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Modelling swift heavy ion irradiation in iron

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ABSTRACT

Swift heavy ions moving in metals lose most of their energy to inelastic scattering of electrons. The energy deposited in the electronic system is transferred into the atomic system via electron–ion interactions and can lead to melting and creation of new damage and also annealing of pre-existing atomic defects. Using a combination of molecular dynamics and a consistent treatment of electron energy transfer and transport we have modelled experiments performed in Fe to investigate the annealing effect and damage creation under electronic excitations. We observe both annealing and new damage creation at low and high electronic stopping, respectively. Rapid separation of interstitial atoms and vacant lattice sites is seen due to efficient transport via replacement collision sequences. Our results suggest that the role of electronic excitation can be significant in modeling of the behaviour of metals under swift heavy ion irradiation and attempts to modify metals via ion implantation.

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1. Introduction

The selection of structural materials for fusion power plants requires an understanding of the process of energy exchange between atoms and electrons in high energy events far from equilibrium [1]. Microscopic materials modification by ion irradiation also requires that damage be controlled and manipulated [2]. A swift heavy ion with MeV–GeV energy will undergo inelastic collisions with electrons, exciting electrons along its path. Such electronic excitation can affect bulk and surface properties, with applications ranging from fusion reactor first wall and blanket candidate material validation to laser ablation and ion beam implantation.

It has long been established in experimental studies that high levels of electronic excitation affect damage formation processes; causing local melting, amorphisation, phase transitions and latent track formation. Tracks have been observed in both insulators and metals, however, the conditions for track formation and the structure of the tracks varies considerably between materials [3]. The rapid recovery of charge neutrality in metals, due to high electron mobility results in damage that is dominated by melting within the thermal spike model. The situation is more complex in semiconductors and insulators due to persistent excitations such as excitons. The interatomic interaction may also be modified by electronic excitations in insulators [4], semiconductors [5] and metals [6,7]. This will lead to soft phonon modes which may contribute to the primary damage state. This may contribute to the radial shock wave caused by thermal expansion.

Experiments have shown different behaviour among pure metals under swift heavy ion irradiation. Inelastic collisions of the swift heavy ion with electrons cause damage production in some metals, while in others enhanced defect recovery and annealing are observed [9]. Experiments in Fe, using an undamaged lattice, showed that low levels of electronic stopping (the amount of energy lost to the electrons per unit length) led to less damage than that predicted solely by atomic collisions due, to annealing of primary damage caused by atomic collisions. At high levels of electronic stopping ($(\frac{dE}{dx})_e > 40$ keV nm^{-1}), the damage efficiency was higher than that calculated theoretically [10,11]. When the sample is doped with defects before undergoing irradiation Fe showed annealing of pre-doped defects [12]. Both defect annealing and damage creation were attributed to electronic excitations.

The early ideas of Lindhard and Scharff [13] have been developed and implemented in the SRIM code which allows calculation of high energy ion ranges and energy deposition due to elastic

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nuclear and inelastic electronic collisions. However, this is limited to the binary collision approximation and cannot describe defect recombination. Swift heavy ion irradiation is often interpreted in terms of a simple two temperature model with melting inferred when the atomic temperature rises above the melting temperature. Wang et al. used such a method, coupled with other techniques, to model swift ion irradiation in metals [14]. Molecular dynamics has the advantage of providing detailed information on the atomic level, which cannot be gained from experimental studies or simpler simulation techniques.

However, since the range of a swift heavy ion is of the order of microns, classical molecular dynamics is incapable of simulating such an event as a series of atomic collisions. It is, therefore, necessary to model the track of excited electrons along the path of the ion as it loses energy and slows down. Electronic energy loss has been modelled as a damping force in the atomic equations of motion in the simulation of displacement cascades [15–17]. The same approach cannot be used to model swift heavy ion irradiation, where the energy is deposited primarily into the electronic system, as there is no consistent way to transfer the deposited energy into the atomic system.

Classical molecular dynamics traditionally confines the role of the electrons to the interatomic potential, neglecting the effect of electronic excitation and subsequent energy redistribution. We have developed a technique for modelling electronic effects by coupling a molecular dynamics simulation to a continuum model for the electrons allowing electronic excitation, definition of a local electronic temperature and feedback of energy lost to the electrons back to the ions. The aftermath of the passage of a swift heavy ion is modelled by initially setting a central column of electrons to an elevated temperature. The atoms and electrons exchange energy via electron–phonon coupling, conserving energy, at a rate dependent on the local temperature difference between the lattice and the electrons [18].

Our previous simulations of displacement cascades investigated the variation of electron–ion coupling parameter and showed that the inclusion of electronic effects gave rise to reduced residual damage [19]. Work on high energy events, where energy is initially deposited into the electron system, highlighted a sensitive dependence of the degree of melting on the electronic thermal parameters [20]. Cascades and ion tracks represent the extremes of the radiation energy spectrum, but in realistic scenarios a material will be subject to irradiation at a range of different energies. An understanding of the cumulative effects of both nuclear displacements and electronic excitations is required, on an atomic level, to determine defect distributions for input into models of damage evolution on longer timescales [21].

In this paper we investigate both defect annealing and creation by swift heavy ions. The atomic configuration resulting from a 30 keV cascade was used as the starting configuration for the ion track simulation. Some of the energy initially deposited in the electron system is transferred into the atoms before diffusing away. The mechanisms for annealing of pre-existing defects and the creation of new damage were investigated for a range of electronic stopping power.

2. Method

A classical molecular dynamics simulation, using the DL_POLY package [22], was coupled to a continuum model for the electrons. A system of 986,078 Fe atoms in a cubic cell of size 226 Å interacting via the magnetic potential of Dudarev and Derlet [23] was used. The electronic temperature is defined on a coarse-grained lattice that is superimposed onto the atomistic simulation. The coarse-grained electron temperature cells are cubic (side-length 22.64 Å) and the central $9 \times 9 \times 9$ cells overlap with the lattice as in Fig. 1. The atomic system was divided into atomic energy cells and periodic boundary conditions were applied.

The simulation proceeds by iterating the atomic equations of motion using the leapfrog Verlet method, and the heat diffusion equation, using a finite difference method, at each molecular dynamics timestep. Energy is exchanged between the lattice and electrons, conserving energy, using a modified Langevin formalism where the lattice is effectively thermostatted to the local electronic temperature. Energy is removed by diffusion to the boundary of the electron system where a constant temperature of 300 K is imposed, which represents the rest of the lattice. The electron system extends beyond the atomic system and is divided into $9 \times 100 \times 100$ equally sized cubic cells allowing a broad diffusive temperature profile to form; relaxing to the ambient temperature far from the radiation event. The simulation proceeded until a stable damage state was reached and the initial and final defect distributions were compared. Further details of the model can be found in [18,20].

Since the range of an ion at a stopping power of order 10 keV nm^{-1} is much greater than the length scales accessible by atomistic simulation, we cannot model the ion explicitly. Instead we model the track of excited electrons by initiating the simulation with a central region of excited electrons. Fig. 1 shows this schematically. The initial temperature of the excited column of electrons was calculated from the energy deposited in the electronic system per unit length (the stopping power), the electronic specific heat and the area of the excited column to give an energy deposition corresponding to a given value of stopping power. Cylindrical symmetry was imposed along the track axis, which was parallel to the cascade knock-on atom velocity. Periodic boundary conditions were imposed in the electron system in the direction of the track axis, and the temperature fixed at 300 K on the boundaries in the other directions.The electronic energy is treated using a continuum model described by the following heat diffusion equation:

$$C_e \frac{\partial T_e(x,y,z)}{\partial t} = \nabla(\kappa_e \nabla T_e(x,y,z)) - g_1[T_e(x,y,z) - T_a(x,y,z)] + g_2 T'_a(x,y,z). \quad (1)$$

Here κ_e is the electronic thermal conductivity, C_e is the electronic specific heat, T_e and T_a are the electronic and atomic temperatures, respectively, T'_a is a temperature derived from the subset of atoms in the stopping regime and g_1 and g_2 are the electron–phonon coupling and electronic stopping strengths, respectively. A tanh form was used for the electronic specific heat C_e entering the heat diffu-

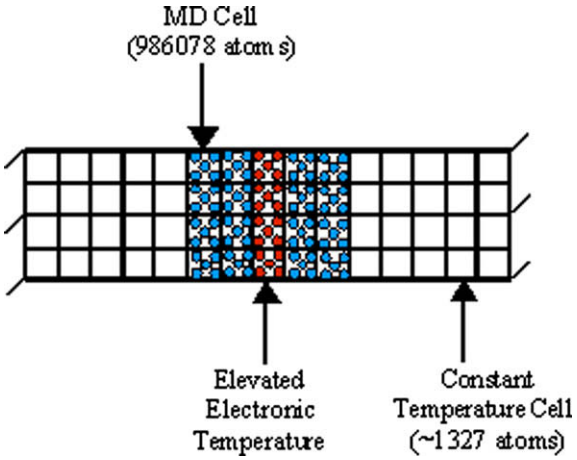

Fig. 1. Schematic of MD cell and initial electronic excitation. The number of cells has been reduced for clarity.

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