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Effects of electronic excitation on cascade dynamics in nickel–iron and nickel–palladium systems☆

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ABSTRACT

Using molecular dynamics simulations and the two-temperature model, we provide a comparison of the surviving damage from single ion irradiation events in nickel-based alloys, for cascades with and without taking into account the effects of the electronic excitations. We find that including the electronic effects impacts the amount of the resulting damage and the production of isolated defects. Irradiation of nickel–palladium systems results in larger numbers of defects compared to nickel–iron systems, with similar numbers of isolated defects. We additionally investigate the mass effect on the two-temperature model in molecular dynamics simulations of cascades.

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Nickel-based concentrated solid solution alloys consist of two or more metal elements of almost equal concentration, and form single-phase fcc alloys with random site occupancy. Due to their chemical complexity, they exhibit unusual thermal, electric and mechanical properties [1–7], which make them good candidates for nuclear applications, where resistance to radiation is required. It has been shown, both in experiments [8,9] and simulations [10–12], that the compositional differences, with components such as Mn, Cr, Fe, Co and Pd, yield different responses to radiation. The response to radiation includes both the effects of the nuclear energy loss, the energy transfer from the ion to the nuclei of the target material, and the electronic energy loss, the transfer of energy to the electrons. Recent molecular dynamics (MD) [11–13] simulations have shown that the electronic effects in ion irradiation of solid solution alloys with components of similar mass affect both the total defect production and the distribution of defects into clusters.

Most of the possible components listed above, including the base material, Ni, are of similar mass, with Pd being the only species to have a significantly larger mass. In order to investigate the effect of the mass of the components on damage production and cluster formation, we provide here a comparison of the damage produced in nickel–iron and nickel–palladium solid solution alloys. We perform Ni ion cascade simulations where the primary knock-on atom (PKA) has 30 keV or 50 keV energy, with and without the electronic effects in equiatomic NiFe and NiPd, $Ni_{80}Fe_{20}$, and $Ni_{80}Pd_{20}$. Additionally, we investigate the effect of the atomic mass in classical MD and two-temperature (2T-MD) model cascades, by setting the mass of Pd atoms equal to the mass of Fe, leaving the rest of the parameters unchanged, and compare the resulting damage.

In classical MD simulations of irradiation, the electronic effects are not taken into account, and the energy is conserved. When the electronic stopping is considered, energy is lost from the atomic system to the electrons. In the 2T-MD model as described by Duffy and Rutherford [14,15], energy deposited to the electronic system due to the electronic stopping can be retributed to the atomic system, depending on the local temperature difference between the two subsystems. The electronic temperature evolution is described by a heat diffusion equation for the electronic system. The 2T-MD model is described in detail elsewhere [12,16].

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Table 1
2T-MD model parameters for the four systems. v_c is the cut-off velocity, γ_s is the electronic stopping parameter, t_{eph} the e–ph coupling activation time, κ_e the electronic thermal conductivity and g_p the e–ph coupling parameter.

	2T-MD model parameters			
	NiFe	$Ni_{80}Fe_{20}$	NiPd	$Ni_{80}Pd_{20}$
v_c (Å ps^{-1})	54	54	31.5	31
γ_s (ps^{-1})	0.59	0.59	0.52	0.56
t_{eph} (ps)	0.2	0.2	0.1	0.1
κ_e (W m^{-1} K^{-1})	21	46.4	30	43
g_p ($\times 10^{17}$ W m^{-3} K^{-1})	8.78	8.48	16.8	21.1

The irradiation simulations are performed using the DL_POLY [17] MD package, which includes the 2T-MD model [14,15]. We provide a graphical description of the model in Fig. S1 of the Supplementary material. For the nickel–iron systems, we use an embedded atom method (EAM) type potential of Bonny et al. [18], and for the nickel-palladium systems we use the EAM-type potential described in Ref. [19]. The systems are cubic with periodic boundary conditions. The 30 keV cascades were performed in systems consisting of about 2.5 million atoms and the 50 keV cascades in systems consisting of about 3.6 million atoms, to ensure the recoil range is contained within the box. All systems are equilibrated under the constant pressure and temperature ensemble using a 0.001 ps timestep at 300 K prior to irradiation. The PKAs of the 30 keV cascades were chosen to be about 45 Å from the MD box boundaries, while the 50 keV PKAs were about 60 Å from the MD box boundaries. With the box centered at (0, 0, 0), all cascades were initiated near the (−x /2, −y /2, −z /2) corner of the cubic boxes, directed inwards and towards the center. We have applied an 8 Å wide boundary thermostat in all systems for all three irradiation conditions, where the velocities are scaled according to a Gaussian distribution, to prevent energy from re-entering the MD box, mimicking the bulk sample. A variable timestep, which changes in response to the dynamics of the system, is used for the cascade simulations to account for the faster atomic motion at the beginning of the simulation, when the cascade develops, and the gradual slowing down as the system cools at later stages. The cascades were run for about 60–75 ps simulation time, which was achieved within 40,000–60,000 steps, depending on the cascade development and therefore the variable timestep, which initially is started at 0.0125 fs. Four of the 50 keV electronic stopping cascades were complete within 30,000 steps (45 ps simulation time), when the system has already relaxed and the number of defects produced is stable (see stable number of displaced atoms in the example in supplementary material Fig. S2, where it is shown that the relaxation takes place within the first 10 ps), therefore we did not continue them further. The classical MD cascades are performed in the canonical ensemble, and the in-cascade electronic stopping energy is removed from the system via a friction term, calculated with the use of the Stopping and Range of Ions in Matter (SRIM) software [20]. In the 2T-MD model simulations, additionally to the electronic stopping, the electron–phonon (e–ph) interactions are taken into account, as shown in the modified equation of motion (Eq. (1)):

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

where the friction term is $\gamma_i = \gamma_s + \gamma_p$ for $v_i > v_c$ or $\gamma_i = \gamma_p$ for $v_i \leq v_c$, and m_i is the mass of atom i with velocity v_i and v_c is the cut-off velocity with a value corresponding to twice the cohesive energy of the system [21]. The e–ph interactions are activated at time t_{eph}, determined by the thermalization time in the cascades with electronic stopping only.

The electronic temperature evolution is described by the heat diffusion equation:

$$Ce \frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_\alpha) + g_s T'_\alpha, \quad (2)$$

where C_e is the heat capacity, k_e is the electronic thermal conductivity, T_e and T_a are the electronic and atomic temperatures, respectively, and g_s and g_p are the electronic stopping constant and the e–ph coupling constant, respectively. The electronic stopping constant g_s is related to the friction term γ_s via $g_s = 3N' k_B \gamma_s / (\Delta V m)$, where N' is the number of atoms with velocities larger than v_c within a coarse-grained cell with volume ΔV, k_B the Boltzmann constant and m the atom mass. The energy exchange depends on the local temperature difference, as expressed by the second term in the right side of the equation. The third term is the energy exchange due to the electronic stopping mechanism, where T'_α has units of temperature, and is calculated from the average kinetic energy of the subset of atoms that are subject to the electronic stopping, i.e. their velocity is larger than a cut-off value v_c.

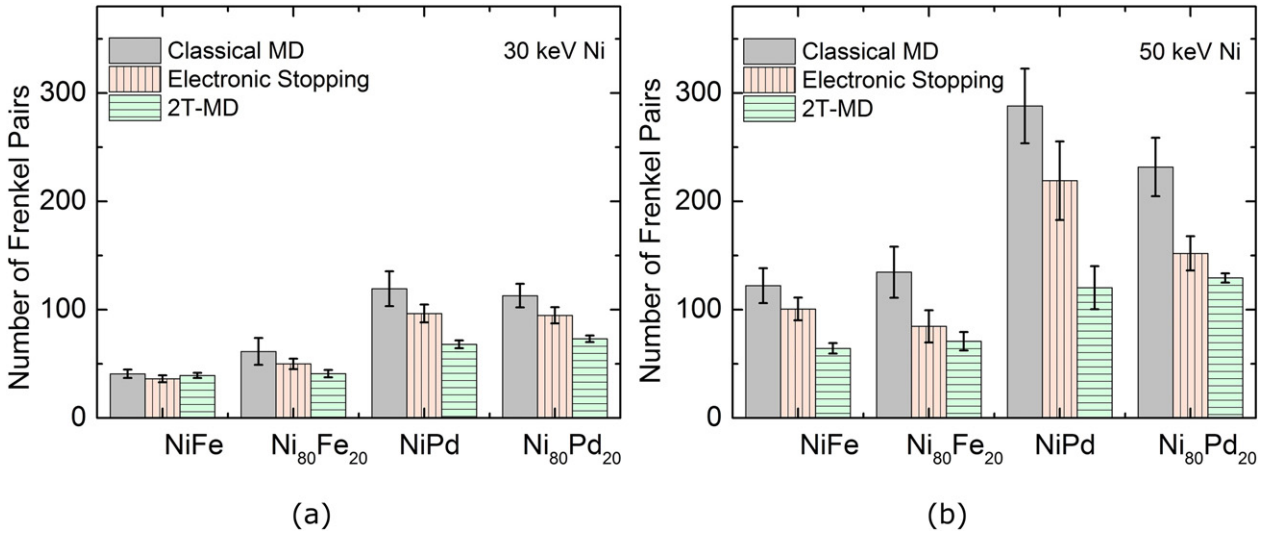

Fig. 1. Average surviving number of defects (Frenkel pairs) for the three irradiation models at the end of the simulation time, for (a) 30 keV and (b) 50 keV Ni ion cascades. The error bars represent the standard error over twelve cascade events for each case.

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