Electronic effects in high-energy radiation damage in iron

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Abstract

Electronic effects have been shown to be important in high-energy radiation damage processes where a high electronic temperature is expected, yet their effects are not currently understood. Here, we perform molecular dynamics simulations of high-energy collision cascades in α-iron using a coupled two-temperature molecular dynamics (2T-MD) model that incorporates both the effects of electronic stopping and electron–phonon interaction. We subsequently compare it with the model employing electronic stopping only, and find several interesting novel insights. The 2T-MD results in both decreased damage production in the thermal spike and faster relaxation of the damage at short times. Notably, the 2T-MD model gives a similar amount of final damage at longer times, which we interpret to be the result of two competing effects: a smaller amount of short-time damage and a shorter time available for damage recovery.

Keywords: radiation damage, molecular dynamic simulations, iron, electronic effects, high-energy collision cascades

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

1. Introduction

Structural damage induced by ions carrying energies lower than 100 keV is mainly due to ballistic processes [1]. On the other hand, at high energy, most of the damage is believed to be due to electronic effects [2]. Molecular dynamics (MD) simulations have been used to describe radiation damage effects induced when an energetic particle interacts with matter, creating a collision cascade [3–6]. When fast-moving atoms interact with the matter, they lose part of their energy due to their interaction with the electrons. The importance of this interaction in the dynamics of a cascade was first mentioned by Flynn and Averback [7] and the challenge has been to develop models to include the effects of electronic stopping and the electron–phonon (e–p) interactions in MD simulations.

These models include proposals by Caro and Victoria [8], Finnis et al. [9], Ivanov and Zhigilei [10] and Duffy and Rutherford [11].

Although electronic stopping has been commonly taken into account in cascade simulations [12–28], there are no systematic studies that include a dynamic, location-dependent description of how the e–p coupling affects the atom dynamics in collision cascades. Examining this issue is especially important in high-energy cascades, where the electronic excitations matter most. In such events, the high-energy ions lose a significant amount of their energy due to inelastic electronic scattering [11] and high electronic temperatures are expected. In order to approach high-energy events in a more realistic way it is essential to study the effects of the interaction of the atoms with the electrons.
In this paper we study these effects in high-energy cascades in bcc-Fe, a base material for ferritic–martensitic bcc steels, which are the main candidate materials for the structural and plasma-facing components of future fusion reactors [29, 30]. We investigate the effect of the e–p coupling in high-energy cascades in bcc–iron by comparing cascades where the energy loss due to electronic stopping has been included in the simulations with cascades where both the electronic stopping and the e–p interaction, as well as the energy feedback from the electronic to the atomic system, are included. We refer to the first set of simulations as ‘friction cascades’ and to the second set of cascades, implementing the full 2T-MD, as ‘2T-MD cascades’. We see decreased damage production in the thermal spike and faster relaxation of the damage at short times for the 2T-MD cascades. At longer times the 2T-MD model gives a similar amount of final damage, which we interpret to be the combination of two competing effects: a smaller amount of short-time damage and a shorter time available for damage recovery.

2. Methods

2.1. The model

The Duffy and Rutherford 2T-MD model [11, 18] is implemented in DL_POLY code [31, 32] version 4.04. It represents the heat exchange between the ionic and electronic subsystems. Inelastic electronic scattering and e–p coupling result in energy loss by the atomic system, which is deposited in the electronic system. The energy feedback from the electronic to the atomic system, which we interpret to be the combination of two competing effects: a smaller amount of short-time damage and a shorter time available for damage recovery.

The evolution of the electronic temperature is described by the heat diffusion equation given below (see equation (6)).

The equation of motion has the form of a Langevin equation:

\[
m v_i(t) = F_i(t) - \gamma_i v_i + \tilde{F}(t),
\]

where \( m \) is the mass of atom \( i \) and \( v_i \) is its velocity, \( F_i(t) \) is the force due to the surrounding atoms of \( i \) at time \( t \), \( \gamma_i \) is the friction coefficient and \( \tilde{F}(t) \) is a random stochastic force term that is determined by the local temperature of the electronic system (electronic temperature) \( T_e \). The evolution of the electronic temperature is described by the heat diffusion equation given below (see equation (6)).

The friction term is a sum of two parts: a term that accounts for the effect of electron stopping \( \gamma_s \), which is applied for velocities of atoms larger than a cut-off value \( v_c \), and a term that accounts for the e–p interaction \( \gamma_p \).

\[
\gamma_i = \gamma_s + \gamma_p \quad \text{for } v_i > v_c
\]

\[
\gamma_i = \gamma_p \quad \text{for } v_i \leq v_c.
\]

The cut-off velocity \( v_c \) corresponds to energy \( E_c \), which in metals is often taken as approximately double the system’s cohesion energy [34] in order to differentiate ballistically moving atoms (with energy in excess of cohesion energy) from those oscillating. In insulators, it has been shown that the band gap governs the electronic energy losses during the radiation damage process [35, 36].

The magnitude of the stochastic force \( \tilde{F}(t) \) is related to the friction coefficient by the fluctuation-dissipation theorem and the energy exchange drives the atomic system to the temperature of the electronic subsystem [11]. We assume that atoms gain energy only from the e–p interactions and not from electronic stopping, and that the stochastic force is proportional only to the e–p interaction friction coefficient \( \gamma_p \).

\[
(\tilde{F}(t')) \cdot (\tilde{F}(t)) = 2k_B T_e \gamma_p \delta(t' - t).
\]

The MD simulation is coupled to a continuum model for the electronic temperature, which evolves using a heat diffusion equation:

\[
C_e \frac{\partial T_e}{\partial t} = \nabla (\kappa_e \nabla T_e) - g_p (T_e - T_a) + g_s T'_a.
\]

where the second and third terms on the right-hand side of the equation represent energy exchange with the lattice via e–p interactions and electronic stopping, respectively. The second term represents energy exchange with the atomic system energy due to the difference between the atomic system temperature \( T_a \) and the electronic system temperature \( T_e \). The third term is a source term that describes the energy lost by the atomic system due to electronic stopping. \( C_e \) and \( \kappa_e \) are the electronic specific heat capacity and thermal conductivity, respectively. The atomic temperature \( T_a \) is calculated from the average kinetic energy of the atoms in a coarse-grained cell. \( T'_a \) also has dimensions of temperature and is calculated from the average kinetic energy of the subset of atoms with energy greater than twice the cohesive energy of the system [33]. \( g_p \) and \( g_s \) are the e–p and electronic stopping coupling constants respectively.

The energy loss \( \Delta U_i \) of an atom \( i \) with velocity \( v_i \) at each timestep with value \( \Delta t \) due to a friction force \( F_i \) is

\[
\Delta U_i = F_i v_i \Delta t = \gamma_i v_i^2 \Delta t.
\]

In a coarse-grained cell \( J \) with constant electronic temperature, the total energy loss will be

\[
\Delta U_J = \Delta t \sum_{i \in J} \gamma_i v_i^2 = \Delta t \sum_{i \in J} \gamma_p v_i^2 + \Delta t \sum_{i' \in J} \gamma_s v_i'^2,
\]

where the second sum is over the atoms that have velocities larger than the cut-off velocity that corresponds to double the cohesive energy of the system. The energy gain of the electronic system at each timestep is

\[
\Delta U_{eg} = g_p T_a \Delta V \Delta t + g_s T'_a \Delta V \Delta t.
\]

Equating \( \Delta U_J \) and \( \Delta U_{eg} \) gives

\[
\sum_{i \in J} \gamma_p v_i^2 = g_p T_a \Delta V
\]

\[
\sum_{i' \in J} \gamma_s v_i'^2 = g_s T'_a \Delta V
\]
so $T_\alpha$ and $T'_\alpha$ are defined as

$$\frac{3}{2} k_B T_\alpha = \frac{1}{N} \sum_{i\in J} m_i v_i^2$$

and the coupling constants $g_p$ and $g_s$ as

$$g_p = \frac{3Nk_B\gamma_p}{\Delta Vm}$$

$$g_s = \frac{3N'k_B\gamma_s}{\Delta Vm},$$

where $N$ is the number of atoms in a coarse-grained cell $J$ with volume $\Delta V$, $k_B$ the Boltzmann constant and $N'$ the number of atoms with velocities larger than $v_i$ in the cell $J$.

As described in [11], the electronic stopping power is proportional to the ion velocity,

$$\frac{dE}{dx} = \lambda E^{1/2}$$

$$m \frac{du}{dt} = \left( \frac{m}{2} \right)^{1/2} u$$

and the constant of proportionality $\lambda$ is determined from the Lindhard and Scharff model [37]. Equation (17), from equation (1) gives

$$\gamma_s = \lambda \left( \frac{m}{2} \right)^{1/2} u$$

and the corresponding relaxation time for electronic stopping is

$$\tau_s = \frac{m}{\gamma_s} \left( \frac{2m}{\lambda} \right)^{1/2}.$$  

The timescale for energy loss due to e–p interactions is

$$\tau_p = \frac{m}{\gamma_p}$$

or from equation (14)

$$\tau_p = \frac{3nk_B}{g_p}$$

with $n$ being the number of atoms per unit volume.

The heat diffusion equation is solved using a finite difference (FD) method. Energy lost by the atoms, due to the friction term, is input into the local FD cell at each MD timestep. The electronic temperature simulation cell is extended beyond the atomistic simulation cell, and each coarse-grained cell of the electronic grid has length of about 3 Å. For the electronic grid we are using Robin boundary conditions. We are using a variable timestep for the solution of the FD model, which depends on the electronic temperature gradient and is typically smaller than the MD timestep. The e–p coupling is modeled by a source/sink term in the heat diffusion equation that depends on the difference between the local electronic and lattice temperatures and the e–p coupling constant. An equivalent amount of energy is removed/added locally to the MD cell by a Langenvin thermostat via $\dot{F}(t)$, which depends on $T_e$.

2.2. Simulations

We assume that the e–p coupling process ($g_p$) is not initiated until 0.3 ps, as the lattice temperature is ill-defined before this. Until this time of the simulation only the electron stopping mechanism is active, while there is a time-frame when both the electronic stopping and e–p interaction mechanisms are active. This approximate value was computed by looking at the convergence of kinetic and potential energies (i.e. thermalization) in the friction cascades. The $C_e(T_e)$ parameterization was obtained through ab initio calculations, as described in [38].

The heat capacity given for a range of electron temperatures can be found in [39]. The temperature dependence of electronic thermal conductivity was assumed to be $\kappa_e(T_e) \sim \frac{C_e(T_e)}{T_e(300 \text{ K})}$. In fact we would expect the electronic thermal conductivity to decrease as the lattice temperature increases, but the simple model of the $1/T$ dependence overestimates this effect, as the ionic temperatures can be locally very high. Also the $\tau_e = 1/T_e$ dependence is neglected in the electron–phonon coupling ($\gamma$) and therefore for consistency it is neglected in the expression for $\kappa$ (assuming e–p coupling and thermal conduction are linked). Reduced electronic thermal conductivity would contribute two effects: quenching (1 ps) and annealing at (1–100 ps), which would potentially decrease the resultant point defect number. However, this does not impact the general conclusion [10, 40]. We further assume no ionic temperature dependence in $\kappa_e(T_e)$ and a constant value of $\gamma$ [38], due to the large uncertainty.

The electronic stopping friction term $\gamma_s$ corresponds to a value of 1 ps$^{-1}$ and the cut-off velocity is set to 54 Å ps$^{-1}$, as described in [41]. In this work, in addition to the previously implemented electronic stopping energy loss mechanism, the exchange of the energy between the atomic and electronic systems is included. The friction coefficient $\gamma_p$ due to e–p interactions corresponds to a coupling parameter value of $g_p = 5.4822 \times 10^{18}$ W m$^{-3}$ K$^{-1}$ [39] and is set equal to 1.56 ps$^{-1}$. A value of $\kappa_e = 80.2$ W m$^{-1}$ K$^{-1}$ for the thermal conductivity at room temperature [42] is used.

We are simulating cascades of 100 and 200 keV Fe primary knock-on atoms (PKA) in bcc-Fe in systems that consist of 30, 50 and 100 million atoms. The atoms contained in the boundary of the MD box, in a layer of about 1 Å thickness, are connected to a thermostat at 300 K. A variable timestep with a maximum value of $1.28 \times 10^{-3}$ ps is used to describe the atomic motion throughout the cascade development and relaxation. We simulate 12 directions of the PKA on up to 65 000 parallel processors of the HECToR National Supercomputing Service [43].

For α-Fe, we have used an embedded-atom potential [44], optimized for better reproduction of several important properties of α-Fe, including the energetics of point defects and their clusters (M07 from [45]). At distances shorter than 1 Å the interatomic potentials were joined to short-range repulsive ZBL potentials [46]. The joining was calibrated against the threshold displacement energies [45]. The resulting thresholds were found to be in as good agreement with experiments as the best previous potentials [45, 47].
3. Results and discussion

Table 1. \(N_{\text{disp}}\) and \(N_{\text{def}}\), calculated using the sphere criterion, at the peak of the damage (1–2 ps) and at the end of the simulation. The standard error of the mean is shown in the brackets, calculated over six events. \(\tau_{\text{disp}}\) and \(\tau_{\text{def}}\) are read-off from figure 1.

| PKA energy       | \(N_{\text{disp}}\) | \(N_{\text{def}}\) | \(N_{\text{disp}}\) | \(N_{\text{def}}\) | \(\tau_{\text{disp}}\) (ps) | \(\tau_{\text{def}}\) (ps) |
|------------------|--------------------|-------------------|--------------------|-------------------|----------------|----------------|
| 100 keV—friction | 89 000 (26 000)    | 146 000 (47 000)  | 19 000 (2000)      | 1100 (200)        | 7              | 10             |
| 100 keV—2T-MD    | 33 000 (2000)      | 61 000 (3000)     | 13 000 (700)       | 1000 (100)        | 2              | 5              |
| 200 keV—friction | 503 000 (98 000)   | 982 000 (193 000) | 66 000 (6000)      | 2000 (400)        | 10             | 20             |
| 200 keV—2T-MD    | 52 000 (6000)      | 97 000 (11 000)   | 23 000 (2000)      | 1700 (100)        | 2              | 5              |

For 100 and 200 keV cascades simulated in different knock-on directions. Specifically, with \(N_{\text{disp}}^P\) we refer to the peak of displaced atoms and with \(N_{\text{def}}^P\) to the peak of the defect atoms, often referred to as the thermal spike [50–52]. \(N_{\text{disp}}^P\) and \(N_{\text{def}}^P\) correspond to the number of displaced and defect atoms in long simulation times (the flat lines in figure 1). \(\tau_{\text{disp}}\) is the time during which the elastic recombination of displaced atoms takes place and corresponds to the width of \(N_{\text{disp}}^P\) (\(N_{\text{disp}}^P\) includes elastic deformation [41]). \(\tau_{\text{def}}\) is the relaxation time during which the dynamic annealing of the defects takes place and corresponds to the width of \(N_{\text{def}}^P\).

Figure 1. \(N_{\text{disp}}\) and \(N_{\text{def}}\) (sum of interstitials and vacancies) from 100 keV (top) and 200 keV (bottom) knock-on atoms, for different PKA directions. Dotted lines represent the friction cascades, while the solid lines are for the 2T-MD cascades. We see more damage production at the peak for the 2T-MD cascades, and less recombination at the end of the simulation time. Both models result in a similar amount of final damage at longer times.
Figure 2. Maximum electronic and atomic temperatures for 200 keV (left) and 100 keV (right) 2T-MD cascade simulations, for six events. The ill-defined lattice temperature reaches past $10^7$ K initially. After 0.3 ps, which is the thermalization time, electronic energy is fed back to the lattice and the ionic temperature starts dropping below $10^4$ K. At around 6 ps the electron–ion temperatures are equilibrated.

Figure 3. Maximum atomic temperatures for 200 keV (left) and 100 keV (right) 2T-MD cascade simulations, for six events. Here we compare simulations where the local COM momentum is subtracted (red dashed lines) for the local atomic temperature calculation with the original runs, where COM motion is not removed (black solid lines). The runs where local COM momentum is removed show no significant difference in comparison to the original runs.

As seen in figure 1 and table 1, there is a significant difference in $N_{\text{disp}}$ and $N_{\text{def}}$ as well as in $\tau_{\text{disp}}$ and $\tau_{\text{def}}$ for both models and simulated energies. First, both $N_{\text{disp}}^0$ and $N_{\text{def}}^0$ are smaller for the 2T-MD cascades as compared to the friction cascades. Second, $\tau_{\text{disp}}$ and $\tau_{\text{def}}$ are shorter for the 2T-MD cascades, corresponding to about 3 ps and 5 ps for $N_{\text{disp}}^0$ and $N_{\text{def}}^0$ respectively, for both simulated energies. These differences are due to faster quenching of the thermal spike in the 2T-MD model that includes the e–p coupling and the additional energy transfer channel. In effect, the e–p coupling removes energy from the thermal spike and electronic thermal conductivity transports it from the simulation cell. This additional energy loss mechanism in the 2T-MD model is also responsible for the smaller amount of unrecombined damage at long times, $N_{\text{disp}}^{\text{def}}$, as is seen in figure 1.

An interesting insight comes from the examination of $N_{\text{def}}^0$, which quantifies the final amount of damage in the structure and ultimately governs the radiation response of the system. We observe that $N_{\text{def}}^0$ is similar in both 2T-MD and friction models (see figure 1 and table 1). This effect can be understood on the basis of two competing mechanisms. On one hand, faster energy transfer to the electrons reduces the short-time displaced atom production, $N_{\text{disp}}^0$. On the other hand, faster energy transfer also reduces the time of the thermal spike in figure 1, which is the time that is available for most efficient and fast recombination in the highly mobile and disordered state. As a result, $N_{\text{def}}^0$ in the 2T-MD cascades are similar to $N_{\text{def}}^0$ in the friction cascade, where the initial amount of damage, $N_{\text{def}}$, is larger but the relaxation time is longer. Figure 2 shows the maximum electronic and atomic temperatures for 100 keV and 200 keV 2T-MD cascades, where for all simulations the atomic temperature is higher than the electronic temperature, meaning that the electronic system acts as a heat sink. This is in agreement with lower energy (10 keV) 2T-MD cascades in iron [11]. The heat transfer relaxation time, as read from these plots, is about 6 ps. In our simulations we have not subtracted the center of mass (COM) momentum from each ionic grid cell. We have repeated a number of runs where we removed local COM momentum for the calculation of the local ionic temperature and it showed no significant difference in comparison to the original runs.

Comparison of the maximum ionic temperature for the original simulations and the simulations where the COM momentum is removed is shown in figure 3. Here we see that the maximum ionic temperature for the two methods of calculating the ionic temperature almost coincide. In figure 4 we see the total energy of the system for a 100 keV friction cascade and for a 100 keV 2T-MD cascade for the same direction of the PKA. The energy is normalized to unity. The energy loss is about the same for
Figure 4. Total energy of the system for a representative 100 keV friction cascade (dotted line) and a representative 100 keV 2T-MD cascade (solid line) for the same direction of the PKA. The energy is normalized to unity.

Figure 5. Two representative 100 keV cascades for the same PKA direction for the friction mechanism and the full 2T-MD. The PKA moves from the top left to the bottom right corner. (a) Displaced atoms for a friction cascade (top) and for a 2T-MD cascade (bottom). (b) Corresponding defect atoms for the friction (top) and the 2T-MD cascade (bottom). The vacancies (interstitials) are shown in purple (green). The simulation box length is 700 Å. The friction cascade size and 2T-MD cascade size are 300 Å and 500 Å, respectively. The snapshots are at 0.1, 2.5 ps and 48 ps for the friction cascade and at 0.1, 0.5 and 63 ps for the 2T-MD cascade. We used Atomeye software [53] to visualize cascade evolution.

In figures 5 and 6 we show representative 100 and 200 keV cascades for the same PKA direction, showing the effects discussed above. Figure 5 shows three different time-frames of the relaxation of two representative cascades in a 30 million atom system, for a 100 keV Fe PKA. Figure 5(a) shows the displaced atoms for a friction cascade (top) and for a 2T-MD cascade (bottom). Figure 5(b) shows the defects for the same cascades. The middle frames demonstrate the difference in displaced (about 70,000 for friction and 40,000 for 2T-MD cascade) and defect atoms (115,000 for friction and 70,000 for 2T-MD cascade) for the two mechanisms. The peak for the 2T-MD cascade is at a shorter time, 0.4 ps, than for the friction cascade, 2.5 ps, demonstrating faster relaxation. \( N_{\text{disp}} \) corresponds to 20,000 and 15,000 for friction and 2T-MD cascades respectively, as shown in figure 1. \( N_{\text{def}}^f \) is 2000 for the friction and 2000 for the 2T-MD cascade.

Smaller \( N_{\text{disp}}^p \), \( N_{\text{disp}}^d \) and \( N_{\text{disp}} \) and shorter \( t_{\text{disp}} \) and \( t_{\text{def}} \) for 2T-MD cascades are also demonstrated in figure 6, where the snapshots of two typical 200 keV collision cascades at three different stages of development are shown. Displaced atoms are shown in figure 6(a) for a friction cascade (top) and a 2T-MD cascade (bottom), and defect atoms are shown in figure 6(b). \( N_{\text{def}}^f \) for both mechanisms is 1,500 atoms. For both the 100 keV and the 200 keV cascades, shown in figures 5 and 6 respectively, we can see that the two models result in different shapes of the cascade.

The discussion of the large-scale analysis above focused on the comparison of the dynamics of the two models. Defect analysis results at the local level are summarized in table 2, where statistics for the defect clusters for the friction and 2T-MD cascades of this paper are given. As discussed above, the difference in the number of Frenkel pairs (FP) between the two models is small. Similar statistics of defect
analysis were obtained for the 100 keV friction and 2T-MD cascades. As shown in the table, we observe statistically significant differences in the defect arrangement in clusters for the 200 keV cascades. In particular, the number of isolated vacancies and interstitials is about two times higher for the 2T-MD results than for the friction model. The number of SIA clusters is much smaller for the 2T-MD model at 200 keV. This shows that the differences in 2T-MD model and friction model cascade dynamics (see above) can have significant effects on damage clustering.

4. Conclusion

Previous works on cascades in Fe have shown that the fraction of damage in clusters depends both on the interatomic potential and the way electron–phonon coupling and electronic stopping is included in the cascades [27, 54]. The fraction of damage in large clusters, in turn, may have a major effect on the long-timescale evolution of damage, and is hence a crucial issue for developing predictive radiation-damage modeling [55]. Moreover the results in the current work show that treating the electron–phonon coupling in a local way may have a major effect on the fraction of damage in clusters. Taken together, these results show that accurately assessing the reliability of primary radiation damage simulations in metals requires consideration of both the interatomic potentials and a local model for the electron–phonon coupling. Furthermore, current work on tungsten shows that the results of the e–p coupling are not generic, which supports that these effects should be investigated for each material individually rather than making extrapolations of results in one material to another, even for cases such as iron and tungsten, which both have the bcc structure. The results of the work presented here show that a realistic approach to high-energy events by treatment of the electronic effects locally is essential, as these effects can significantly affect the arrangement of the defects in clusters, and consequently the long-term performance of the material.

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