Scripta Materialia 154 (2018) 25–29

Contents lists available at ScienceDirect

Scripta Materialia

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

Regular article

Dislocation-assisted linear complexion formation driven by segregation

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ARTICLE INFO

Article history:
Received 12 April 2018
Received in revised form 9 May 2018
Accepted 10 May 2018
Available online xxxx

Keywords:
Complexions
Dislocations
Segregation
Precipitation

ABSTRACT

Atomistic simulations are used to study linear complexion formation at dislocations in a body-centered cubic Fe-Ni alloy. Driven by Ni segregation, precipitation of the metastable B2-FeNi and stable $L1_0$-FeNi phases occurs along the compression side of edge dislocations. If the Ni segregation is not intense enough to ensure precipitate growth and coalescence along the dislocation lines, linear complexions in the form of stable nanoscale precipitate arrays are observed. Critical conditions such as global composition and temperature are defined for both linear complexion formation and dislocation-assisted precipitation.

Thermodynamically-stable grain boundary structures, known as *complexions*, have been intensively studied in recent years because of their significant impact on the mechanical [1,2] and transport [3] properties of both coarse-grained and nanocrystalline materials [4–6], as well as thermal stability [7,8]. Often formed due to dopant segregation, grain boundary complexions behave as equilibrium "phase-like" structures and can experience something similar to phase transitions, changing their type with respect to the system's temperature and composition [7,9]. Nevertheless, such complexions exist only in the form of the planar structural defects, requiring the surrounding bulk to be in equilibrium.

Extending the concept of interfacial complexions to one-dimensional defects, or *linear complexions*, Kuzmina et al. [10] reported chemical and structural states confined at dislocations in a bcc Fe-9 at.% Mn alloy. These authors demonstrated that the structure and composition of these linear complexions correspond to an fcc Fe-Mn austenite structure. The phenomenon that Kuzmina et al. observed was heterogeneous second phase precipitation, caused by the local stress field and compositional inhomogeneity around the dislocations. Similar types of phenomena have been investigated both theoretically [11–15] and experimentally [16–19] in earlier studies as well. A theoretical investigation by Cahn [11] applied equilibrium thermodynamics to determine how the system's general characteristics such as Burger vector and supersaturation affect heterogeneous nucleation on dislocations. Recent theoretical works on this topic have used phase-field [14,15] and kinetic Monte Carlo [12,13] methods to investigate the kinetics of the nucleation, growth, and coalescence of a second phase. Nevertheless, the large number of empirical parameters that are needed limits the applicability of such models, providing only a qualitative agreement with experimental results. On the other hand, systematic experimental investigations have also been restricted due to the small size of precipitates formed along the dislocation lines and only a limited number of the binary and ternary alloy systems such as Al-Li [16], Al-Cu [17], Al-Ag-Cu [18], α-Fe-Nb-C [19] have been studied. These studies reported heterogeneous nucleation of precipitate arrays along the dislocation lines, which competes with homogeneous nucleation inside the grain to influence the final microstructure. The control of second-phase precipitation is extremely important for improving thermal stability (Zener pinning) [20,21] and precipitation hardening [22,23]. The linear complexions found by Kuzmina et al. [10] existed as arrays of stable nanoscale-size precipitates, which could potentially improve both the thermal stability and the strength of polycrystalline alloys. As a whole though, questions remain about how to control the process of second-phase precipitation and complexion formation on dislocations.

In this work, we report on atomistic simulations of segregation-induced formation of the intermetallic linear complexions confined at edge dislocations, using α-Fe doped with Ni. The metastable B2-FeNi intermetallic phase is first formed on dislocations and then partially transformed to the stable $L1_0$-FeNi intermetallic compound. It is important to note that this B2 phase is very small, meaning it would likely be invisible to electron diffraction techniques such as those used in Ref. [10]. This highlights the utility of atomistic simulations to identify nanoscale details of complexion transformations. Nucleation of the $L1_0$-FeNi phase on dislocations occurs for a wide range of the global compositions and annealing temperatures outside of the two-phase coexistence region on the equilibrium Fe-Ni phase diagram. For some of these compositions and temperatures, homogeneous nucleation is thermodynamically-restricted and the final microstructure is determined by

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https://doi.org/10.1016/j.scriptamat.2018.05.014
1359-6462/

dislocation-assisted precipitation, being limited by the amount of dopant segregation. For other cases, the solute segregation is strong enough to form large, bulk-like precipitates at the dislocations. Finally, if a balance is reached, true linear complexions in the form of nanoscale precipitate arrays can be formed along the dislocation lines.

Atomistic simulations were carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software package [24] and an embedded-atom method (EAM) interatomic potential for the Fe-Ni system [25]. The samples were equilibrated with a hybrid Monte Carlo (MC)/Molecular Dynamics (MD) method, in which every MC step was followed by an MD equilibration over 100 integration steps of 1 fs each. MC steps were performed in the variance-constrained semi-grand canonical ensemble using a parallel algorithm developed by Sadigh et al. [26], which allows the system to reach the thermodynamic equilibrium state relatively quickly for a given composition and temperature. Semi-grand canonical ensemble is well-suited to explore phase transformations in multicomponent crystalline solids [26,27], while it is also commonly used to investigate the formation of grain boundary complexions [7,9]. In turn, MD steps were performed in an isothermal-isobaric ensemble at zero pressure, allowing the system to relax the local strain variations associated with solute segregation and phase transformations. A convergence criteria was used that requires the absolute value of the potential energy gradient over the final 20 ps to be less than 1 eV/ps. When this value is reached, the simulation cell has reached an equilibrium configuration and no major structural changes would be observed after this point. The equilibrium atomic structures were analyzed by polyhedral template matching (PTM) [28] and visualized with the OVITO software [29]. In all atomic snapshots, atoms were colored according to their crystal structure: violet – bcc Fe-Ni solid solution, green – $L1_0$-FeNi, red – B2-FeNi. The position of the dislocation core was determined by the dislocation extraction algorithm (DXA) [30] as implemented in OVITO.

A bcc Fe single crystal with one positive and one negative edge dislocation was first created, as shown in Fig. 1(a). The edge dislocations were inserted by (1) removing one-half of the YZ atomic plane in the center of a sample and (2) equilibrating the system using molecular statics at zero pressure. Two types of simulation cells, "long" and "short" in terms of dimensions in the Z-direction, were considered. Both cells had dimensions of 23 nm and 24 nm in the X- and Y-directions, respectively. The dimensions of the Z-direction were equal to 75 nm and 7.5 nm for the long and short cells, respectively. The long samples equilibrated at 500 K were used to qualitatively characterize all aspects of the second-phase precipitation along the dislocation lines. Compositions in a range from 1 to 4 at.% Ni were considered. Because the long samples were computationally expensive, the short samples were used for more systematic studies over a broader range of global compositions (1–7 at.% Ni) and temperatures (300–800 K).

First, we investigated how a gradual increase in dopant concentration affects the structure of the long samples at 500 K. At global compositions below ~2 at.% Ni, the dopant atoms segregate to the compression

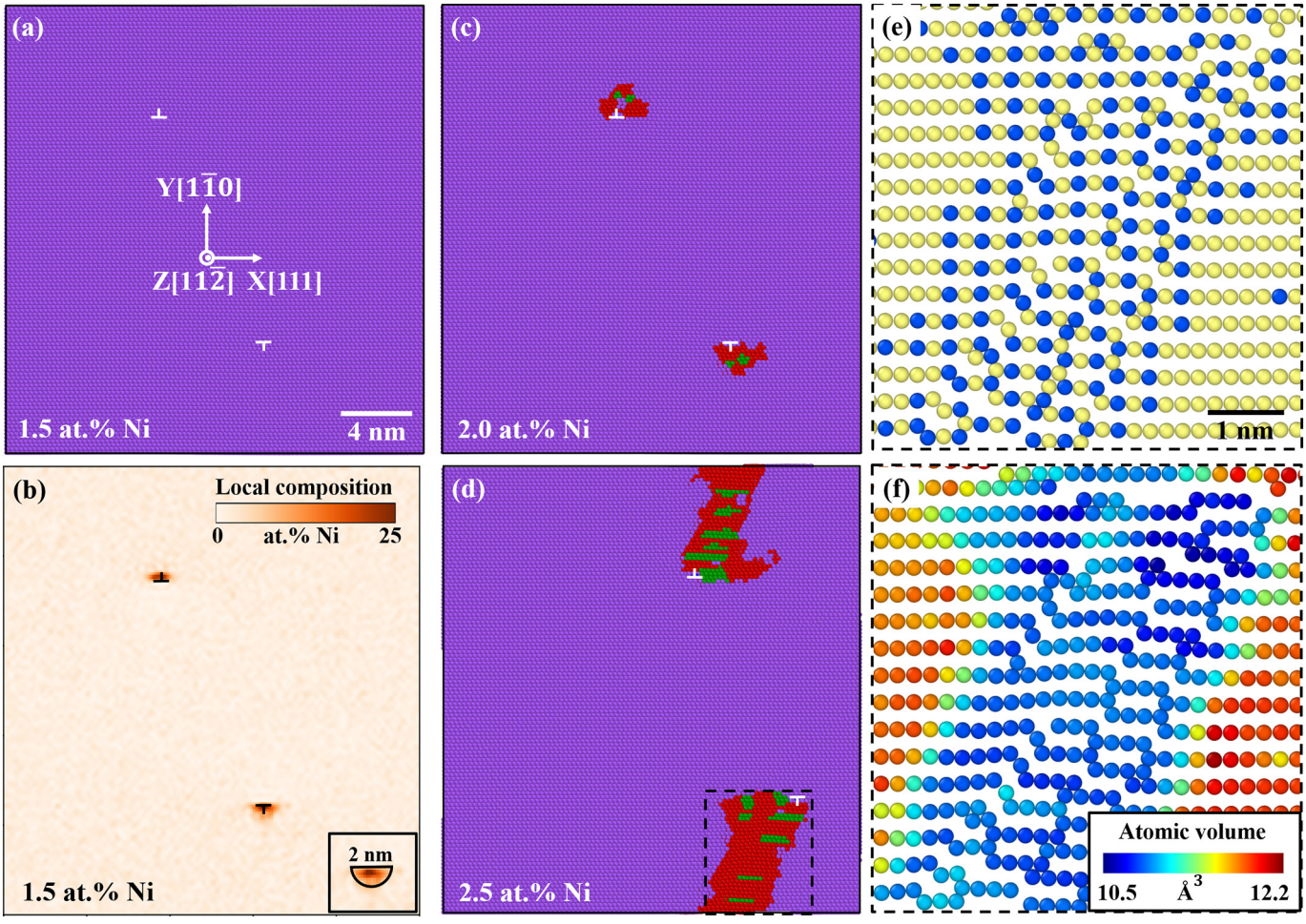

Fig. 1. (a) View along the XY plane of the long simulation cell with two dislocations containing 1.5 at.% Ni and equilibrated at 500 K, as well as (b) the corresponding composition distribution. The small box at the right bottom corner of (b) shows the zone of intensive dopant segregation on the compression side of the lower dislocation. The B2 + $L1_0$ phase precipitation is shown for the long samples with (c) 2.0 at.% Ni and (d) 2.5 at.% Ni at 500 K. Atoms in (a)–(d) are colored according to their alloy type: violet – bcc Fe-Ni solid solution, green – $L1_0$-FeNi, red – B2-FeNi. A slice along one atomic plane, limited to the dashed box in (d), is shown in (e, f). In these images, the atoms are colored according to (e) atom type (yellow – Fe, blue – Ni) and (f) atomic volume. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)