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Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation

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Abstract—We propose an approach for the computationally efficient and quantitatively accurate prediction of solid-solution strengthening. It combines the 2-D Peierls–Nabarro model and a recently developed solid-solution strengthening model. Solid-solution strengthening is examined with Al–Mg and Al–Li as representative alloy systems, demonstrating a good agreement between theory and experiments within the temperature range in which the dislocation motion is overdamped. Through a parametric study, two guideline maps of the misfit parameters against (i) the critical resolved shear stress, τ_0, at 0 K and (ii) the energy barrier, ΔE_b, against dislocation motion in a solid solution with randomly distributed solute atoms are created. With these two guideline maps, τ_0 at finite temperatures is predicted for other Al binary systems, and compared with available experiments, achieving good agreement.

Keywords: Solid-solution strengthening; DFT; Peierls–Nabarro model; Ab initio; Al alloys

1. Introduction

By using ab initio methods, two kinds of approaches are usually employed to simulate solid-solution strengthening. The first one utilizes the materials properties calculated from ab initio calculations as the input to the solid-solution strengthening models developed in the framework of linear elasticity theory (e.g. [7–12]). This approach is very efficient, but the linear elasticity models used cannot properly describe dislocation cores. Consequently, the predictions can be qualitatively incorrect. For example, in the case of Al–Mg and Al–Li solid solutions, the strengthening capability of Li in Al is predicted to be higher than that of Mg, but the experimentally detected strengthening shows the opposite behavior (for details see Appendix A).

The second approach is to fully describe the interaction between the dislocation core and the solute atom(s) by the ab initio method. Simulations based on this approach should hence describe the solid-solution strengthening [3–6] and softening [13] very accurately. The approach is, however, time consuming, computationally demanding and thus not entirely suitable for rapidly predicting solute strengthening in model alloy systems, and large-scale systematic alloy screening.

In this study we aim at merging the advantages of the two approaches outlined above, and at developing a computationally efficient and quantitatively accurate approach to the prediction of solid-solution strengthening. In the first step, the dislocation core is described by the 2-D Peierls–Nabarro model [1,2]. In the second step, the pressure and displacement fields obtained from the 2-D Peierls–Nabarro model are used to capture the interaction between a solute and a straight dislocation. The third step is to homogenize this "dislocation–single solute" interaction effect into a net "dislocation–multiple solute" interaction form by using the solid-solution strengthening model recently developed by Leyson et al. [3–5] for calculating the critical resolved shear stress (CRSS) at 0 K and finite temperatures. This solid-solution strengthening model is a Labusch-type weak pinning model [14–16]. In principle, the third step could be alternatively replaced by a Friedel–Fleischer-type strong pinning model [17,18]. It has been observed, though, that for most cases, when the temperature is above 78 K and the solute concentration is above 0.01 at.%, the Labusch-type model becomes more appropriate compared to the Friedel–Fleischer-type model [19]. Thus, considering the Labusch-type model is likely to be suited for most engineering solid-solution alloys.

This paper is organized as follows: Section 2 outlines the theoretical methods employed in this study, including the solid-solution strengthening model developed by Leyson et al. [3–5], the 2-D Peierls–Nabarro model developed by Schoeck [1,2], and the corresponding ab initio calculations

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to obtain the necessary material properties to carry out the predictions; in Section 3.1, the dislocation–solute interactions in Al–Mg and Al–Li are to be shown; in Section 3.2, we present the predicted critical resolved shear stress vs. temperature curves of Al–Mg and Al–Li solid solutions compared with experiments; in Section 3.3, we employ a parametric study to show the dependence of the solid-solution strengthening capability on the strengthening parameters which are defined in Section 2.2.2; in Section 3.4, we compare the predictions by the parametric study described in Section 3.3 with the previous studies in which the dislocation–solute interactions are directly calculated by the ab initio method [3,4], and the experiments [62,63]; Section 4 summarizes our findings.

2. Methodology

In this section, we present the approach in a reverse manner, because the necessary input parameters are from the previous step(s). First we briefly describe the solid-solution strengthening model developed by Leyson et al. [3–5]; then the 2-D Peierls–Nabarro model used in this study, and how the dislocation–solute interaction energies are calculated from the 2-D Peierls–Nabarro model; finally we present the ab initio calculations used to obtain the necessary materials properties to carry out this approach.

2.1. Solid-solution strengthening model [3–5]

The solid-solution strengthening model developed by Leyson et al. [3–5] is related to the Labusch model for dense solute arrays [14–16]. This model describes the following process: in an infinite crystal of a pure metal, a single isolated dislocation is at its minimum energy, hence it assumes a straight form. In a solid solution with randomly distributed solute atoms, a straight dislocation should spontaneously bow-out, relaxing to its energetically favorable shape due to the local arrangement of the solutes. The final relaxed shape of the dislocation results from two competing processes. First, the binding energy (E_p) of the dislocation to the local region is decreased, while, second, the line energy (E_{el}) is increased due to the bow-out configuration. The bow-out shape is characterized by two parameters: the characteristic segment length (L_c) and the characteristic bow-out distance (ω_c), both of which can be determined by minimizing the total dislocation energy ($E_{tot}=E_p+E_{el}$). At 0 K, the critical resolved shear stress (CRSS) corresponds to the applied stress which is required to move a dislocation segment of characteristic length (L_c) over a characteristic bow-out distance of (ω_c). At finite temperature, the movement of the dislocation can be thermally activated. The details of the analytical derivation of this model can be found in Refs. [3–5].

To carry out this model, the dislocation–solute interaction energy is required. This interaction energy can be approximated by elastic models (e.g. [8,9]), or fully by ab initio calculations (e.g. [3–6]). In this study, the interaction energy is determined by using the 2-D Peierls–Nabarro model suggested by Schoeck [1,2].

It should be mentioned that the dislocation line tension has to be incorporated into this analysis for describing the bow-out of the dislocation. In the previous work of Leyson et al. [3,4], the dislocation line tension of Al was obtained from atomistic simulations (embedded atom method (EAM) potential). In this study, the dislocation line tension of Al is obtained from the isotropic linear elasticity [20], which is justified since Al has a relatively low elastic anisotropy with a Zener ratio of $A_Z \approx 1.3$. The line tension obtained from isotropic linear elasticity is 0.43 eV/Å for edge and 1.58 eV/Å for screw dislocations. The order of magnitude of these values is the same as those obtained from atomistic simulation, namely 0.25 eV/Å [3] or 0.47 eV/Å [4] for edge, and 1 eV/Å for screw dislocations [21]. The elastic constants used to determine the line tension are obtained by ab initio calculations in conjunction with Hershey's homogenization method [27] (see Section 2.3).

2.2. Dislocation–solute interaction by 2-D Peierls–Nabarro model

As described in the previous section, the solute position dependent dislocation–solute interaction energy is required to carry out the solid-solution strengthening model by Leyson et al. [3–5]. In this study, the interaction energy is obtained by inserting the misfit parameters into the pressure and displacement field obtained from the 2-D Peierls–Nabarro model. In this section, we first briefly describe the 2-D Peierls–Nabarro model developed by Schoeck [1,2], and then introduce the misfit parameters, i.e. volume and misfit parameters.

2.2.1. Equilibrium dislocation configuration using the 2-D Peierls–Nabarro model [1,2]

In the 2-D Peierls–Nabarro model developed by Schoeck [1,2], the equilibrium configuration of a straight dislocation is determined by minimizing the dislocation energy with respect to the adjustable geometrical parameters in the trial functions:

$$u_{\parallel} = \sum_i \left(\frac{Z_i}{\pi} \arctan\left(\frac{x + d_i}{\omega_i} \right) + \frac{Z_i}{2} \right)$$
$$u_{\perp} = \sum_i \left(\frac{Y_i}{\pi} \arctan\left(\frac{x + k_i}{v_i} \right) + \frac{Y_i}{2} \right) \quad (1)$$

where $u_{\parallel}$ and $u_{\perp}$ are the displacement profiles which are parallel and perpendicular to the total Burgers vector, respectively; Z_i and Y_i are the Burgers vectors of the fractional dislocations which are parallel and perpendicular to the total Burgers vector, respectively; d_i and k_i are positions of the fractional dislocations; ω_i and v_i are the width of the fractional dislocations. The trial functions serve to approximate the displacement profiles of the fractional dislocations. The dislocation energy comprising the elastic energy and the misfit energy can be calculated using the trial functions together with the knowledge of the elastic modulus and the γ-surface of the pure metal in consideration. The dislocation energy is minimized with respect to Z_i, Y_i, d_i, k_i, ω_i, and v_i, with one constraint that the sum of Burgers vectors of the fraction dislocations must be the same to the Burgers vector of the dislocation.

In this study, the equilibrium configuration of the straight dislocation in pure Al is determined by assuming two triplet partial dislocations as proposed in Ref. [1]: