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Short communication

Effects of the electron-phonon coupling activation in collision cascades

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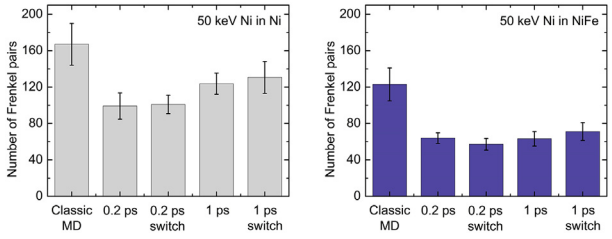
HIGHLIGHTS

- The electron-phonon interactions in irradiation affect the energy dissipation.
- The resulting damage depends on the electron-phonon interaction activation time.
- The electronic stopping acts on the ions before the electron-phonon interactions.

GRAPHICAL ABSTRACT



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ABSTRACT

Using the two-temperature (2T-MD) model in molecular dynamics simulations, we investigate the condition of switching the electronic stopping term off when the electron-phonon coupling is activated in the damage production due to 50 keV Ni ion cascades in Ni and equiatomic NiFe. Additionally, we investigate the effect of the electron-phonon coupling activation time in the damage production. We find that the switching condition has negligible effect in the produced damage, while the choice of the activation time of the electron-phonon coupling can affect the amount of surviving damage.

Molecular dynamics (MD) simulations is a technique that has been widely used to investigate ion irradiation effects in matter [1,2]. Using the equation of motion to calculate the atom trajectories and describe the system status at any point during the simulation, MD simulations are an important tool to gain insights at the atomic level, and provide information on the processes that take place in very small length-scales, in the range of a few angstroms, within time-scales of some tens of picoseconds. For energy events of up to a few keV, this classical approach for ballistic collision processes is accurate, and has revealed important information on primary radiation damage processes and cluster formation [3–9]. For irradiation with ions of higher energy (from a few tens of keV), the two-temperature (2T-MD) model [10,11] in MD simulations is a more realistic approach, as it takes into account the energy exchange between the atomic and the electronic subsystems [12,13]. In the 2T-MD model, the excited electrons can act as a heat sink or a heat bath [10,14], which can affect damage production, defect recovery and cluster formation.

Recent simulations of 30 and 50 keV Ni cascades in Ni and Ni-based solid solution alloys [15,16] have shown that, compared to

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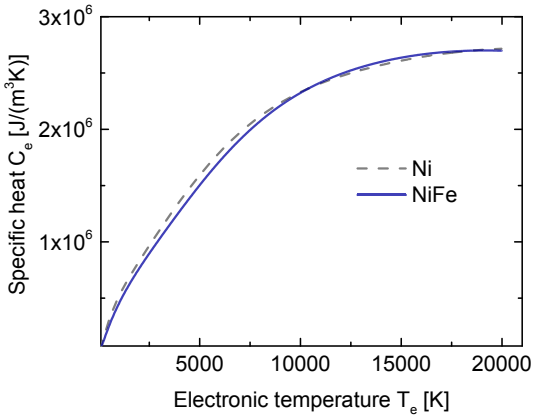

Fig. 1. Specific heat capacity for a range of the electronic temperature for Ni (grey dashed line) and equiatomic NiFe (blue solid line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

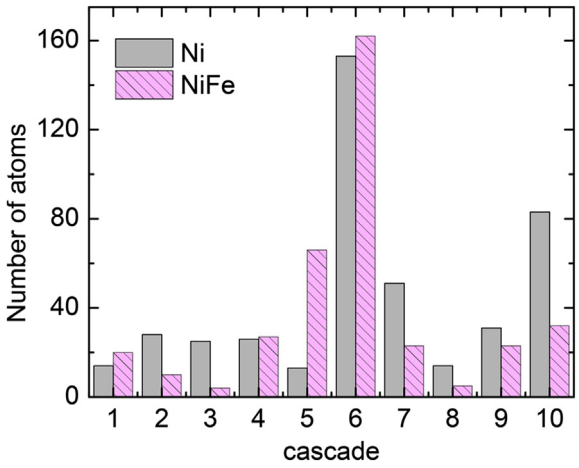

Fig. 3. Number of atoms with velocity higher than the cut-off value at 0.2 ps simulation time in 50 keV Ni ion cascades in Ni and NiFe. For 1 ps activation time, all atoms have velocities smaller than the specified cut-off.

classical MD cascades and cascades where only the electronic stopping are taken into account, the 2T-MD model, which includes the electron-phonon (e-ph) coupling in addition to the electronic stopping, results in a smaller amount of damage and more isolated vacancies and interstitials. In the present paper, we investigate the effect of deactivating the electronic stopping mechanism when the e-ph coupling is turned-on, as well as the effect of the e-ph coupling activation time in the damage production.

For our simulations we use the MD package DL_POLY [17], where the 2T-MD model [10,11] algorithms are incorporated. In the 2T-MD model, as described by Duffy and Rutherford [10,11], the equation of motion used in classical MD simulations is modified (Eq. (1)), and contains a friction term γ_i to include the energy loss to electrons, and a term (stochastic force $\mathbf{F}_i(t)$) to include the energy gain due to interactions with the electrons of the system. The friction term γ_i consists of a term γ_s for the electronic stopping, and a term γ_p to account for the e-ph coupling, which is activated at time t_{eph}.

$$m_i \frac{\partial \mathbf{v}_i}{\partial t} = \mathbf{F}_i(t) - \gamma_i \mathbf{v}_i + \tilde{\mathbf{F}}(t) \tag{1}$$

In our first study case, which we will call Case I, the electronic stopping is activated at the beginning of the simulation, and it is still active when the e-ph coupling is activated at t_{eph}. The electronic stopping is applied only to atoms that move with velocity larger than a specified cut-off value v_c:

$$\gamma_i = \gamma_s + \gamma_p \quad \text{with} \quad \gamma_s = 0 \quad \text{for} \quad v_i \le v_c, \tag{2}$$

where m_i is the mass of atom i with velocity v_i, and the value of v_c corresponds to energy double the cohesive energy of the target system [18]. An atom with velocity corresponding to twice the cohesive energy will travel distance equivalent to the range of the interatomic potential in the time needed for the neighboring atoms to respond to the impulse of the moving atom [10]. Other suggested values for these parameters can be found in Refs. [19–22].

In the second case, which we will refer to as Case II, the electronic stopping, similar to Case I, is activated at the beginning of the simulation and is applied to atoms with velocities larger than v_c, but it is turned-off at t_{eph}, when the e-ph coupling is turned-on:

$$\begin{aligned} &\gamma_i = \gamma_s \ \text{for} \ t < t_{eph} \quad \text{and} \\ &\gamma_i = \gamma_p \ \text{for} \ t \ge t_{eph}, \\ &\text{with} \quad \gamma_s = 0 \ \text{for} \ v_i \le v_c \end{aligned} \tag{3}$$

We additionally investigate the effect of the e-ph activation time in the damage production from 50 keV Ni cascades in Ni and

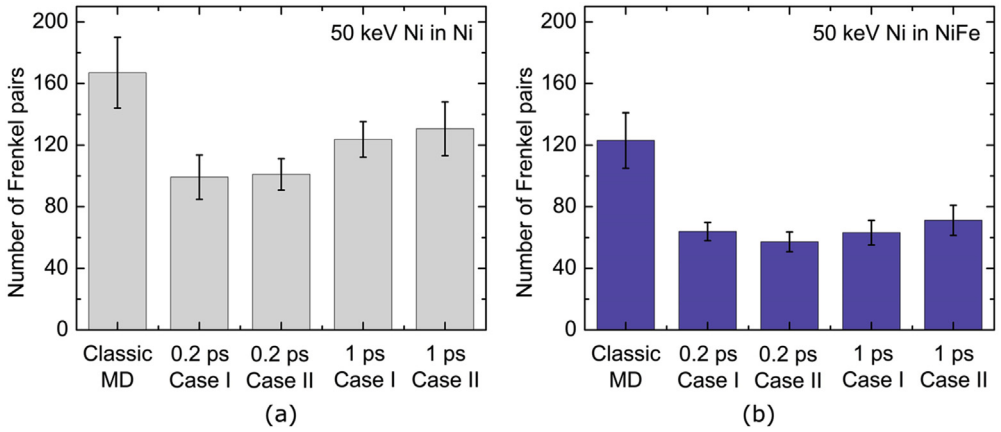

Fig. 2. Average surviving number of defects (Frenkel pairs) at the end of the simulation time for 50 keV Ni cascades in (a) Ni and (b) NiFe. The error bars represent the standard error over ten cascade events. Results for classical MD simulations from Ref. [15] is provided for comparison.