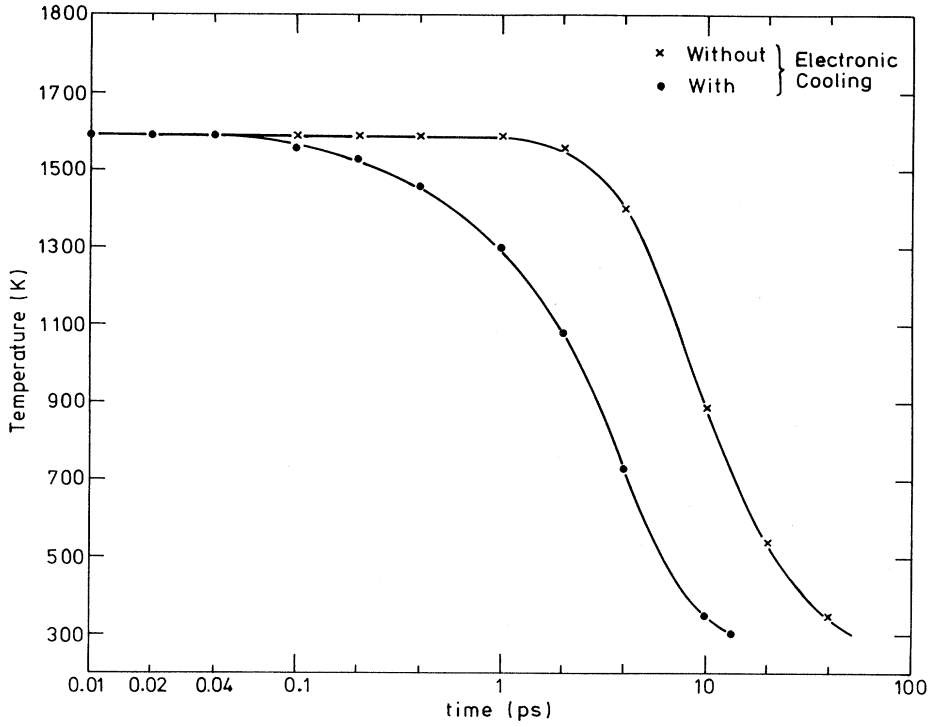

FIG. 3. Cooling rate of a 5-keV cascade in copper, calculated with and without electronic cooling.

curve for such a cascade shows the cascade cooling faster than the period of one lattice vibration. Although our thermal model of the interaction becomes unphysical at such rapid cooling rates, the message is clearly that electronic conduction cannot be ignored.

ATOMISTIC SIMULATION WITH MD

Implementation of the above ideas into a MD code requires the definition of both ion and electron local temperatures. However, we have seen that, in most cases, where the above equations are expected to remain good approximations, T_e remains close to ambient temperature because the time scale for conduction through the electron gas is usually much shorter than the time scale for loss of energy of ions to electrons. In this case the equation of motion of the ions needs to be modified to add the effect of the term introduced by Eq. (12). Two ways to deal with this suggest themselves. One possibility is to scale all ionic velocities after each time step by an appropriate amount depending on the local temperatures. An alternative approach, and the one adopted here, is to apply a damping force $\mathbf{F}_i$ to each ion in the form

$$\mathbf{F}_i = -\mu \mathbf{v}_i \ , \tag{17}$$

as has been suggested by other authors.[11] The rate of change of thermal energy is then

$$\mathbf{F}_i \cdot \mathbf{v}_i = -\mu \mathbf{v}_i \cdot \mathbf{v}_i \ , \tag{18}$$

which we equate to $(\partial/\partial t)(3k_B T_i)$. Hence, from Eq. (12) we have

$$-\mu \mathbf{v}_i \cdot \mathbf{v}_i = -3k_B \alpha (T_i - T_e) \ . \tag{19}$$

Finally, using (19) and the following expression for T_i:

$$T_i = \frac{m v_i^2}{3k} \ , \tag{20}$$

where m is the ion mass, we may write the equation for μ as

$$\mu = \alpha m \left[\frac{T_i - T_e}{T_i} \right] . \tag{21}$$

This equation presents a problem as $\mathbf{v}_i$ tends to zero (which will often be the case in a vibrating solid) because T_i will also go to zero, causing the expression for μ to become singular. To avoid this possibility, we have introduced a smooth cutoff to μ at $T_e/20$ by rewriting (21) as

$$\mu = \alpha m \frac{T_i - T_e}{[T_i^2 + (T_e/20)^2]^{1/2}} \ , \tag{22}$$

where the factor $\frac{1}{20}$ has been chosen to be compatible with the time steps used in our MD code when atoms are thermally vibrating. In this way the value of μ becomes constant when an atom comes to rest. Test calculations with the atoms at the same temperature as the electrons

show that the above cutoff has no appreciable effect on the vibrations of the atoms over the time scale of cascade calculations. It is found that vibrating atoms can sustain their temperature to better than 1 K over times of the order of 10 ps with this approximation. It has also been verified that, when the atom temperature is initially higher than that of the electrons, then it will steadily fall towards the electron temperature with a time constant given by $\tau=\alpha^{-1}$, in good agreement with similar continuum calculations.

COMPARISON WITH OTHER WORK

Caro and Victoria[11] have described a scheme to add a velocity-dependent damping term to the ionic equation of motion to simulate the electron-ion interaction over the whole range of energies encountered in the cascade, from the collisional phase through to the thermal phase. An empirical interpolation scheme is proposed to smoothly connect the "stopping power regime" and the "thermal regime" of the electron-ion interaction by varying the coupling according to the local electronic density encountered by a moving ion. Detailed comparison with the present work is difficult since no relationship between the ion energy and the electronic density encountered is given in Ref. 11; however, it is clear that the thermal model we have presented above will tend to underestimate the damping in the collisional phase in comparison. This should not be a serious error, however, since most ion-ion collisions are at a glancing angle and, in terms of the description of Caro and Victoria, the electronic density encountered by the ions will not differ greatly from the equilibrium value. A comparison of the present model with Ref. 11 can be obtained by noting that our product αm is the same as their β at high temperature. If we assume the electron density is given by the conduction electron density in Cu, then we find $\beta=2.7\times10^{-14}$ kg/s while $\alpha m=2.4\times10^{-14}$ kg/s, in satisfactory agreement.

The problem of the electron-ion interaction has been considered by Kaganov *et al.*[15] who derived the following expression for α:

$$\alpha=\frac{\pi^2}{6}\frac{m_e s^2 n_0}{\tau\Theta_D\sigma\rho}\ , \tag{23}$$

where m_e is the electron mass, s is the speed of sound in the solid, and n_0 is the number density of electrons. If we substitute expressions for the free-electron density of states, Fermi energy, and Debye wavelength[16] into our expression for α, Eq. (12), and also make the assumption that $T_i\approx T_e$, we obtain a similar result but with the coefficient $\pi^2/6$ replaced by $108^{1/3}/Z^{2/3}$, where Z represents the number of free electrons per atom. The agreement between these two equations then is satisfactory in the free-electron approximation; however, our expression clearly has the greater generality since it takes the band structure of the solid into account via the factor γ_e.

MD SIMULATIONS

The above formalism has been implemented in a recent version of the MD code[17] MOLDY and used to study the effects of electron-phonon coupling on displacement cascades in copper using a modified Ackland *et al.* many-body potential between the atoms.[18] The original Ackland potential does not contain a short-range repulsive core potential and, as a result, it allows Cu atoms to pass through one another at energies greater than around 60 eV. A short-range Born-Mayer-type potential has been incorporated in such a way that the fitted properties, such as single-crystal elastic constants, cohesive energy, etc., are unaffected. The coefficients of the potential were adjusted to give the best fit to the measured threshold displacement energies for a range of crystallographic directions. The resulting fit is close to the well-known Gibson 2 repulsive potential commonly used in simplified cascade simulations. The atoms were thermally equilibrated at 100 K for around 10 ps ($\sim$150 vibrations) before the cascade was initiated. We have chosen to simulate a 500-eV knockon event in the $\langle 345\rangle$ direction with the primary atom situated near the center of the block. Four different levels of electron-phonon interaction were introduced, ranging from a zero interaction, as currently assumed in MD cascade simulations, to the strong interaction predicted for nickel. Periodic boundary conditions are employed which have the advantage that the cascade does not necessarily have to evolve in the center of the block. The block size is chosen so that replacement collision sequences are contained within the block and do not overlap with one another through the faces as a consequence of the periodic boundary conditions. For the 500-eV cascades, a block of 6912 Cu atoms ($12\times12\times12$ unit cells) was used. The computer-generated pictures in Fig. 4 show a three-dimensional view of the cascade according to the criteria: (i) atoms displaced by more than one-quarter of a lattice constant from any lattice site are shown as solid squares, and (ii) vacant lattice sites, defined as having no atom within one-quarter of a lattice constant of the site, are shown as open squares. It is a general feature of cascade simulations that very small changes in the initial conditions often produce large differences in the final defect configuration. Ideally, one would average over many simulations to reduce statistical fluctuations before producing quantitative results;[14] however, qualitative conclusions can be drawn from the results of just a few simulations and it is in this spirit that we present the following results.

For an electron temperature of 100 K we find, from Eq. (12), that the coupling constant for Cu is $\alpha m=2.49\times10^{-14}$ kg/s, while for Ni it is 7.98×10^{-13} kg/s, which is around a factor of 30 stronger. We have also made MD simulations for the intermediate value of 2.5×10^{-13} kg/s, corresponding to ten times that of Cu (or one-third that of Ni). In Fig 4 we present a comparison of the evolution of a 500-eV cascade in the $\langle 345\rangle$ direction of a Cu lattice, with the above coupling constants. The atom vibrations had previously been equilibrated at a temperature of 100 K (corresponding to a classical kinetic energy of $\frac{3}{2}$ kT, which is intended to

simulate the residual thermal motion of the atoms at low temperature. The weak electron-phonon coupling in Cu has little effect on the peak disorder at 0.2 ps but reduces the final defect yield from five to four Frenkel pairs (FP). With the strong coupling to be expected in Ni, the defect yield was reduced to only two FP. The cascade structure at 0.2 ps shows that strong coupling appreciably retards the propagation of the replacement collision sequences,

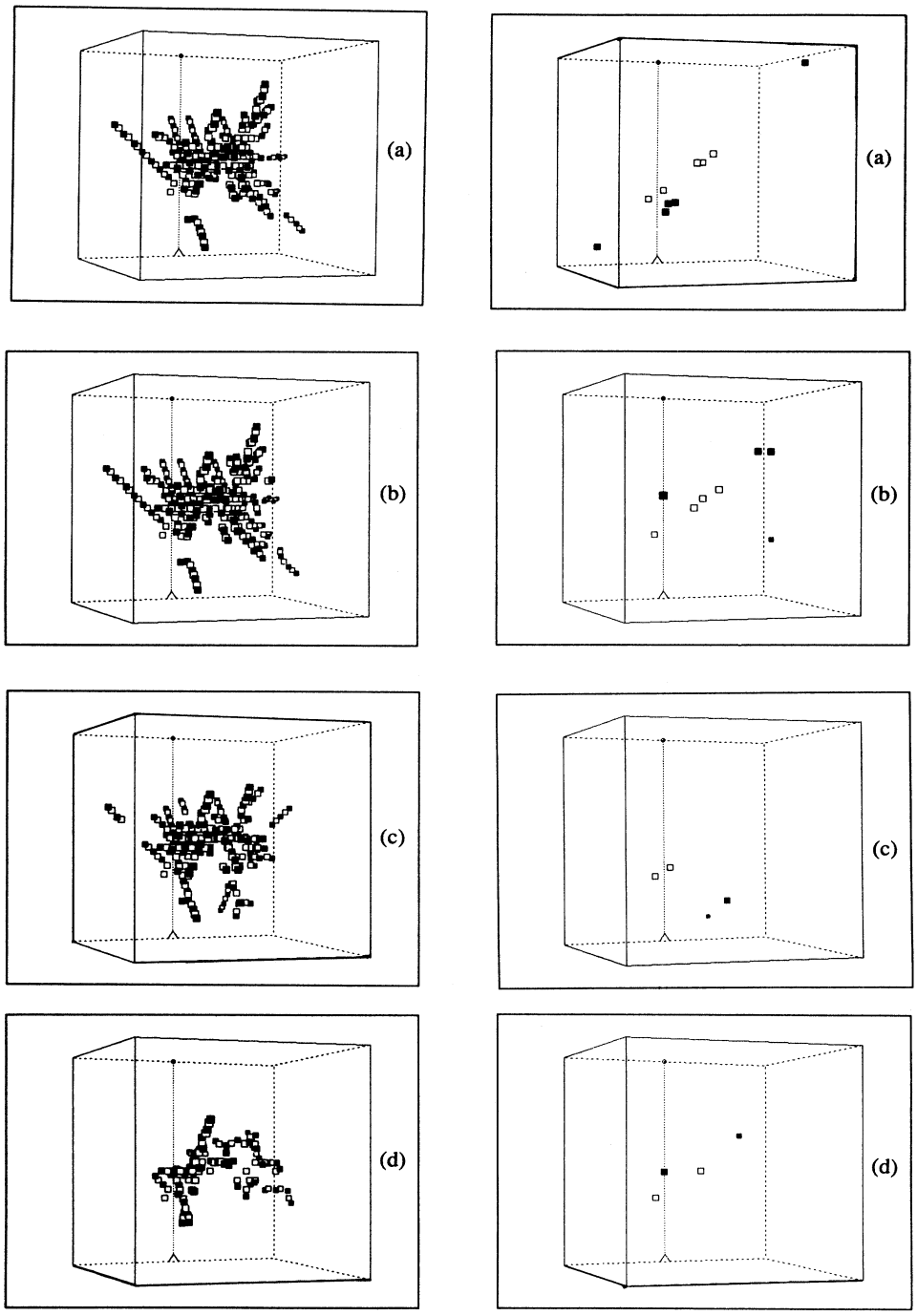

FIG. 4. The effect of different electron-phonon coupling strengths on the evolution of a 500-eV cascade in copper. Interstitials are shown as solid squares and vacancies as open squares. The left-hand column shows the defect configuration 0.2 ps after the primary event while the right-hand column is after 7 ps. The coupling strengths used are those corresponding to (a) zero coupling, (b) copper, (c) ten times that of copper (or one-third that of nickel), (d) nickel.

thus the overall effect is not dissimilar to a reduction in the cascade energy.

We have not observed any obvious quenching in of defects during these and other similar cascade simulations which have been made in the energy range 250 eV to 1 keV; however, this could well occur at energies above 1 keV, where a quasiliquid zone is likely to be formed at the center of the cascade. This formation of a liquidlike zone has been observed by other workers in 5-keV cascades.[19] The electron-phonon coupling would shorten the lifetime of such a zone, which might enhance the defect yield.

CONCLUSIONS

We have derived equations governing the thermal interaction of electrons and phonons in the cooling phase of energetic displacement cascades and have obtained numerical solutions of these equations for 2-keV cascades in both Ni and Cu. These calculations confirm that cascades in Ni should quench much faster than those in Cu. Our approach demonstrates the importance of the ratio of two parameters in determining the efficiency of electronic cooling of the cascade region: T_0, the temperature at which the electron-phonon mean free path reduces to the radius of the Wigner-Seitz sphere and γ_e, the coefficient of the electronic heat capacity. We have shown quantitatively that current MD simulations of displacement cascades underestimate the rate of removal of energy from the cascade region during the cooling phase by neglecting the electron-phonon interaction and have incorporated a model of this interaction into the MD code MOLDY. The surprising result of these simulations is that, in materials where the electron-phonon interaction is stronger and heat transfer from the cascade region is enhanced during the cooling phase, defect production is actually inhibited as atomic configurations which would result in high residual defect concentrations are less likely to develop. We have not observed a quenching in of defects during the MD simulations, however, with higher-energy cascades we believe this is possible.

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