Acta Materialia 116 (2016) 136–142

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

The effect of alloying nickel with iron on the supersonic ballistic stage of high energy displacement cascades

Laurent Karim Béland*, Yuri N. Osetsky, Roger E. Stoller

Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6138, USA

ARTICLE INFO

Article history:
Received 13 April 2016
Received in revised form
8 June 2016
Accepted 14 June 2016

Keywords:
Radiation damage
Nickel
Nickel-iron
Molecular dynamics
High-entropy alloys

ABSTRACT

Previous experimental and theoretical studies suggest that the production of extended defect structures by collision cascades is inhibited in equiatomic NiFe, in comparison to pure Ni. It is also known that the production of such extend defect structures results from the formation of subcascades by high-energy recoils and their subsequent interaction. A detailed analysis of the ballistics of 40 keV cascades in Ni and NiFe is performed to identify the formation of such subcascades and to assess their spatial distribution. It is found that subcascades in Ni and NiFe are created with nearly identical energies and distributed similarly in space. This suggests that the differences in production of extended defect structures is not related to processes taking place in the ballistic phase of the collision cascade. These results can be generalized to other, more chemically complex, concentrated alloys where the elements have similar atomic numbers, such as many high-entropy alloys.

1. Introduction

The study of radiation damage in Ni-based alloys is relevant because they act as a good model system for the austenitic stainless steels that are broadly used nuclear power applications. While it is well known that the microstructure of post-irradiation alloys critically depends on composition, many of the physical underpinnings of these different responses are still a mystery, which often leads to somewhat *ad hoc* material design rules. Recently, concentrated single-phase alloys, also known as high-entropy alloys, were proposed as potentially radiation-tolerant materials [1,2]. These alloys possess a simple face centered cubic structure (fcc), but are made of several principle elements (such as NiFeCoCrMn), in contrast with conventional alloys that typically contain only one principle component. This high chemical complexity was shown to reduce electronic [2,3] and phonon [4] mean free paths, as well as slow down defect mobility [5,6]. While these properties are known to be important for radiation damage evolution, the mechanisms that explain energy dissipation and defect production in these systems remain largely unexplored.

An important aspect of radiation response and damage accumulation is related to primary damage production. Investigation of such damage production is typically done by simulating the collision cascades produced by primary knock-ons atoms (PKAs) of high-energy particules. Such molecular dynamics studies are now practically routine. Their results are usually characterized in three main dimensions: number of defects produced, distribution defect cluster (size, composition and number) and order/disorder transitions. In the case of concentrated alloys, notable investigations have focused on NiAl [7–9] and NiAg [10] alloys, which tend to amorphize under such conditions, CuAu [10], and $Fe_{90}Cr_{10}$ [11–13], which is of interest for next-generation power plants. The latter case has shown little differences in defect production and defect cluster size. In contrast with the FeCr case, recent studies in concentrated solid solutions (NiFe [13,14,2,15,16], NiCr [16], NiCo [2,15], and NiCoCr [17]) indicate that such alloying has an important effect on both the number of stable defect produced and the distribution of defect clusters. Understanding the physical processes dictating the radiation response in these materials is an important step towards a better understanding of the high-entropy alloys that are composed of the same elements as these binary and ternary alloys.

For example, in the case of equiatomic NiFe and NiCo alloys [15], it was found that, for PKA energy of 20 keV or less, damage reduction can be explained by the energetics of short-range interatomic interactions and by reduced thermal conductivity [4,2], in comparison to pure Ni. Stiffer short-range interactions in the alloys, relative to pure Ni, lead to less damage formation during the

* Corresponding author.
E-mail address: belandlk@ornl.gov (L.K. Béland).

http://dx.doi.org/10.1016/j.actamat.2016.06.031
1359-6454/

supersonic stage of the collision cascade. Low thermal conductivity in the alloys, relative to pure Ni, extends the lifetime of the thermally enhanced recovery stage, which favors the self-annihilation of defects. However, it was found that these mechanisms cannot explain primary damage reduction at higher PKA energies, e.g. at 40 keV. These higher energies are of particular importance since they directly generate extended defect structures such as stacking fault tetrahedra and dislocations loops that are difficult to explain by classical nucleation mechanisms driven by point defect aggregation. These larger defects are significant because of their prominent role in radiation-induced microstructural evolution and mechanical property changes [18].

In this article, the differences in primary defect production in Ni and NiFe at 40 keV is investigated in further detail. A review of the current state of knowledge is presented, which highlights the importance of the formation and interactions of subcascades. Such subcascades are then identified and characterized in both materials. A careful comparison is performed and discussed.

2. A brief review

2.1. Three phases of collision cascade

Collision cascades have historically been divided in two stages, the ballistic stage and a thermally enhanced recovery stage [20]. More recently, a careful analysis indicated that the ballistic stage can be further split into a supersonic and a sonic phase [19]. These can be identified by a change in slope of a logarithmic time-profile of the number of Frenkel pairs (N_{FP}) during a cascade, as illustrated in Fig. 1.

High-energy recoils involving kinetic energies larger than the displacement threshold take place during the first stage, i.e. the supersonic phase. As evidenced in Refs. [19,21], these recoils lead to concerted motion of atoms. Low-density pockets of atoms are formed, surrounded by a high-density, supersonic pressure wave, involving pressures of the order of tens of GPa. A few hypersonic recoils will escape the pressure wave, eventually creating their own low-pressure pockets (i.e. subcascades). The supersonic shockwave creates permanent defects along its trajectory, given the high kinetic energies and pressures involved. It was also shown that the

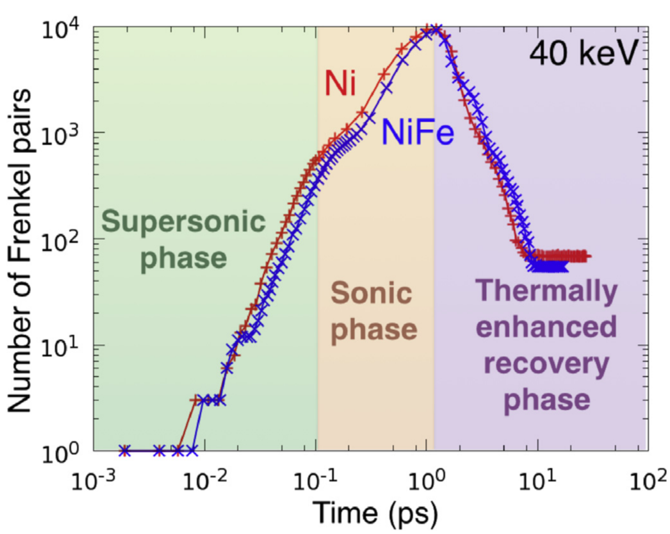

Fig. 1. Typical time profiles of the number of defects during 40 keV cascades in Ni and NiFe. The three stages of the cascade [19] are illustrated by the background colour. Notice the change in the log-log slope at 0.1 ps. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

interaction of these subcascades leads to the formation of extended defects (see sub Section 2.3 for more details).

As the supersonic shockwave propagates and is attenuated, the kinetic energy of the fastest atoms in the system will become lower than the displacement threshold energy. This corresponds to the moment the shockwave enters the sonic regime. In other words, the atoms no longer have enough energy to knock their neighbors permanently out of position after this point in time. In that sense, the supersonic shockwave is a destructive wave, while the sonic wave is non-destructive. In a previous account of cascades in Ni and Ni-alloys [15], the N_{FP} at this supersonic-sonic transition point (or transonic N_{FP}) was averaged over several dozens of runs. Naturally, this quantity is roughly proportional to cascade energy $E^{cascade}$. More interestingly, it was found that each material had its own characteristic transonic $N_{FP}/E^{cascade}$. Furthermore, the average number of stable FP found in a given material and a given PKA energy is proportional to its average transonic N_{FP}. This relationship is especially strong for PKA energy lesser than 20 keV. This evidence is consistent with the idea that permanent displacements are created during the supersonic stage and that they are no longer created after the supersonic-sonic transition.

It should also be noted that the relationship between transonic N_{FP} and the stable N_{FP} breaks down for PKA energies larger than 20 keV [15,22]. This observation is unexplained and is the focus of the current study. It is known that at these energies, fragmentation and subcascade formation becomes important. This is a complex fractal process, that has profound consequences on primary damage production [23–25].

The second stage corresponds to the sonic shock propagation. While no new permanent defects are created, many elastic displacements are created, which register as a large spike in the number of FP, as identified by atomic displacements or Wigner-Seitz analysis (e.g. around 1 ps in Fig. 1). This process is reversible and does not increase the number of miscoordinated atoms. The time-profile of N_{FP} can take different shapes in the sonic phase, that depend on the details of the classical potential at hand [20,15]. Once again, the displacements caused by this sonic shockwave are transient, corresponding to elastic shifts of atoms that eventually recover their original positions. Nonetheless, these elastic shockwaves may have other effects. They may interact with the preexisting microstructure and influence its evolution. Likewise, they may displace defect precursors created by the supersonic shockwave and thus influence extended defect formation. Also, during the sonic stage, which lasts nearly 1 ps, atoms and defect precursors inside the sphere formed by the shockfront evolve rapidly, given the high temperatures (thousands of Kelvins) near the center of the subcascades. This leads to both aggregation and recombination of defects.

A rapid decrease of N_{FP} is observed during the third stage, i.e. the thermally enhanced recovery. The system recovers from the elastic displacements created during the sonic stage and the cores of the subcascades cool down and densify. The center of the subcascades core, which are initially in a liquid-like state (i.e. are miscoordinated), recrystallize. Depending on thermal conductivities, temperatures at the center of the subcascade cores remain over 1000 K for a few ps to more than 10 ps. This can be especially long in concentrated alloys, where lattice and electronic thermal conductivities can be quite low [4,2,15,26]. At these elevated temperatures, coarsening and annihilation of defects and defect precursors is quite important. This influences both the magnitude of defect production and the nature of the defects.

2.2. The supersonic to sonic transition and the importance of short-range interatomic interactions

In another study [21], it was found that the transonic $N_{FP}/E^{cascade}$