Journal of Alloys and Compounds 700 (2017) 106–112

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Two-temperature model in molecular dynamics simulations of cascades in Ni-based alloys

Eva Zarkadoula [a, *], German Samolyuk [a], William J. Weber [b, a]

[a] Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
[b] Department of Materials Science & Engineering, University of Tennessee, Knoxville, TN 37996, USA

ARTICLE INFO

Article history:
Received 18 October 2016
Received in revised form
22 December 2016
Accepted 31 December 2016
Available online 3 January 2017

Keywords:
Molecular dynamics
Two-temperature model
Electronic effects
Nickel-based alloys
Cascades

ABSTRACT

In high-energy irradiation events, energy from the fast moving ion is transferred to the system via nuclear and electronic energy loss mechanisms. The nuclear energy loss results in the creation of point defects and clusters, while the energy transferred to the electrons results in the creation of high electronic temperatures, which can affect the damage evolution. We perform molecular dynamics simulations of 30 keV and 50 keV Ni ion cascades in nickel-based alloys without and with the electronic effects taken into account. We compare the results of classical molecular dynamics (MD) simulations, where the electronic effects are ignored, with results from simulations that include the electronic stopping only, as well as simulations where both the electronic stopping and the electron-phonon coupling are incorporated, as described by the two temperature model (2T-MD). Our results indicate that the 2T-MD leads to a smaller amount of damage, more isolated defects and smaller defect clusters.

1. Introduction

During irradiation, fast moving particles lose energy both to the atoms of the system and to the electrons. In the low energy regime the electronic energy loss can be considered insignificant, and in the high energy regime most of the energy deposition is to the electrons. In the intermediate energy range, the effects of the electronic excitations are not well understood. While the damage at intermediate energies is primarily due to ballistic processes, which result in the creation of point defects and defect clusters, high electronic temperatures are expected that can affect damage production and evolution. Molecular dynamics (MD) simulations are a tool widely used for cascade modeling, where the main damage mechanisms are the ballistic processes, and have provided valuable information on the primary stages of the damage formation [1–3], which takes place in very short time scales. Generally, and until recently, the electronic excitations are usually not taken into account, or are included partially in the simulations, as a friction term for the electronic stopping. The importance of energy deposition to electrons in radiation damage has been shown over the years [4–8] in efforts to include the electronic effects in MD simulations. Recent studies [9–13] have employed the electronic energy dissipation fully, in terms of both the electronic stopping and the electron-phonon (e-ph) interactions, by implementing the two-temperature model (2T-MD), as described by Duffy and Rutherford [8,14], in MD simulations of high-energy cascades, which have clearly demonstrated that the electronic excitations can affect the cascade evolution.

In the present work, we investigate the effects of the electronic excitations from irradiation of nickel-based concentrated solid solution alloys with the face-centered cubic (fcc) structure. Unlike traditional alloys, these are random solid solutions consisting of two or more fcc or body-centered cubic (bbc) metals, forming single phase alloys. Due to their good thermal, electric and mechanical properties [15–21], single-phase concentrated solid-solution nickel-based alloys are of increasing interest in nuclear energy applications, where high radiation resistance is important. In such applications, the materials interact with highly energetic particles, that transfer energy both to the atomic and the electronic subsystems of the target.

To investigate the response of the materials to the combined action of the nuclear and the electronic energy loss, we perform irradiation simulations both with and without the electronic effects taken into account, and compare the resulting damage. First, we perform classic MD simulations of 30 keV and 50 keV Ni ion cascades in $Ni_{80}Fe_{20}$ (NiFe), $Ni_{80}Cr_{20}$ (NiCr), and $Ni_{40}Fe_{40}Cr_{20}$ (NiFeCr),

* Corresponding author.
E-mail address: zarkadoulae@ornl.gov (E. Zarkadoula).

http://dx.doi.org/10.1016/j.jallcom.2016.12.441
0925-8388/

where the electronic excitations are ignored. Second, we include the electronic stopping in the cascade simulations, but only as a friction term in the equations of motion; and last, we take into account the electron-phonon (e-ph) interactions, in addition to the electronic stopping mechanism, by using the 2T-MD model. By implementing the 2T-MD model for the simulation of irradiation damage in these systems, the electronic energy transport and redistribution to the lattice is included in the simulations, and the materials' electronic properties, such as the electronic thermal conductivity and specific heat capacity, are taken into consideration in the cascade evolution.

2. Methods

For our simulations, we used the MD package DLPOLY [22], where the 2T-MD model is implemented. The 2T-MD describes the energy exchange between the atomic and the electronic subsystems, coupling in this way the atomic properties to the properties of the electronic system. In high irradiation events, energy is transferred from the atomic system to the electronic system due to the inelastic electronic scattering and the interactions of the electrons with the phonons. Depending on the local temperature difference, part of this energy deposited in the electronic system is returned to the atomic system, while another part is diffused via the electrons. This energy transfer between the atomic and the electronic subsystems is expressed via the heat diffusion equation (Eq. (1)), where C_e is the heat capacity, k_e the electronic thermal conductivity, T_e and T_a are the electronic and atomic temperatures, respectively, and g_s and g_p the electronic stopping constant and the e-ph coupling constant, respectively. The second term in the right side represents the energy transfer due to the e-ph interactions, which depends on the local temperature difference, and the third term is the energy exchange due to the electronic stopping mechanism. 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 which corresponds to twice the cohesive energy of the system [23].

$$Ce\frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_\alpha) - g_s T'_\alpha, \quad (1)$$

The constants g_s and g_p are expressed as:

$$g_p = \frac{3Nk_B\gamma_p}{\Delta V m_i} \quad (2)$$

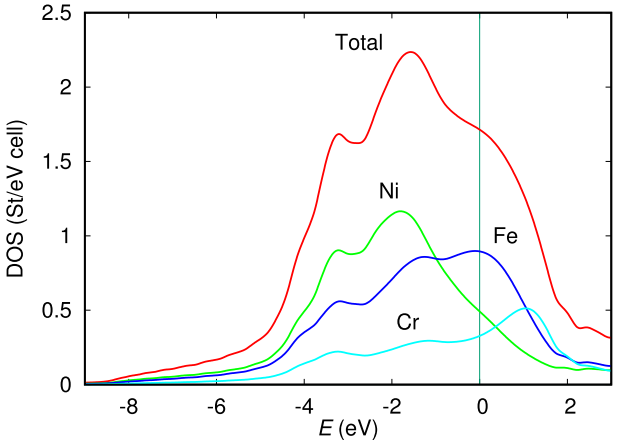

Fig. 1. The total and partial electronic density of states calculated in NiFeCr alloy. The Fermi energy corresponds to zero energy.

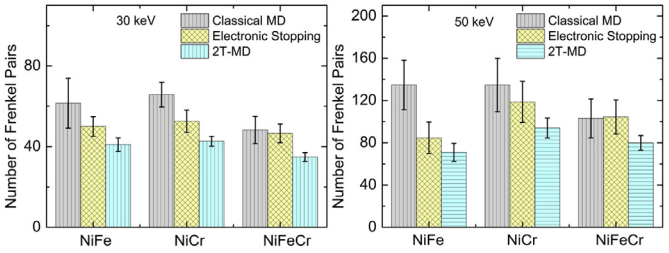

Fig. 2. Average surviving damage at the end of the simulation time for 30 keV (left) and 50 keV (right) Ni cascades in $Ni_{80}Fe_{20}$, $Ni_{80}Cr_{20}$, and $Ni_{40}Fe_{40}Cr_{20}$. Results for classical MD simulations, electronic stopping-only simulations and the 2T-MD model are plotted. The standard error over twelve cascade events is shown.

$$g_s = \frac{3N'k_B\gamma_s}{\Delta V m_i} \quad (3)$$

where m_i is the mass of atom i, N is the number of atoms in a coarse-grained cell of volume ΔV, k_B the Boltzmann constant, and N' the number of atoms with velocities larger than v_c.

In the 2T-MD model, where the electronic effects are taken into account, the simple equation of motion used in the classic MD simulations (Eq. (4)) is modified (Eq. (5)) to include the electronic stopping as a friction term γ_s, a friction term γ_p to account for the e-

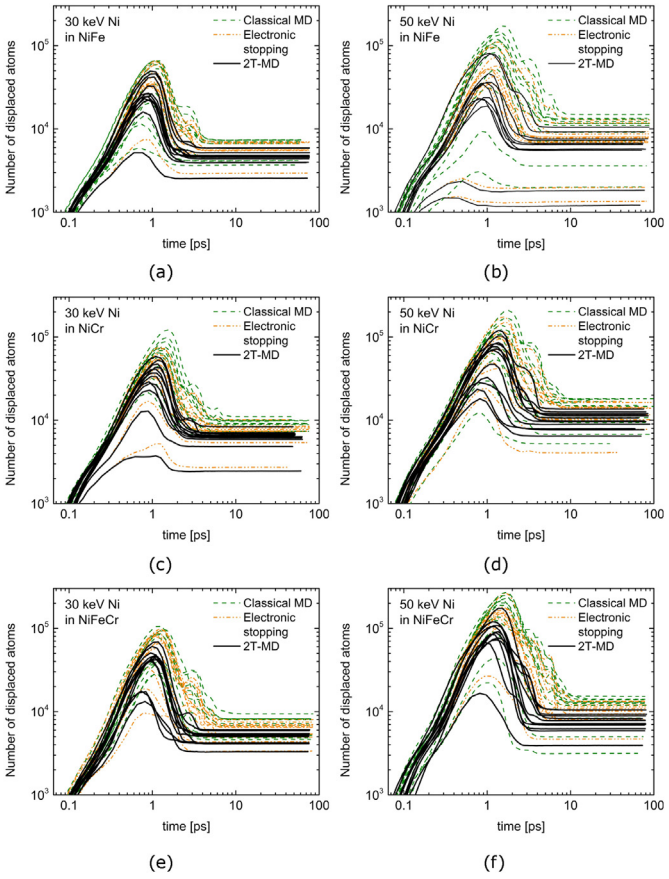

Fig. 3. The evolution of the number of displaced atoms with time for 30 keV and 50 keV Ni cascades in (a)–(b) NiFe, (c)–(d) NiCr, and (e)–(f) NiFeCr. The green dashed lines correspond to classical MD cascades, the orange dotted lines to electronic-stopping-only cascades, and the solid black lines to 2T-MD model cascades. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)