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Misfit dislocation networks in semi-coherent miscible phase boundaries: An example for U–Zr interfaces

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ABSTRACT

Semi-coherent cube-on-cube miscible U–Zr interfaces were studied using molecular dynamics simulations. The misfit accommodation of such semi-coherent phase boundaries was characterized by a two-dimensional dislocation network model utilizing a combination of theoretical predictions and analysis of the atomic system. The dislocation networks were discussed for various stacking orientation of the adjoining phases in terms of the composition of the dislocation sets, the partitioning between edge and screw components and the associated residual elastic fields. These analyses showed that the patterning of the network of dislocations forming these phase boundaries results from the competition between a structurally-driven process (i.e., function of the lattice misfit) and a chemically-driven process (i.e., due to the miscibility between U and Zr).

1. Introduction

The structure and properties of heterophase boundaries (also referred to as phase boundaries) are important microstructural factors controlling the formation, morphology and stability of multiphase metallic alloys [1,2]. The nature of such interfaces in terms of coherency (coherent, semi-coherent or incoherent) is classically characterized by the lattice mismatch between both phases $\epsilon^{m,S} = 2\frac{\ell_\alpha - \ell_\beta}{\ell_\alpha + \ell_\beta}$ (ℓ_α and ℓ_β representing the lattice constants of each phase α and β), resulting in the formation of interfacial defects such as dislocation networks [3]. The state of interfacial coherency depends not only on the physical and the chemical natures between both phases, but also on external factor such as the temperature or the stress field. For a coherent phase boundary, the mismatch is completely accommodated by straining both phases. In the case of a semi-coherent phase boundary, localized misfit dislocation networks are responsible for compensating uniform far-field elastic fields, while an incoherent phase boundary is the result of two rigid semi-infinite media in rigid contact [3,4]. In the general case where one phase precipitates from the other and the two host metallic elements are (at least partially) mutually miscible, it is unlikely that the phase boundaries will be incoherent. If the interface is coherent, thermodynamic properties of the individual phases generally draw more interest than the interface and are well studied by researchers [5,6]. Additionally, incoherent and semi-coherent boundaries between immiscible metals have attracted significant attention owing to the development of engineered multilayered materials [7–10] for improved strength, toughness and radiation resistance.

From a theoretical standpoint, the characterization of the structure of interfaces in terms of dislocation network and the nature of those dislocations is commonly performed through the analysis of the geometrical compatibility and/or the elastic distortion near the interface. Thus, the Frank-Bilby formalism [11–13] is a widely used approach to determine the intrinsic dislocation content of a general boundary. Extensions of this classical formalism have been proposed to account for anisotropic elasticity or the elastic relaxations from the in-plane dislocation configurations [14,15]. Alternatively, interphase boundaries have also been extensively examined through the use of atomistic simulations. The objectives of such computational studies differ from theoretical ones', as they center not only on the interfacial defect structures [8,16], but also on additional thermodynamic and kinetic properties of the interface [7,10,17]. Analysis techniques such as disregistry [13,16] or the Dislocation Extraction Algorithm (DXA) [18–21] are now frequently used to analyze and quantify interfacial dislocation networks. The materials systems studied are commonly interfaces between immiscible metal solids such as Cu–Nb [8,10] or Ag–Ni [1,22], for example.

In comparison, incoherent and semi-coherent phase boundaries between miscible materials are more commonly encountered in structural materials but less studied. Buried in the bulk, such interfaces are not easily amenable to surface characterization probes.

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Thermodynamic, kinetic and physical properties of the individual phases warrant and attract significant attention. However, these types of phase boundaries between two miscible phases play an important role in determining key properties such as interphase decohesion, crack propagation, or interfacial solute segregation. An illustration of such interfaces can be found in U–Zr binary alloys which exhibit a tendency to phase separate into U-rich and Zr-rich precipitates. Depending on alloy compositions as well as heat treating/cooling conditions, complex interfacial features such as lamellar, acicular and Widmanstätten microstructures can be observed [23–25]. Both U and Zr have non cubic native structures at room temperature (orthorhombic and hexagonal) and transform to the cubic bcc structure at higher temperatures. Within this temperature regime, the two metals form a bcc solid solution which upon cooling leads to a high temperature miscibility gap in which both bcc phases (γ-U and β-Zr co-exist). With lattice constants $\ell_U = 3.442$ Å and $\ell_{Zr} = 3.553$ Å, the natural lattice mismatch $\epsilon_{U/Zr} = 0.0317$. It is expected that the U–Zr interface will be semi-coherent with the lattice mismatch being accommodated by misfit dislocations. Previous investigations into this alloy system have focused primarily on the structure and properties of the bulk phases as a function of the alloy composition and on thermodynamically driven phase formation [26,27]. Interphase boundaries in U–Zr alloys, however, have received little to no attention so far. Neither U nor Zr lends itself easily to atomistic study or experimental observation and the alloy system described above presents a rich variety of interfacial configurations. Before venturing into studying boundaries between the complex crystal structures, we can investigate an extreme bound of these phase boundaries, namely cube-on-cube U–Zr interface boundaries. Such a set of boundaries may exist in the miscibility gap (albeit with some mutual solubility) and are also precursors of the phase separation into the intermetallic δ and the orthorhombic α phases. Unlike in immiscible boundaries, the competition between elastic interfacial interactions due to misfit dislocations and chemical interactions due to the miscibility plays a crucial role in the formation and stability of dislocation networks in miscible semi-coherent interfaces and the associated interfacial properties.

In what follows, the non-uniform dislocation structure of miscible semi-coherent bcc/bcc U–Zr interfaces is systematically characterized using atomistic simulations. Misfit dislocation networks and their characters are investigated as functions of various interfacial misfit strains and surface orientations. Section 2 describes details of the atomistic simulation and methods used to characterize the interface dislocation structure. Section 3 provides a description of the misfit dislocation patterning characteristics for the various stacking orientations and misfit strains explored. Section 4, concludes this study with a discussion of the miscible interface properties, with a particular emphasis on the respective contributions from the dislocation–dislocation elastic interactions on one hand and chemical interactions due to the miscibility between U and Zr on the other.

2. Methodology

2.1. Atomistic modeling of semi-coherent U–Zr interfaces

The atomistic simulation code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator [28]) was used to generate and configure the relaxed atomistic configurations of semi-coherent U–Zr phase boundaries. In this work, the Modified Embedded Atom Method (MEAM) interatomic potential developed by Moore et al. [26] for U–Zr alloys was employed to describe interatomic interactions in the vicinity of U–Zr interfaces. This interatomic potential has been developed for simulating γ-U–Zr alloy phase, and considered the anisotropic bonding at the rigid bi-crystalline interfaces. As the basis for this study, the optimized, relaxed structures of pure bcc U and pure bcc Zr were first obtained using bulk molecular static simulations. The resulting lattice constants and per-atom bulk energy were calculated to be $\ell_U = 3.442$ Å, $E_U^{bulk} = -5.287$ eV and $\ell_{Zr} = 3.535$ Å, $E_{Zr}^{bulk} = -6.2$ eV respectively. These properties were fairly consistent with other first principle simulation results, and closely matched experiment data with $\ell_U^{exp} = 3.198$ Å [29] and $\ell_{Zr}^{exp} = 3.574$ Å [30]. As evident by the proximity of the lattice constants ℓ_U and ℓ_{Zr}, the two pure bcc phases share highly similar structures. Such similarity in lattice constants eliminates most incoherent interfaces, which are highly disordered interfaces and thermodynamically unfavorable. The two remaining types are the coherent interface and the semi-coherent interface. The former results from distributed intra-phase strains, creating perfect lattice match; the latter accommodates the lattice mismatches in forms of periodic localized dislocations. Comparably, the dislocation features affect the interfacial characteristics far more prominently, hence the main focus of the study is on the semi-coherent interfaces.

Various stacking orientations were considered within the atomistic simulations based on the most energetically favorable cube-on-cube interfaces between U and Zr, namely only the {001}, {110}, {111} and {112} boundary planes. For each of these orientations, various interfacial structural mismatches were considered by varying the overlap between the surface lattice vectors of each phase during the matching process between both materials. Within the atomistic model, the structural mismatch $\epsilon^{m,S}$ is classically defined as $\epsilon^{m,S} = 2\frac{m\ell_U - n\ell_{Zr}}{m\ell_U + n\ell_{Zr}}$ [4,31], where (m, n) are scaling factors (integers) corresponding to lattice multiplicities of their respective ensemble. Considering the lattice size difference between U and Zr, the scaling factors were chosen such that $m > n$, with the extra lattices residing exclusively in the smaller U lattice. A 5% mismatch upper limit was also imposed on the scaling factor selection to improve the natural viability of the interfaces. The mismatched ensemble lattices selected for simulations range from 2.4% ($m = 20$, $n = 19$) to 5.3% ($m = 13$, $n = 12$) depending on the combination of the scaling factors (m, n).

Simulation setups are typical of semi-rigid bi-crystalline contact interfaces. To accommodate the lattice misfit and achieve commensurability in the contact planes, one lattice was isotropically stretched/deformed by $\epsilon^{m,S}$ to match dimensions of the adjoining other lattice. Deformations in this study were imposed on the Zr supercells due their lower scaling factor n, where edge dislocations would be absent. Periodic boundary conditions were applied to the simulation cell in all directions, matching the periodic nature of the semi-coherent interface structures. The periodic boundary condition also generated a secondary stacking interface in the transverse direction. To minimize any interface-interface interactions, each initial ensemble was constructed with a minimum height of ≈ 100 Å.

To generate variations in the initial interfacial structures, the Γ-surface technique [10,32] was adopted. Stacking variations were created by incremental displacements of one superlattice relative to the other in the interfacial plane. The process is typically arduous due to the small displacement increments (1 Å) need to cover the superlattice surface. Fortunately for systems of misfit interface, due to the repeating nature of both superlattices, the number of unique stacking variations is greatly reduced. Accordingly, the displacement shifts were conducted over a 5×5 grid across a single lattice surface with increments between 0.7 Å and 1.2 Å, generating 25 structural variants per orientation.

Following the construction of each interface, molecular statics simulations were performed to generate the energy-optimized interfacial structures. An isobaric-isothermal (NPT) ensemble with a zero pressure constraint was applied to each system to allow strain redistribution and dislocation formation. Energy minimization was conducted over maximum 200, 000 iterations using the Conjugate Gradient (CG) algorithm; energy and force convergence were set to 10^{-15}.

2.2. Characterization of interface dislocation structure

The characterization of networks of misfit dislocations was accomplished using an atomistic computational algorithm that identifies all