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GeV ion irradiation of NiFe and NiCo: Insights from MD simulations and experiments☆

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ABSTRACT

Concentrated solid solution alloys have attracted rapidly increasing attention due to their potential for designing materials with high tolerance to radiation damage. To tackle the effects of chemical complexity in defect dynamics and radiation response, we present a computational study on swift heavy ion induced effects in Ni and equiatomic Ni -based alloys ($Ni_{50}Fe_{50}$, $Ni_{50}Co_{50}$) using two-temperature molecular dynamics simulations (2T-MD). The electronic heat conductivity in the two-temperature equations is parameterized from the results of first principles electronic structure calculations. A bismuth ion (1.542 GeV) is selected and single impact simulations performed in each target. We study the heat flow in the electronic subsystem and show that alloying Ni with Co or Fe reduces the heat dissipation from the impact by the electronic subsystem. Simulation results suggest no melting or residual damage in pure Ni while a cylindrical region melts along the ion propagation path in the alloys. In $Ni_{50}Co_{50}$ the damage consists of a dislocation loop structure (d = 2 nm) and isolated point defects, while in $Ni_{50}Fe_{50}$, a defect cluster (d = 4 nm) along the ion path is, in addition, formed. The simulation results are supported by atomic-level structural and defect characterizations in bismuth-irradiated Ni and $Ni_{50}Fe_{50}$. The significance of the 2T-MD model is demonstrated by comparing the results to those obtained with an instantaneous energy deposition model without consideration of e-ph interactions in pure Ni and by showing that it leads to a different qualitative behavior.

1. Introduction

A major challenge in materials science is to understand and predict materials behavior when exposed to ion irradiation. To this end classical molecular dynamics (MD) simulations are often used [1–3]. They provide an atomic-level view of the system under ion study, but do not include a description of the electronic subsystem and are, therefore, limited in applicability to events that involve a low or negligible level of electronic excitations and ionizations.

Several approaches have been developed to address this issue. A prominent method among these is the so-called two-temperature molecular dynamics (2T-MD) model. The model assumes the thermalization of the electronic subsystem and charge neutrality. With these simplifications, the energy dissipation in the electronic subsystem and its coupling to the atomic subsystem can be included without the drastic increase of computational cost that follows from an explicit quantum mechanical description of the excited electronic subsystem.

The term swift heavy ion (SHI) is commonly used to describe ions that are heavier than carbon and with a kinetic energy over 0.5–1 MeV per nucleon depending on the atomic mass. SHIs deposit their energy mostly to the electrons along their path before

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the nuclear stopping takes over at the end of the ion range. Resolving the mechanisms of radiation damage by SHIs is a long-standing challenge in the study of ion-matter interactions [4], and the two-temperature approach depicts one possible path forward. According to the model, in metals, the deposited energy can be expected to dissipate effectively in the electronic subsystem due to high electronic thermal conductivity, and cause only a moderate effect. However, the electronic energy loss is known to cause, for example, an anomalous annealing of recoil-induced damage in nickel [5] and damaged structures along the ion path in titanium, i.e. ion tracks that are observable by transmission electron microscopy. They seem to consist of dense dislocation loop networks [6]. In the intermetallic compound Ni–Zr_2, amorphous and quasi-continuous tracks have been reported to form [7]. MD simulations of SHI impacts in metals predict the formation of dislocation loops in Fe and W [8].

Recently, Ni-based single-phase concentrated solid solution alloys (CSAs) have gained interest due to their unique physical properties and dramatically enhanced irradiation performance. Among these CSAs, several have been shown to have less damage accumulation than pure Ni when exposed to ion irradiation within the elastic energy loss regime, at least under room temperature irradiation to a low dose [9,10] and elevated temperature to a high dose [10]. As a general trend, the more chemical disorder exists in CSAs, the better radiation resistance is observed. In this Article, to investigate the effect of the alloy composition and chemical disorder in the electronic stopping regime, we have chosen to study Ni, $Ni_{50}Fe_{50}$ and $Ni_{50}Co_{50}$ using 2T-MD simulations. The ion (1.542 GeV Bi) was selected so that its nuclear stopping power ($dE/dx_{nucl} = \sim 0.1$ keV nm^{-1}) is negligible and the electronic stopping power at its maximum (peak dE/dx_{ele} ranges from 62.28 keV nm^{-1} in $Ni_{50}Fe_{50}$ to 68.85 keV nm^{-1} in Ni), as summarized in Table 1.

In chemically disordered alloys, a stronger effect from the electronic energy loss is expected due to the significantly reduced electron mean free paths (MFPs) compared to pure metals [11]. Therefore, CSAs are ideal systems to test different theoretical approaches for modeling electronic energy loss in metallic targets. It is also noteworthy that the MFPs depend on the alloying elements and concentration, which can be tuned. Moreover, as pointed out in a recent review [11], CSAs hold distinctive links between tunable scattering processes and energy dissipation, as well as unique correlations between modified energy landscapes and various defect dynamic processes.

Besides importance from a fundamental research perspective, the development and study of the 2T-MD model are relevant for a variety of applications. For example, the model has been shown to have an effect on the residual defect concentration after a recoil simulation at an energy regime relevant for fusion reactor wall materials [12]. We note that the effects of high energy ions are also discussed using the Coulomb explosion [13] and other models in which the interatomic forces are significantly modified [4]. The two-temperature approach and its extensions are under active research also in the laser community [14,15].

2. Methods

2.1. The 2T-MD model

The two-temperature model for radiation damage was introduced in the work of Lifshitz, Kaganov and Tanatarov [16,17]. Separate temperatures are assigned to the atomic and electronic subsystems, noted as T_a and T_e, respectively, that evolve according to a heat equation. An additional sink/source term, H, is added to describe the heat absorbed or emitted by the atoms via the electron-phonon coupling. The spatiotemporal evolution of the thermal energy in the electronic subsystem is given by

$$\frac{\partial E_e}{\partial t} = C_e \frac{\partial T_e}{\partial t} = \nabla \cdot (K_e \nabla T_e) + H \quad (1)$$

Here C_e is the electronic heat capacity and K_e the electrical heat conductivity. It is useful and conventional to write $H = G(T_a - T_e)$ since, in a high-temperature approximation, H is directly proportional to the temperature difference and G is, therefore, a constant. In general, G, as well as the rest of the parameters, depend on the electronic and atomic temperature. An often-used practice, which we adopt here, is to consider the electronic temperature dependence of all the parameters only, since the values depend more on T_e than T_a. In the original formulation of the model, accompanied by Eq. (1), there is another heat diffusion equation for the atomic subsystem. Here the 2T-MD model is a compelling alternative and uses molecular dynamics instead. The interaction potential of MD describes e.g. mass transport, pressure waves, superheating and coupling between the optical and acoustic phonon modes [14]. Thereby the number of poorly characterized parameters is substantially reduced.

To connect equation (1) to a MD simulation, the simulation space is divided into small cells, so that equation (1) can be solved on a Cartesian grid. Within each cell, an atomic temperature is calculated from the kinetic energies of atoms. Each cell is assigned an electronic temperature that is evolved by a finite difference (FD) solution of Eq. (1). To represent the energy exchange via e-ph interactions, the MD equation of motion is complemented with a thermostatting term that can add kinetic energy to the atoms or remove it. Several adaptations of the term can be found in the literature (see Supplementary material for more discussion). We use here a simplified version of the one presented in Ref. [18] that has been implemented in the PARCAS simulation code [19,20]. The heat is exchanged in accordance with equation (1) by a damping force in the MD equations of motion [21].

$$F_i = -\nabla V(\{\bar{r}_i\}) + \xi m_i \bar{v}_i$$

The magnitude of ξ is chosen so that the increase in kinetic energy per MD time step corresponds to HV_{cell}, where V_{cell} is the volume of the finite difference grid cell used to solve equation (1). m_i is the mass of the i:th ion, $\bar{r}_i$ the position and $\bar{v}_i$ the velocity. V is the interatomic potential (in this work, given by Ref. [22]). By taking the derivative of the kinetic energy of the atoms within a cell, it follows that [18].

Table 1
Experimentally-determined densities and SRIM-predicted stopping powers and ion ranges for 1.542 GeV Bi ions in Ni and Ni alloys.

Crystal	Density (g/cm^3)	Density (MD simulation, g/cm^3)	Electronic stopping power (keV/nm)	Nuclear stopping power (keV/nm)	Ion range (μm)
Ni	8.908	8.84	68.8	0.128	28.26
$Ni_{50}Co_{50}$	8.8484	8.75	66.6	0.122	28.96
$Ni_{50}Fe_{50}$	8.2326	8.28	62.8	0.113	30.49