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Dislocation cross-slip in fcc solid solution alloys

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ABSTRACT

Cross-slip is a fundamental process of screw dislocation motion and plays an important role in the evolution of work hardening and dislocation structuring in metals. Cross-slip has been widely studied in pure FCC metals but rarely in FCC solid solutions. Here, the cross-slip transition path in solid solutions is calculated using atomistic methods for three representative systems of Ni-Al, Cu-Ni and Al-Mg over a range of solute concentrations. Studies using both true random alloys and their corresponding average-alloy counterparts allow for the independent assessment of the roles of (i) fluctuations in the spatial solute distribution in the true random alloy randomness and (ii) average alloy properties such as stacking fault energy. The results show that the solute fluctuations dominate the activation energy barrier, i.e. there are large sample-to-sample variations around the average activation barrier. The variations in activation barrier correlate linearly with the energy difference between the initial and final states. The distribution of this energy difference can be computed analytically in terms of the solute/dislocation interaction energies. Thus, the distribution of cross-slip activation energies can be accurately determined from a parameter-free analytic model. The implications of the statistical distribution of activation energies on the rate of cross-slip in real alloys are then identified.

1. Introduction

Materials design for enhancing the performance of metals used in load bearing structural components requires mechanistic understanding of the underlying microscopic processes that control the mechanical properties. Plastic deformation in polycrystalline metal alloys is controlled by the motion of, and interactions between, lattice dislocations. There are many different aspects of dislocation motion and interactions. One important process is cross-slip, the process by which dislocations change glide planes. Cross-slip is restricted to dislocations having screw character, where the dislocation line direction $\boldsymbol{\xi}$ is parallel to the dislocation Burgers vector $\mathbf{b}$, $\boldsymbol{\xi}\cdot\mathbf{b}=0$, so that the dislocation glide plane $\boldsymbol{\xi}\times\mathbf{b}$ is not uniquely defined. Cross-slip contributes to dislocation multiplication, due to double-cross-slip [1], and to dislocation annihilation, due to cross-slip of oppositely-signed screw dislocation gliding on nearby parallel planes [2]. Cross-slip also allows dislocations to overcome obstacles, such as precipitates [3,4]. These microscopic processes determine the macroscopic stress-strain evolution of the material, and this has driven the extensive study of cross-slip processes and mechanisms in metals [5–28].

In FCC metals, cross-slip has been invoked to explain several meso- and macroscopic aspects of deformation, in particular specific forms and transformations of the dislocation network. For example, the prevalence of edge dislocation dipoles in stage I of FCC single crystal deformation is explained by mutual annihilation of screw segments through cross-slip [29–31]. Other structures whose formation is thought to involve cross-slip are dislocation sheets [32] and persistent slip bands [33]. Recently, the importance of cross-slip for network formation has been shown using dislocation dynamics simulations [23] and dislocation-based plasticity models [34]. Cross-slip has also been incorporated into models for macroscopic plastic behavior of FCC metals, specifically work hardening and dynamic recovery [35–37], creep at intermediate homologous temperatures [38–41] [1] and the copper-brass texture transition [45–48]. Cross-slip is also postulated to be involved in the transition between stage II and stage III deformation, see e.g. Refs. [8,49–51] and [52], p. 154, although there is some controversy here.

Here, we focus on the cross-slip mechanism and the associated activation energy ΔE_{act}. Any higher-level modeling effort that

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[1] See also the discussion in Refs. [42,43] as well as the review [44].

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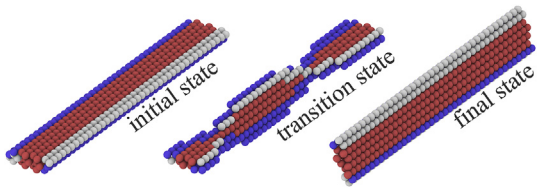

Fig. 1. Typical states during dislocation cross-slip in average Ni-15 at.% Al. The transition state was calculated with the string method [58], see Sec. 2.2. Atoms are colored according to their common neighbor value [59] (red = HCP, blue = BCC, white = other). Atoms in FCC coordination are not shown. Ovito [60] was used for visualization. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

strives to be predictive requires this fundamental information. Specifically, ΔE_{act} for the appropriate length of cross-slipping segment (see below) is required to calculate the rate r of cross-slip. Since cross-slip is a thermally activated mechanism, this rate can be described by an Arrhenius law of the form

$$r(T) = \nu \exp\left(-\frac{\Delta E_{\text{act}}}{kT}\right), \tag{1}$$

where k is the Boltzmann constant, T is temperature, and ν is an attempt frequency.

The most prominent mechanism for cross-slip in FCC is the Friedel-Escaig [7,8] (F-E) mechanism. The F-E mechanism assumes that the initial dislocation, dissociated into Shockley partial dislocations on an initial glide plane [53], must constrict locally to form a Stroh constriction [54] from which the dislocation can cross-slip and begin dissociating on another glide plane. The transition state of the F-E mechanism consists of a short section of dislocation dissociated on the cross-slip plane with the remainder of the dislocation residing on the original glide plane, and with two constrictions joining the two regions segments (see Fig. 1). Escaig initially calculated the activation energy for this mechanism using a linear and isotropic elastic dislocation line tension approach. Since then, several workers have proposed improvements or more elaborate calculations [55] [17,56]. The F-E mechanism is also seen in atomistic transition path calculations [57].

The F-E mechanism generally predicts a high activation energy, making cross-slip unlikely at room temperature. Since cross-slip is implicated in many processes at such moderate temperatures, there has been effort to examine cross-slip associated with heterogeneous mechanisms. The cross-slip energy barrier can be reduced to roughly one half of the homogeneous nucleation value if cross-slip is nucleated at a pre-existing constriction, e.g. a jog, as first considered by Escaig [8] [2]. In the past two decades, atomistic models have confirmed that heterogeneities like jogs [22,62], intersections with forest dislocations [63–66] or surfaces [67] can significantly reduce the activation energy.

In most studies to date, the metal is assumed to be pure. Extension to alloys is primarily considered by assuming that the effects of alloying are limited to changing the relevant average material properties entering the F-E model. In particular, alloying is considered mainly to change the stacking fault energy γ_{sf}, with decreases in γ_{sf} leading to wider dissociation of the initial partial dislocations, and thus a higher energy for forming the constriction. A more accurate dimensionless measure for the dissociation width, and hence the tendency for cross-slip, is $\gamma_{\text{sf}}/\mu b$, the ratio of stacking fault energy to shear modulus and Burgers vector magnitude [68]. However, this reduction to a single parameter is a simplistic model of the alloying effect that misses important mechanisms identified here. Surprisingly, there have been few dedicated studies of alloying effects on FCC cross-slip to date.

Andrews et al. [69] developed an elastic model to compute the energy to form a Stroh constriction using a line tension model, but with the assumption of solute segregation to the dissociated dislocation. The assumption of segregation leads to strong pinning of the initial dislocation, leading to very high energy barriers for cross-slip (e.g. in Cu-Zn, from approximately 1.64 eV at 0.0025 at.% Zn to ca. 10.8 eV at 20 at.% Zn). This assumption is probably not valid for considering materials being deformed steadily at normal strain rates and moderate temperatures, where solute diffusion is too slow to cause significant segregation near dislocations that are temporarily pinned at obstacles. An atomistic study of cross-slip in solid solutions without segregation was conducted by Du et al. [70], who calculated the activation energy for cross-slip in Ni-2 at.% Al and Ni-10 at.% Al, using the Nudged Elastic Band [71] method. The activation energy increased by 0.2 eV if an Al-Al solute pair was formed in the process, due to strong Al-Al near-neighbor repulsion in Ni-Al; this result will echo our broader findings below. A similar methodology was used by Wen et al. for Ni with very ordered arrangements of interstitial H solutes [72,73]. Overall, however, there are no systematic studies of cross-slip in realistic fcc solid solution alloys that would reveal the clear effects of alloying on this important process.

In the present paper, we study the effect of substitutional solutes on the cross-slip activation energy ΔE_{act} in random FCC solid solutions. We compute the activation energies in a set of model alloys (Ni-Al, Cu-Ni, and Al-Mg) over a range of concentrations using atomistic transition path calculations. These calculations show that the activation energy is a random variable with large fluctuations around the mean value. The large fluctuations found over the length of the critical cross-slip nucleus indicate that cross-slip in alloys can be initiated at the statistically easiest region for cross-slip along a long dislocation line. Therefore, average-alloy models are not useful for judging the ease of cross-slip in alloys, and an understanding of the distribution of activation energies is necessary. We show that the activation energy for a specific random distribution of solutes is closely correlated with the energies of the dislocation in the initial and final states. We then develop an analytic model to compute the standard deviation in energy between initial and final states, and validate the model against the simulations. The analytic model in tandem with the observed correlation then allows for an accurate estimate of the statistical variations in cross-slip activation barrier in terms only of the fundamental solute/screw-dislocation interaction energies. These energies can be obtained not only from semi-empirical interatomic potentials (as done here) but also from first-principles studies, enabling for prediction of cross-slip in alloys that do not yet exist or for which there are no reliable interatomic potentials.

The rest of the paper is organized as follows. In the first two sections, we describe the setup of the transition path calculations. The first section presents calculations using the “average atom” interatomic potential for a desired alloy, which accurately captures the cross-slip behavior in the absence of fluctuations in local solute distributions, thereby providing the average reference cross-slip barrier *as if* the alloy was a pure element. The second section describes the transition path calculations in the true random alloys. The resulting transition paths and activation energies are presented in Sec. 3, demonstrating the statistical variations in activation barrier. The correlation between activation barrier and energy difference between initial and final states is also shown. An analytic model for the statistical distribution of activation energies is then

[2] Note also that Escaig incorporated another kind of heterogeneity in his model by assuming that the dislocation is piled up against an unspecified obstacle on the glide plane, see Ref. [61] and the discussion therein.