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Acta Materialia 60 (2012) 2350–2358

Acta MATERIALIA

www.elsevier.com/locate/actamat

Prediction of thermal cross-slip stress in magnesium alloys from a geometric interaction model

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Received 12 April 2011; received in revised form 10 November 2011; accepted 3 January 2012
Available online 1 March 2012

Abstract

We develop a geometry-based model from first-principles data for the interaction of solutes with a prismatic screw dislocation core, and predict the thermally activated cross-slip stress above room temperature in Mg alloys. Electronic structure methods provide data for the change in prismatic stacking fault energy for different possible fault configurations for 29 different solutes. The direct solute–dislocation interaction energies for solutes that produce stable prismatic screw dislocation cores (K, Na, Sc and Ca) is correlated with stacking fault misfits. This geometric interaction model produces similar prediction errors for all 29 solutes. The model predicts alloys with cross-slip stresses lower than pure Mg for three previously considered solutes (K, Na and Sc) and three new solutes (Ca, Y and Zr). The model also qualitatively confirms the experimental observation that Mg–Li alloys have lower cross-slip stress than pure Mg. In particular, low concentrations of Y are predicted to significantly decrease the cross-slip stress in Mg.

Keywords: Magnesium alloys; Dislocations; Plastic deformation; Cross-slip; Density functional theory

1. Introduction

Expanding the use of the lightweight structural metal Mg—as a replacement for Al and steels in automotive applications [1]—requires the solution of a variety of metallurgical issues [2], including formability. Current Mg alloys require temperatures near 300 °C for forming (e.g. warm stamping) to activate the five independent slip systems required by the von Mises criterion [3]; this is in part due to the large anisotropy between basal and prismatic slip [4]. Cross-slip of *a*-type dislocations from the (0 0 0 1) basal plane onto the $(0\ 1\ \bar{1}\ 0)$ prismatic plane requires large stresses or high temperatures. Experimentally, few solutes have been found to lower the stress for cross-slip: Al and Zn lower the stress at low (below room) temperatures [5], while Li can lower the cross-slip stress in both regimes [6–9]. The difficulty of performing experiments to measure cross-slip stresses for alloys—requiring single-crystal samples oriented for prismatic slip—is compounded by the possibility that, like solid-solution softening in body-centered cubic (bcc) alloys [10], it may occur over a limited concentration and temperature range. Hence, we have developed new state-of-the-art first-principles predictions of solute–dislocation interactions coupled with computational modeling of thermally activated cross-slip in the presence of solutes to guide the design of new Mg alloys that can be formed at temperatures below 300 °C [11].

In previous work, we developed a numerical model (and analytic approximation) to predict basal to prismatic cross-slip stress in Mg in the presence of solutes from density-functional theory (DFT) dislocation–solute interaction data [11]. The results were limited to solutes that would not destabilize the prismatic screw dislocation core after substitution. Despite this limitation, three binary alloys—Mg–K, Mg–Na and Mg–Sc—were predicted to lower the

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1359-6454/$36.00
doi:10.1016/j.actamat.2012.01.004

thermally activated cross-slip stress. The thermal cross-slip model was based on changes in prismatic kink energies in the presence of a random field of solutes; the double-kink nucleation model is valid above room temperature up to approximately 700 K. The model [11] has been validated both by comparing the mechanism against *in situ* characterization of cross-slip [12–14] in this temperature regime and the measurement of single-crystal cross-slip stress with temperature [15]. Prismatic kinks must nucleate, separate and propagate along the line in the presence of a random field of solutes; the solutes produce distributions of enthalpy barriers for these processes. The solute distribution is assumed to be random to describe the flow of dislocations after breaking away from any kind of initial solute field, but excluding solute drag. The effect of multiple solutes is considered to be additive, and solute–solute interaction energies which could produce short-range ordering of the solutes is ignored. This model has analytic dilute-limit predictions of changes in cross-slip stress as well as non-dilute predictions.

The previous predictions required that solutes not destabilize the prismatic core to compute an interaction energy; however, other solutes may reduce the stress for cross-slip as long as the energy of solutes in a prismatic core was reduced relative to the same site in the basal screw dislocation core. Here, we develop a geometry-based model for the interaction energy of solutes with a prismatic screw dislocation core that is optimized to reproduce direct interaction data [11]. This model allows the prediction of interactions with prismatic cores for 29 solutes (the same considered in an earlier study of basal strengthening [16]) whether the interaction is attractive or repulsive. Combined with our model for thermally activated cross-slip [11], we predict changes in cross-slip stress with temperature and concentration. Of the 29 solutes, six lower the cross-slip stress: Ca, K, Na, Sc, Y and Zr. The interaction of Li is weaker than the prediction error of our model, though it is consistent with experimental observations of softening. We connect the prismatic stacking fault geometry to the prismatic screw dislocation core geometry to quantitatively correlate changes in stacking fault energy to interaction energies, and hence predict the cross-slip stress of binary Mg alloys. Hence, we can predict new, more formable Mg alloys from solute misfit data.

2. Computational methodology

To model the interaction of solutes with the Mg prismatic screw dislocation core, solute interactions with the prismatic stacking faults were calculated within DFT using VASP [17,18]. We use a plane-wave basis set with the projector augmented-wave (PAW) method [19] with potentials generated by Kresse and Joubert [20]. The Perdew–Wang 91 generalized gradient approximation exchange–correlation potential [21] and a plane-wave kinetic energy cutoff of 273 eV for pure Mg ensures accurate treatment of the potentials. Plane-wave cutoffs and electronic configurations for the PAW potentials for solutes in Mg are provided in Table 1. To calculate the chemical misfits for solute X in Eq. (1), we calculate stacking faults with a $5\sqrt{3}a \times 2a \times 2c$ (Mg_{79}–X_1) supercell and a $1 \times 17 \times 16$ k-point mesh with a Methfessel–Paxton smearing of 0.5 eV; atoms are relaxed normal to the fault plane to within 5 meV Å^{-1}, for an energy accuracy of 5 meV. Energies of individual Mg atoms at different planes in the stacking fault (see below) are also computed with an embedded atom method (EAM) potential [22]; it has been validated with basal and prismatic screw dislocation core structures and stacking fault energies in Mg [23]. The screw dislocation core geometries with Burgers vector $\vec{b} = \frac{a}{3}[2\,\bar{1}\,\bar{1}\,0]$ have previously been calculated for the basal geometry [23] and prismatic geometry [11].

3. Results

Fig. 1 shows the possible prismatic $(0\,1\,\bar{1}\,0)$ stacking fault geometries and energies in magnesium from PAW and EAM. The prismatic plane is corrugated, with two possible choices of cut plane for the stacking fault, "easy" and "hard," with unrelaxed planar separations $\frac{a}{\sqrt{3}}$ and $\frac{a}{2\sqrt{3}}$, respectively. Atoms across the fault plane are displaced by $b/2 = \frac{a}{6}[2\,\bar{1}\,\bar{1}\,0]$ relative to their bulk positions to form an unstable stacking fault. The hard stacking fault is more than twice the energy of the easy stacking fault at the $\frac{a}{6}[2\,\bar{1}\,\bar{1}\,0]$; this is due to the displacement of twice the number of nearest-neighbor bonds relative to the easy fault. Inside of the prismatic screw dislocation core, displacements corresponding to both faults appear. Moreover, there are two possible sites for solute substitution, and similarly, both geometries appear in the prismatic screw dislocation core. The EAM calculations agree well with the PAW potential. In addition, the EAM potential provides information about the partitioning of energy between the two planes: the energy change for a Mg atom in the easy fault is $E_{\text{E1}}^{\text{Mg-prism}} = 74$ meV for the first plane and $E_{\text{E2}}^{\text{Mg-prism}} = 54$ meV for the second compared to bulk; while for the hard fault, the Mg atom energy is $E_{\text{H1}}^{\text{Mg-prism}} = 205$ meV for the first plane and $E_{\text{H2}}^{\text{Mg-prism}} = 23$ meV for the second compared to bulk. This energy is not known from DFT, only the total fault energy. We use these changes to determine what fraction of the stacking fault energy change is due to a solute.

Table 1 gives the solute misfits—changes in stacking fault energies—for 29 different substitutional solutes in Mg. To predict the solute energies in the prismatic core, we need to know how the stacking fault displacements change the energy of solute compared with bulk. For each solute, we compute the energy with the solute in the bulk and in each of the two planes for each fault, with relaxation normal to the fault plane. We then subtract the energy of the remaining Mg atoms in both planes of the fault, so that only the change in energy of the solute atom remains. This subtraction is equivalent to subtracting off the total fault energy without a solute and adding in the energy for a Mg atom at the substitutional site. Finally, we scale the