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Atomistic simulations of interaction between basal <a> dislocations and three-dimensional twins in magnesium

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ABSTRACT

Dislocation slip and twinning are equally important in the plastic deformation of hexagonal close packed crystals. Basal slip and extension $\left\{10\bar{1}2\right\}<\bar{1}011>$ twins can be activated concurrently in magnesium and, as a result, complex dislocation-dislocation, twin-twin, and dislocation-twin interactions take place and determine the hardening behavior. Here, using atomistic simulations, we study the latter mechanism, namely, the interactions between basal <***a***> dislocations and a three-dimensional (3D) $\{10\bar{1}2\}$ twin. According to our findings, a basal screw dislocation can fully transform into the twin via multiple cross-slip between basal and prismatic planes in the matrix. This process causes the formation of jogs and basal stacking faults in the matrix, and prismatic <***a***> dislocations in the twin. We also find that a basal mixed dislocation cannot directly transform into the twin. Instead, it dissociates into twinning dislocations, resulting in a change in twin thickness and the formation of basal/prismatic steps. When the dislocation interacts with the lateral twin boundary, slip transformation in the twin is accomplished through the gliding of either ½<***a***+***c***> or <***a***+***c***> on the prismatic plane in the twin. Accompanying the gliding of ½<***a***+***c***>, a prismatic stacking fault is created inside the twin. By accounting for the 3D character of the dislocation-twin reactions, our results extend our understanding of slip transformation into a twin, the formation of basal and prismatic stacking faults in matrix and twin, and the role that local stresses and the lateral boundary of the twin play in this process.

1. Introduction

Dislocation slip and twinning are equally important in the plastic deformation of hexagonal close packed (hcp) crystals [1–4]. For Mg and Mg alloys, the primary deformation mechanisms at room temperature are basal <***a***> slip ($\{0001\}<11\bar{2}0>$) and $\left\{10\bar{1}2\right\}<\bar{1}011>$ extension twin. Prismatic <***a***> slip $\left\{10\bar{1}0\right\}<11\bar{2}0>$ and pyramidal <***a***+***c***> slip $\left\{11\bar{2}2\right\}<\bar{1}\bar{1}23>$, are difficult to activate due to the low mobility of the associated dislocations. A considerable amount of work has been devoted to understanding the mechanisms and mechanics of plastic deformation associated with dislocation slip and twins in hexagonal close packed crystals. The studies regarding dislocations have concentrated on structure, energy, and motion of dislocations, and on their interactions in the framework of dislocation configurations [5–9]. Because basal slip and extension twinning are concurrently activated, complex dislocation-twin [10–27] and twin-twin interactions [28–35], take place and affect strain hardening. In the case of twin-twin interactions, twin-twin boundaries (TTBs) form that subsequently affect the twinning, de-twinning, and slip processes [36–38]. Such mechanism is particularly relevant in connection with cyclic loading [39]. With increasing loading cycles, more TTBs form, and the stability of TTBs requires increasing stresses in order to activate de-twinning, which results in increased strain hardening [32,39].

Although twins are 3-dimensional domains, practically all the work done on dislocation-twin and twin-twin interactions regards the twins as two-dimensional entities, sectioned along the plane that contains the propagation and normal direction [17,18,40–42]. Traditionally, TEM and EBSD studies analyze two-dimensional

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sections of twins, and only recently results from serial sectioning that capture the volumetric shape of twins in AZ31 Mg have been reported [43]. Also recently, Liu et al. [44] have characterized experimentally and via molecular dynamics method (MD) the structure of the 'lateral' side of $\{10\bar{1}2\}$ twins in Mg. Gong et al. further studied equilibrium and non-equilibrium boundaries associated with 3-D twins by using crystallographic dislocation theory and MD simulations [45]. Luque et al. used MD to study stability of 3D 'terraces' growing on the coherent twin boundary of tensile twins in Mg [46]. We believe that the 3D character of twins has to be accounted for, if one expects to fully understand twin-twin interactions, dislocation-twin interactions, and twin transformation across grain boundaries.

In this work, we use as a guide and reference the extensive 2D knowledge acquired in the last half century, and focus on dislocation-twin interactions in Mg from the 3D perspective. We attempt to improve our comprehension about the barriers that twins represent to dislocation glide, the reactions taking place at the twin interfaces, and the characteristics of dislocation transmutation across the twin. Understanding kinetic processes of the slip-twin interactions in hexagonal materials is an indispensable first step for developing a comprehensive understanding of the role that this mechanism plays on hardening the parent and the twin. The majority of experimental studies have concentrated on the interactions between dislocations and coherent twin boundaries in Mg [4,15,20–22], Zn [14,16,47–49], Zr [50–53], and Ti [54]. Wang and Agnew [20] recently conducted a transmission electron microscopy study of dislocation transmutation across twin boundaries, which confirms some previously proposed dislocation transformation reactions, and reveals $\langle \boldsymbol{c} \pm \boldsymbol{a} \rangle$ dislocations in the vicinity of the twin boundary. In addition, geometry models and atomistic simulations have been used for characterizing the interaction of basal <***a***> dislocation with coherent twin boundary in a 2D framework. The major results can be summarized as follows.

- A screw <***a***> dislocation can directly transmit across the twin boundary without leaving a residual defect at the twin boundary [13,17,55]. This transmission involves cross-slip of the dislocation from basal plane in the matrix to basal or prismatic plane in the twin.
- A mixed <***a***> dislocation cannot directly transform across the twin boundary. Instead, the dislocation dissociates into multiple mobile twinning dislocations, resulting in twinning or detwinning with respect to the gliding and formation of PB steps. A residual defect is left at the TB [18,40,41,56–59].
- Two mixed <***a***> dislocations gliding on a basal plane in the matrix could react to produce one <***a***+***c***> dislocation on the prismatic plane in the twin and a residual dislocation at the interface [13,55]. After the reaction, a <***a***+***c***> dislocation transforms into the twin via gliding on the prismatic plane of the twin.

The interaction between a dislocation and a boundary depends strongly on the slip systems available in the twin, the atomic structure of the boundary, the local stress state, and temperature [2,22,60–62]. The last two factors can be varied with loading conditions, but the first two factors are determined by the geometrical characteristics of the boundary [18]. Regarding the interaction of a dislocation with a 3D twin, there are two geometric factors. Firstly, besides the widely studied coherent twin boundary and its contribution to twin thickening, there are two other characteristic twin boundaries to consider. One is responsible for the forward ('edge') propagation of the twin domain along the twinning shear direction, while the other is responsible for the lateral ('screw') propagation in a direction perpendicular to the growth and the shear directions. These two twin boundaries are associated with the pileup and rearrangement of twin dislocations (TDs) [45]. Secondly, a dislocation with a given Burgers vector may exhibit screw, edge or mixed character, and may approach the twin from different directions. For example, a basal <***a***> dislocation line can be parallel to the coherent twin plane, or parallel to the lateral twin boundary. However, knowledge is missing regarding the interactions between a dislocation and lateral twin boundaries, or how a dislocation transforms across a twin domain when it impinges on different sides of the twin.

In this paper, we conduct atomistic simulations of the interaction processes of basal <***a***> dislocations approaching a three-dimensional (3D) $\{\bar{1}012\}$ twin. In section 2, we describe essential details of simulation models and methods. In section 3, we report on simulation results with respect to the incoming dislocation characters including Burgers vector and line sense and the three twin boundaries. We draw conclusions in section 4. The results provide comprehensive insights of the interactions between a dislocation and a deformation twin.

2. Crystallographic characterization and atomistic simulation

2.1. Crystallographic characterization

In a 3D twin, three types of twin interfaces/facets can be identified, each one related to a different twin propagation direction. For simplicity, a schematic 3D twin domain is presented in Fig. 1, and characteristic boundaries, as identified in experiments and atomistic simulations, are identified. The x-axis coincides with the twin shear direction ($\boldsymbol{\eta} = [10\bar{1}\bar{1}]$), y-axis is along the twin normal ($\boldsymbol{n} = [\bar{7}078]$) and z-axis is along the lateral direction ($\boldsymbol{\lambda} = [1\bar{2}10]$). The three types of twin boundaries/facets (TBs) are associated with the 'normal' (parallel to ***n***), 'forward' (parallel to **η**) and 'lateral' (parallel to **λ**) propagation/growth directions, respectively. The

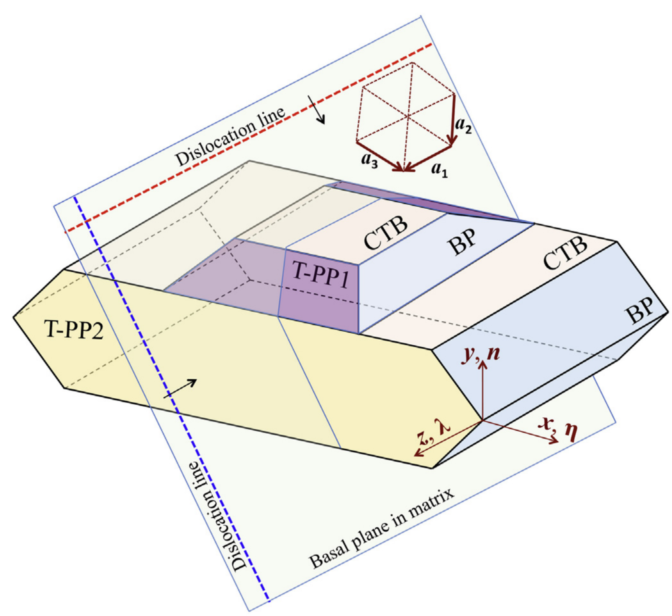

Fig. 1. A schematic three-dimensional twin, showing characteristic boundaries associated with a $\{\bar{1}012\}$ twin and three available basal <*a*> slip vectors. The red and blue dashed lines denote dislocation lines. The red one is parallel to the z-axis and the blue one is along the <*c*> axis. The black arrows indicate the moving direction of the dislocation. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)