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Atomistic simulations of dislocations in a model BCC multicomponent concentrated solid solution alloy

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ABSTRACT

Molecular statics and molecular dynamics simulations are presented for the structure and glide motion of a/2⟨111⟩ dislocations in a randomly-distributed model-BCC $Co_{16.67}Fe_{36.67}Ni_{16.67}Ti_{30}$ alloy. Core structure variations along an individual dislocation line are found for a/2⟨111⟩ screw and edge dislocations. One reason for the core structure variations is the local variation in composition along the dislocation line. Calculated unstable stacking fault energies on the ⟨110⟩ plane as a function of composition vary significantly, consistent with this assessment. Molecular dynamics simulations of the critical glide stress as a function of temperature show significant strengthening, and much shallower temperature dependence of the strengthening, as compared to pure BCC Fe as well as a reference mean-field BCC alloy material of the same overall composition, lattice and elastic constants as the target alloy. Interpretation of the strength versus temperature in terms of an effective kink-pair activation model shows the random alloy to have a much larger activation energy than the mean-field alloy or BCC Fe. This is interpreted as due to the core structure variations along the dislocation line that are often unfavorable for glide in the direction of the load. The configuration of the gliding dislocation is wavy, and significant debris is left behind, demonstrating the role of local composition and core structure in creating kink pinning (super jogs) and/or deflection of the glide plane of the dislocation.

1. Introduction

Recent work has shown that when 5 or more elements are combined in nearly equiatomic concentrations, a new class of materials emerges [1–3]. These materials are called High Entropy Alloys (HEA) stemming from the idea that entropy of mixing may stabilize novel phases in many-component systems. The number of phases in a HEA system can be significantly smaller than the maximum number of phases present at equilibrium as predicted by the well-known Gibbs phase rule [4]. While many alloys that meet the definition of an HEA [5,6] contain multiple phases, including intermetallics [7,8], there are few single-phase solid solution systems [7,9]. These single-phase systems, both FCC and BCC, generally have unusually high yield strength and/or high ductility. The origin of the strengthening in FCC HEAs has been proposed as due to solute/dislocation interactions, that is solution strengthening in concentrated alloys [10]. The origin of the strengthening in BCC refractory HEAs, which retain significant strength up to very high temperatures [11,12], has been discussed in the framework of the elastic interactions of the crystal lattice (caused by different atomic radii and elastic moduli of the alloying elements) with dislocations [13]. However, BCC materials generally deform plastically by a dislocation kink-pair nucleation mechanism for the screw dislocations, which is very sensitive to the precise screw core structure. Thus, the strengthening may arise from local variations in core structure in these compositionally-complex alloys. In this paper, we use atomistic simulations to investigate the origins of strengthening in a model BCC HEA. We show that the true random alloy has a much higher strength than a corresponding "mean-field" material composed of a single atom type but having the same average properties as the true random alloy. Thus, local compositional

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disorder -which is accompanied by local lattice distortions - is the source of the observed strengthening. We also show that the compositional disorder induces significant variations in local core structure along the length of a single dislocation. The measured strength and measured high "effective kink-pair activation energy" are hypothesized to be due to the inhibition of dislocation motion due to the core structure variations.

Atomistic modeling of multicomponent metallic alloys has been challenging since it requires accurate interatomic potentials for all of the interacting elemental components of the alloy. The literature has thus mainly focused on binary systems, such as Ni-Al and Al-Mg, with very detailed tuning of parameters to achieve quantitative predictive capability. However, a suite of potentials for 16 different metallic elements (Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, Zr) was developed some years ago [14] with the aim of maintaining a unified description of all elements such that any combination of these elements could be studied via simulation. The existence of this suite of potentials enables investigation of a very wide scope of possible multicomponent alloys, including High Entropy Alloys. The suite of potentials were fit mainly to elemental properties, and thus properties that were not fit and properties of multicomponent alloys are not assured to be quantitatively accurate. However, the ability to generate model systems of arbitrary complexity presents a huge opportunity to explore and discover mechanisms of deformation in systems where concepts developed for elemental and dilute binary alloys may not apply. Here, we take advantage of these potentials to probe a model BCC HEA material precisely to uncover heretofore unknown mechanisms of plastic deformation. Any new insights into the unusual mechanical behavior of BCC high entropy alloys can be used to guide future alloy discovery.

2. Computational model of the BCC $Co_{16.67}Fe_{36.67}Ni_{16.67}Ti_{30}$ random alloy

A four element Co-Fe-Ni-Ti interatomic potential developed by Zhou et al. [14,15] was implemented in the molecular dynamics (MD) code LAMMPS [16]. An atomistic simulation cell consisting of a BCC lattice with lattice constant of pure Fe (2.86A) was created, with periodic boundary conditions along three orthogonal directions x = [1–10], y = [110] and z = [001], with dimensions of ~300A in each direction (~2 million atoms). BCC lattice sites were randomly occupied by Co, Fe, Ni, and Ti atoms to achieve an average composition $Co_{16.67}Fe_{36.67}Ni_{16.67}Ti_{30}$. The energy of the system was determined as a function of the average lattice parameter of the BCC cell and a minimum-energy lattice parameter of 2.96A was found for the random alloy. The elastic constants C_{11}, C_{12} and C_{44} for the alloy were determined using standard straining methods, yielding $C_{11} = 165.3$ GPa, $C_{12} = 132.5$ GPa, and $C_{44} = 91.9$ GPa. Such values are similar to Fe-36Ni [17]. This shows that the BCC lattice is a local minimum in energy structure at a lattice parameter of 2.96A and is elastically stable for the selected average composition.

A second BCC simulation cell, with a lattice parameter of 2.96A, was created with the three orthogonal axes along x = [111], y = [11–2], and z = [110], with dimensions of approximately 300A in each direction (~2 million atoms). This cell was relaxed using free surface boundary conditions along z and periodic boundary conditions along x and y. The upper half of the simulation cell was then translated with respect to the bottom half the unstable stacking fault vector 1/6[111] and the system was relaxed to equilibrium at zero pressure and temperature. A similar procedure was used with the fault vector 1/3[111]. The resulting unstable stacking fault energies were then computed from energy differences to yield $\gamma_{usf}([111]/6) = 385$ mJ/m^2 and $\gamma_{usf}([111]/3) = 418$ mJ/m^2, values that are comparable to pure V [18]. This shows that the BCC lattice is stable to large shear deformations on the (110) glide plane. Due to the stability of the BCC lattice to Bain deformation, elastic stresses and large shear deformation, a study of the properties of the ⟨111⟩ glide dislocations in the BCC lattice of the random alloy becomes feasible.

To assess the compositional dependence of the unstable stacking fault energies, similar simulations were also performed over a range of alloy compositions Co 0.2–0.5, Fe 0.2–0.5, Ni 0.1–0.3, and Ti 0.2–0.4, with the bcc lattice being unstable for Co > 0.4. Fig. 1 shows the computed $\gamma_{usf}([111]/3)$ as a function of Fe content, for the various Ti, Co, and Ni concentrations. In general, increasing Co, Ni and Ti concentrations tended to decrease $\gamma_{usf}([111]/3)$ while $\gamma_{usf}([111]/3)$ increased approximately linearly with increasing Fe content. Over the composition space studied, $\gamma_{usf}([111]/3)$ ranged from ~380 to 480 mJ/m^2. Similar behavior was found for $\gamma_{usf}([111]/6)$. These results indicate that local concentration fluctuations in the true random model $Co_{16.67}Fe_{36.67}Ni_{16.67}Ti_{30}$ alloy lead to significant local variations in unstable stacking fault energies, which would have an impact on local core structures of dislocations [19].

To study dislocation structure and dynamics, a ½[111] screw dislocation with line direction x = [111], glide direction y = [11–2], and glide plane normal [–110], was inserted into a cell with the edge lengths of X = 300A, Y = 1200A, and Z = 300A, containing 8 million atoms in total. The dislocation was inserted by deforming the atomic positions according to the anisotropic elastic Volterra solution. Conjugate gradient energy minimization was then performed on the initial atomic positions with periodic boundary conditions along the line direction x and fixed boundary conditions along y and z. Similarly, a ½[111] edge dislocation with the line direction along y = [11–2] was introduced inside a cell with dimensions x = 1200A in the glide direction, y = 300A, and z = 300A. Energy minimization was performed using periodic boundary conditions along x (screw) or y(edge) and fixed boundary conditions along y and z (screw) or x and z (edge). To measure the critical resolved shear stress for motion at T = 0 K, a pure shear stress was applied (τ_{xz} on the (–110) glide plane) by straining the atoms to a desired fixed shear strain and then holding the boundary atoms along y and z (an outer layer of atoms with a thickness equal to $2R_{cut}$, where R_{cut} is the cut-off radius of the interatomic potentials) fixed while the remainder of the system was energy minimized. This was repeated for a range of shear stresses. Molecular dynamics simulations were performed to determine the variation of the

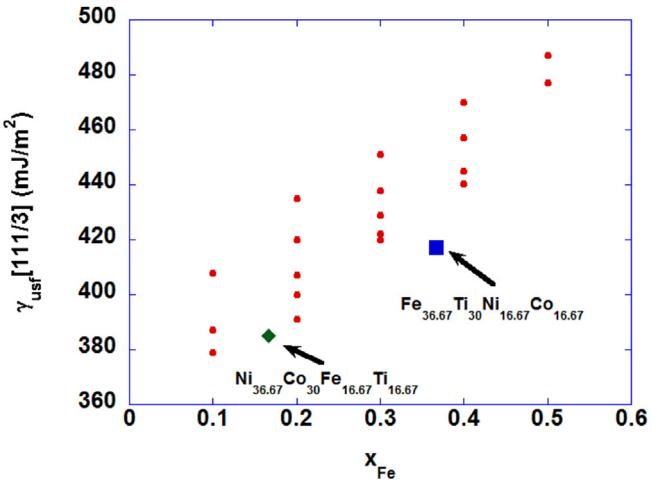

Fig. 1. Unstable stacking fault energy, γ_{usf} [111/3] on the (1–10) plane as a function of Fe concentration, x_{Fe}, in Co, Fe, Ni, Ti based multicomponent random BCC solid solution alloys.