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Connections between the basal I1 "growth" fault and $\langle c + a \rangle$ dislocations

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Abstract

Recently published experimental results have suggested a connection between the I1 basal stacking fault and the non-basal $\frac{1}{3}\langle 11\bar{2}3\rangle$ (i.e. $\langle c + a\rangle$) dislocation, particularly in Mg–Y and Mg–Y–Zn alloys. Deformed Mg–Y alloys contain more $\langle c + a\rangle$ dislocations and I1 faults than pure Mg, and the I1 fault energy has been shown to be significantly reduced by the addition of Y solute atoms using ab initio modeling. The TEM evidence of a possible connection between the two crystal defects is reanalyzed to reveal: (i) a non-planar dissociation of the pyramidal $\langle c + a\rangle$ edge dislocation into the basal plane, resulting in an I1 fault bounded by $\frac{1}{6}\langle 20\bar{2}3\rangle$ partial dislocations; and/or (ii) a new source mechanism involving nucleation of the pyramidal $\langle c + a\rangle$ dislocation from a pre-existing I1 fault. The former reaction is energetically favorable, but non-conservative. The latter is shown to be energetically conceivable for a wide range of fault geometries. The concepts hypothesized in this paper provide explanations for the frequent TEM observation of rectilinear, edge $\langle c + a\rangle$ dislocations in Mg alloys, as well as a possible explanation for the yield strength anomaly observed in Mg and Mg alloy single crystals. Implications for radiation damage in hexagonal close packed metals are also suggested.

Keywords: Magnesium; Zirconium; Hexagonal close packed; Crystal plasticity; Radiation damage

1. Introduction

1.1. Why the interest in $\langle c + a\rangle$ dislocations?

The $\langle c + a\rangle$ dislocation has received much attention in the recent Mg alloy literature [1–10]. It has also been observed or modeled in Ti [11], Zr [12,13], Be [14], generic hexagonal close packed (hcp) crystals [15], as well as ordered intermetallic compounds such as Ti_3Al (e.g. Refs. [16,17]) and semiconductors such as GaN [18,19]. This defect is significant because it is the sole slip dislocation type, as opposed to twinning dislocations, that will enable *c*-axis deformation of hexagonal crystals. Indeed, its operation provides the five independent slip systems requisite for homogeneous deformation of polycrystals. As such, it has been cited as the explanation for the enhanced ductility of various Mg alloys, especially those containing Li [2] or Y [3].In the latter case, the activation of $\langle c + a\rangle$ slip was specifically observed to alleviate the tendency for Mg and its alloys to undergo heterogeneous deformation involving catastrophic shear banding, which otherwise leads to premature failure.

Berghezan et al. [20] presented a list of the possible perfect and partial dislocation Burgers vectors within the hcp crystal structure to explain their TEM observations of Zn. Their list of possible Burgers vectors did not include $\langle c + a\rangle$, presumably because such a dislocation was viewed as having too large a self-energy to occur. In the meantime, there have been numerous observations of $\langle c + a\rangle$ disloca-

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tion activity (even if one restricts attention to Mg and its alloys), by single crystal slip trace analysis [21,22], transmission electron microscopy (TEM) (e.g. Refs. [1–4,23]), and most recently by electron backscattered diffraction (EBSD) slip trace analysis (e.g. Refs. [23–25]). Furthermore, experimentally validated crystal plasticity modeling studies of polycrystalline Mg and Mg alloys have suggested that the critical resolved shear stress to operate this deformation mechanism is not so high, relative to the other slip mechanisms (e.g. Refs. [26,27]), as early oriented single crystals suggested [21,22]. In particular, Y additions were suggested to promote a texture evolution during rolling [3] or plane strain compression [28], which is consistent with the operation of $\langle c+a\rangle$ slip.

Despite all the evidence for $\langle c+a\rangle$ slip, the large Burgers vector means that it is indeed energetically costly, which raises questions about its nucleation and core configuration, not to mention its mobility, once it is formed. The molecular dynamics (MD) study by Nogaret et al. [7], like previous studies of Zr [12,13] and generic hcp metal [15], had suggested that the core configuration of $\langle c+a\rangle$ dislocations in pure Mg is very complex and has a strong character (screw vs. edge) dependence. In contrast, the most recent atomistic study of the $\langle c+a\rangle$ dislocation in Mg [8] employing density functional theory (DFT) suggests a much simpler dissociation reaction into two $\frac{1}{2}\langle c+a\rangle$ partial dislocations on the $\{1\,1\,\bar{2}\,2\}$ planes, regardless of dislocation character. The current paper revisits the topic of $\langle c+a\rangle$ dislocation dissociation from a continuum elasticity perspective and correlates the resulting hypothesis with prior diffraction contrast TEM imaging and mechanical property observations. The conclusions are consistent with high-resolution Z-contrast STEM observations by Yang et al. [8].

1.2. Why the interest in I1 faults?

Berghezan et al. [20] did discuss the I1 "growth" stacking fault and explained how either vacancy or interstitial condensation as a disk within the basal plane would lead to a prismatic loop, bound by a partial dislocation with a Burgers vector of $\frac{1}{2}\langle 0\,0\,0\,1\rangle$ (or $\frac{1}{2}\langle c\rangle$). The resulting stacking fault is high energy, thus it is possible that a $\frac{1}{3}\langle 1\,0\,\bar{1}\,0\rangle$ (or $\langle p\rangle$) Shockley partial dislocation may be nucleated and sweep the entire fault, resulting in an I1 fault that has lower energy, though the self-energy of the bounding $\frac{1}{6}\langle 2\,0\,\bar{2}\,3\rangle$ (or $\langle p+\frac{1}{2}c\rangle$) partial dislocation would, of course, be larger than the original. It is emphasized that the I1 fault is bounded by a sessile, "prismatic" dislocation loop, which can only move non-conservatively, by mass transport (vacancy or interstitial diffusion).

In addition to observing more $\langle c+a\rangle$ dislocations, Sandlöbes et al. [3] observed many I1 faults in the microstructure of the Mg–Y alloy, but not the pure Mg. In the meantime, ab initio electron DFT has been employed to show that Y (and other rare earth element) additions to Mg lower the stacking fault energy of the I1 fault [29,30], as well as that of the I2 Shockley-type fault on the basal plane [31]. A recent modeling survey investigated the effect of a large number of binary alloying additions on the stacking fault energies in Mg [32]. Notably, of the elements investigated, Y was identified as the one that most potently reduces the I1 fault energy. Thus, the observation of an enhanced density of I1 faults in Mg–Y relative to pure Mg conforms with theoretical expectations. What remains unexplained in all these recent publications is the relationship between $\langle c+a\rangle$ dislocations and the I1 fault. For example, the I1 fault has been suggested as a possible heterogeneous nucleation site for $\langle c+a\rangle$ dislocations, owing to the concomitant observation increases in the density of $\langle c+a\rangle$ dislocations and I1 faults in a certain Y-containing Mg alloy relative to pure Mg [3]. However, the details of the proposed $\langle c+a\rangle$ nucleation mechanism are not clear.

Stohr and Poirier [21] observed that $\langle c+a\rangle$ edge dislocations induced during c-axis compression of pure Mg single crystals undergo a non-coplanar dissociation into two $\frac{1}{6}\langle 2\,0\,\bar{2}\,3\rangle$-type partial dislocations on the basal plane within a certain deformation temperature regime characterized by a yield strength anomaly. Obviously, an I1 stacking fault would result from this dissociation reaction. In that important original work, Stohr and Poirier [21] noted that this was a sessile configuration for the $\langle c+a\rangle$ edge dislocation. Poirier [33] later explained that it was an example of a non-conservative (climb-induced) dissociation reaction observed in the high-temperature deformation of ceramics and minerals. Since the required diffusion is thermally activated, this begins to explain the strength anomaly, which has in the meantime been observed by Ando et al. [1,34].

1.3. Objectives and outline

The purpose of the present paper is to (1) consider possible $\langle c+a\rangle$ dislocation dissociation reactions from a isotropic continuum elasticity perspective, (2) evaluate the energetics of a specific $\langle c+a\rangle$ dislocation nucleation mechanism, and (3) present an analysis of previously published TEM images of $\langle c+a\rangle$ dislocations in a Mg–Y alloy to provide evidence for the proposed reactions. Then, it considers the possibility that the proposed reactions explain (4) the appearance of $\langle c+a\rangle$ dislocations and electron-induced radiation damage during TEM observations, and (5) the $\langle c+a\rangle$ slip yield strength anomaly. Finally, (6) an outlook is provide for related future alloy and thermomechanical process design.

2. $\langle c+a\rangle$ dislocation dissociation reactions

Apart from computations of activation barriers associated with dissociation events, continuum dislocation theory can be used to assess the likelihood of dislocation reactions by simple comparison of the resulting energy states. In the following, frequent reference is made to the recently performed atomistic simulations, in order to avoid pitfalls associated with this limitation. This paper is primarily concerned with the dissociation of the $\langle c+a\rangle$ edge dislocation, which lies at the intersection of the $\{1\,1\,\bar{2}\,2\}$ second-order pyrami-