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Solute strengthening in random alloys

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ARTICLE INFO

Article history:

Received 25 May 2016

Received in revised form

16 September 2016

Accepted 27 September 2016

Available online 19 November 2016

Keywords:

Solute strengthening

Mechanical properties

Metallic alloys

Ab initio calculations

Solute-dislocation interactions

ABSTRACT

Random solid solution alloys are a broad class of materials that are used across the entire spectrum of engineering metals, whether as stand-alone materials (e.g. Al-5xxx alloys) or as the matrix in precipitate-strengthening materials (e.g. Ni-based superalloys). As a result, the mechanisms of, and prediction of, strengthening in solid solutions has a long history. Many concepts have been developed and important trends identified but predictive capability has remained elusive. In recent years, a new theory has been developed that builds on one historical model, the Labusch model, in important ways that lead to a well-defined model valid for random solutions with arbitrary numbers of components and compositions. The new theory uses first-principles-computed solute/dislocation interaction energies as input, from which specific predictions emerge for the yield strength and activation volume as a function of alloy composition, temperature, and strain-rate. Being a general model for materials that otherwise have a low Peierls stress, it has broad application and has been successfully applied to Al-X alloys, Mg-Al, twinning in Mg alloys, and recently fcc High-Entropy Alloys. Here, the new theory is presented in a general and systematic manner. Approximations and limiting cases that reduce the complexity and facilitate understanding are introduced, and help relate the new model to various physical features present among the historical array of models, other recent models, and simulation studies. The quantitative predictions of the model in the various materials above is then demonstrated.

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Contents

1. Introduction	661
2. Background	661
3. Theory of solute strengthening	664
3.1. Average matrix in a random alloy	665
3.2. Energy of a straight dislocation segment in a random alloy	666
3.3. Minimum energy configuration of a long dislocation in a random alloy	666
3.4. Thermal activation of dislocation glide	667
3.5. Yield stress versus temperature and strain rate	668
3.6. Activation volume	668
4. Valuable and insightful simplifications	668
4.1. Dilute limit	668
4.2. Elastic interaction model	670
4.3. Additional core contribution: interaction with the stacking fault	671
5. Applications	672
5.1. Al-Mn solid solutions	672

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5.2.	Activation volume of Al alloys	673
5.3.	Mg-Zn solid solutions	674
5.4.	Twinning in Mg	675
5.5.	fcc high entropy alloys	676
6.	Discussion	677
6.1.	Identification of promising materials	677
6.2.	Failures of the theory	678
6.3.	Contribution of screw dislocations to solute strengthening	679
6.4.	Strengthening in other materials	679
6.5.	Flow stress in atomistic simulations	679
6.6.	Alloys with short range order	680
7.	Summary	680
	Acknowledgments	680
	Role of the dislocation core structure	680
	References	681

1. Introduction

To facilitate the development of advanced materials, computational materials science can be used to provide guidelines for design and to give physical mechanistic insight into the origins of experimentally-derived trends. However, robust and predictive models are critical. Predictions of the macroscopic mechanical properties, such as flow stress, work hardening, and fatigue behavior, in metals or other materials undergoing dislocation-mediated plastic flow, hold particular challenges. Such behavior is controlled by phenomena at multiple scales, from atomistic through mesoscale and microstructural scales, and is associated with the collective interactions among defects (solute, dislocations, grain boundaries, precipitates). With rapidly increasing computational power and new methods at all of these various scales, computational metallurgy is entering a new chapter where predictive capability is achievable and having an impact on the design of new materials.

Here, we present recent progress in the modeling of one broad class of materials, random solid solutions. Such materials are some of the most technologically important and/or promising materials: aluminum alloys, such as the 1xxx, 3xxx, 5xxx and solutionized 6xxx series [1] used in automotive applications, austenitic stainless steels [2], many binary alloys such as Ni-Fe and Cu-Ni [3,4], and the emerging high entropy alloys (HEAs) [5–7]. Many precipitation-strengthened alloys also retain some solid solution strengthening that is not negligible. Interstitial solutes, such as hydrogen, carbon, and nitrogen, also confer strengthening that may be beneficial or detrimental, and their high mobility can contribute to dynamic strengthening phenomena.

In the next section, we briefly discuss the main historical concepts that developed over many decades. In subsequent sections, we present the current model framework in general. We then show how the current model encompasses some historical models, in terms of general scaling of strengthening versus material parameters, so that the current model can be seen as a holistic version of the historical models but with precise and computable material parameters. We also note connections to other recent models when pertinent. We then present applications of the model to a sequence of cases, each of which reveals some new features in the solute strengthening that arise naturally from the model due to the different dislocation structures in each case.

2. Background

Solute strengthening arises from the interaction of a dislocation

with the solutes in the lattice. These interactions fall into two basic categories: those where the solute changes or reconfigures the dislocation core structure and those where the solute leaves the topology of the core structure largely intact. When a solute changes the core structure, the strengthening effects depend on the specific details of the interaction and how the core structure is changed [8–11]. We do not envision any general theory for this important class of problems; presumably the changes in structure and associated energies are very specific to the solute, the matrix, and the dislocation character. When a solute distorts the core but does not change it topologically, and/or when solutes outside the core interact through nominally elastic interactions, then a general theory can be developed, and that is the focus of the work presented here.

When solutes do not change the core structure, the fundamental quantity is the interaction energy $U(x_i, y_j, z_k)$ between a straight dislocation at the origin with line direction z and glide direction x , and a solute at position (x_i, y_j, z_k) . At the simplest level, this interaction energy can be modeled as the mechanical interaction energy between the straight dislocation pressure field $p(x_i, y_j)$ and the misfit volume ΔV of the solute with respect to the matrix material. This interaction energy $U_{el}(x_i, y_j) = -p(x_i, y_j)\Delta V$, also referred to as the first order “size” interaction [12], is equal to the work done on the dislocation pressure field by the expansion or contraction of the material upon addition of the misfitting solute atom. This mechanical interaction energy can be generalized to include the interaction energy between deviatoric misfit strains and the deviatoric dislocation stress field (the first order “shape” interaction), which is typically important for interstitial solutes [13–15]. For simplicity here, we focus on misfit volumetric strains that are appropriate for substitutional solutes in cubic matrices [16,17]. The elastic interactions are long-ranged, since the dislocation stress field decays only as $1/r$ with distance r from the center of the dislocation, and give a quantitative description of the solute/dislocation interaction away from immediate dislocation core region [13–18].

When the solute is located within the core region of the dislocation, *i.e.* along the glide plane and within the highly-distorted region of the core, additional effects between the solute and the dislocation can occur. Part of the chemical short-range interaction can be estimated using additional elasticity models. Since the addition of solutes changes the elastic moduli of the material, a solute atom can be envisioned to possess elastic constants that differ from the host matrix, giving rise to an “elastic inhomogeneity” interaction energy [12,19,20]. This interaction decays as $1/r^2$ so is short-ranged and, within linear elasticity, can be simply added to the first-order size interaction. A “second order size” interaction arises when non-linear effects (*e.g.* third-order elastic constants) are

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