Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 90 (2015) 140–150

Acta MATERIALIA

www.elsevier.com/locate/actamat

Non-equilibrium basal stacking faults in hexagonal close-packed metals

X.Y. Zhang,[a] B. Li[b,*] and Q. Liu[a]

[a]School of Materials Science and Engineering, Chongqing University, People's Republic of China
[b]Department of Chemical and Materials Engineering, University of Nevada, Reno, NV 89557, USA

Received 6 December 2014; revised 18 February 2015; accepted 20 February 2015

Abstract—Transmission electron microscopy (TEM) studies were performed to investigate non-equilibrium basal stacking faults (SFs) in deformed hexagonal, close-packed (HCP) metals, i.e., magnesium (Mg), cobalt (Co), titanium (Ti) and a Mg AZ31 alloy. These SFs present a width that is two to three orders of magnitude wider than the equilibrium width of the basal SFs created by partial dislocations. The non-equilibrium basal SFs are often generated inside deformation twins, and in conventional TEM the SFs present a morphology of straight lines well aligned with the trace of the basal planes, and may cross a whole twin. To investigate the mechanism of the formation of the SFs, we performed atomistic simulations. The simulation results show that the formation of the non-equilibrium basal SFs is closely associated with incoherent twin boundary (TB) migration. When the structure of the initial TB is incoherent, basal SFs are nucleated with one end being anchored at the moving TB. SFs subsequently grow along with the moving TB, resulting in SFs with a large width that may cross the whole twin. No Shockley or Frank partial dislocations are involved in the nucleation and the growth of SFs. When the structure of the initial TB is coherent or nearly coherent, no SFs are generated. The non-equilibrium basal SFs interact with prismatic and pyramidal slips, and impede the dislocation slip.

Keywords: Stacking faults; Hexagonal close-packed; Dislocations; Deformation

1. Introduction

Stacking faults (SFs) are often observed in transmission electron microscopy (TEM) studies of crystalline metals with a low stacking fault energy (SFE). SFs are closely related to partial or incomplete dislocations in crystals. For close-packed crystal structures, SFs are formed as partial dislocations are nucleated and glide on the close-packed crystallographic planes. Different from full or complete dislocations, the glide of partial dislocations changes the local structure of the crystal, and hence, excess configuration energy is created. To minimize the energy, a trailing partial dislocation is subsequently nucleated and wipes out the SF until an equilibrium between the SFE and the repulsive force of the partial dislocations is reached [1]. The equilibrium width of an SF (d_0) is inversely proportional to the SFE, i.e., $d_0 \sim 1/\text{SFE}$ [1–3]. If a resolved shear stress is imposed on the slip plane, the actual width of the SF may change as a result of the difference in the shear factors of the two partial dislocations [1,4]. In addition to activities of partial dislocations, SFs can also be formed during crystal growth [5] or by condensation of excess point defects (vacancies or interstitials) produced by irradiation [6–9] or by large strain plastic deformation [10,11], normally on close-packed planes. After collapse of the lattice near the vacancy discs, sessile dislocation loops or SF tetrahedra are formed. In TEM studies, SFs usually present well-defined dark/bright fringes in bright field (BF) or dark field (BF) imaging [12].

SFs in low symmetry, hexagonal-close-packed (HCP) structures are much more complex than those in cubic structures [13–19]. The complexity is manifested by the presence of multiple possible slip systems. So far, three slip systems are confirmed in atomistic simulations: basal slip on the close-packed plane $\{0002\}$ along $\langle 1\bar{2}10\rangle$, prismatic slip on the corrugated plane $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$, and pyramidal slip on the slightly corrugated plane $\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$ [20–23]. The widely cited pyramidal slip system $\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$, i.e., the $\langle c+a\rangle$ slip remains controversial because the interplanar spacing (d) of the $\{11\bar{2}2\}$ ($d=\frac{\gamma\cdot a}{2\sqrt{1+\gamma^2}}$) is only about half of that of the $\{10\bar{1}1\}$ ($d=\frac{\sqrt{3}\cdot\gamma\cdot a}{\sqrt{4\gamma^2+3}}$, a is the lattice parameter and γ the c/a ratio). Dislocation slip is more likely to occur on planes with larger interplanar spacing because the frictional energy barrier is lower. The magnitude of the Burgers vector of a full $\langle c+a\rangle$ ($a\sqrt{1+\gamma^2}$, 0.612 nm for Mg) is so large that dissociation into partial dislocations is expected. Possible dissociation of the $\langle c+a\rangle$ pyramidal slip was studied by a number of researchers using molecular dynamics (MD) simulations [24–27]. But the partial dislocations and the corresponding SFs obtained in the MD simulations have not been confirmed in TEM observations. Dissociation of a prismatic dislocation was first observed in MD

* Corresponding author. Tel.: +1 775 784 4507; e-mail: binl@unr.edu

http://dx.doi.org/10.1016/j.actamat.2015.02.036
1359-6462/

simulations by Liao et al. [28]. Such a dissociation was found to be unstable because the trailing partial was quickly nucleated following the leading partial and wiping out the SF. The leading and the trailing partial then combined into a full dislocation.

In general, SFs in HCP metals are most likely to be observed on the basal plane (0002), because the SFE of the basal plane is relative low. For magnesium (Mg), the basal SFE is about 25–35 mJ/m^2 [21] according to first principles and MD calculations. However, despite the relatively low basal SFEs in HCP metals, the equilibrium width of the basal SFs is usually rather small. Trinkle et al. [21] simulated the dissociation of an edge and a screw basal dislocation in Mg and found that equilibrium width is only 1–3 nm. Such a low split distance is too small to be observed with conventional TEM. Therefore, basal dislocations are usually observed as full dislocation lines in TEM.

However, in the published TEM studies of Mg and other HCP metals, a special type of SF has often been reported. The SFs appear to be straight lines well aligned with the traces of the basal plane, and have a length that is two to three orders of magnitude larger than the equilibrium width of the basal SFs [29–33]. When the specimen was tilted properly, dark/bright fringes may be observed but always less well-defined than those SFs observed on the {1 1 1} close-packed planes of cubic metals. These straight lines were interpreted as basal SFs and are often observed inside $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ deformation twins [30–32]. They have also been observed in grains that do not satisfy the twin orientation relationship. For example, Agnew et al. [33] observed in Mg straight lines that were decorated with dark speckled features. Similar features were also observed in other HCP metals such as Ti and Zr by Song and Gray [34].

The nature of the super-wide basal SFs in HCP metals observed in experiments have not been fully understood yet. The purpose of this study is to investigate the mechanism of the formation of these basal SFs, using TEM and MD simulations. We show that these non-equilibrium SFs are closely associated with the migration of incoherent twin boundaries (TBs) and the glide of the Shockley partial dislocations is not involved.

2. Methods

Three pure HCP metals, i.e., Mg, Co and Ti, and an AZ31 Mg alloy were investigated in this study. Commercially pure Mg was extruded at 593 K with a cross-sectional area reduction rate of about 14. A circular plate was cut from the extruded bar, and the axial direction of the plate is along the extrusion direction. The plate was then annealed at 823 K for 3 h. After annealing, the grain size was approximately 50 μm. Then a specimen for compression was prepared from the annealed plate. The specimen was compressed to failure (~10% engineering strain) at room temperature along the extrusion direction at quasi-static strain rate (10^{-3} s^{-1}). For TEM analysis, thin slices (~600 μm) in thickness were cut off perpendicular to the extrusion direction using a diamond saw, and then mechanically polished to about 130 μm in thickness using a series of sandpapers down to 800 grit number. Three millimeter discs were then mechanically punched off the specimen. The discs were electrochemically polished using a Tenupol-3 electropolisher with a solution of ethanol, nitric acid (20%), and perchloric acid (~2%) at −30 °C. Afterward, the specimen was gently cleaned using ion-milling for about 10 minutes with a low incidental angle and low voltage (2.0 kV). TEM observations were carried out on Philip 420 (120 kV) and CM 300 (300 kV) TEMs.

Separate mechanical tests were performed on cylindrical specimens of high purity (99.99%) Co and α-Ti (99.99%) and the AZ31 Mg alloy (3 wt.% Al, 1 wt.% Zn, balance Mg). The specimens were dynamically compressed at a strain rate 2×10^2–10^3 s^{-1} at room temperature (293 K). The Ti and Co specimens were compressed to ~10% and ~17% plastic strain, respectively. The AZ31 was compressed to ~7%. Thin foils of the deformed Co, Ti and AZ31 Mg specimens were prepared for TEM observations via twin-jet electrochemical polishing. Subsequent TEM observations were carried out on FEI TecnaiF30-G^2 TEM (300 kV). More experimental details of the dynamic testing can be found in [35,36].

To understand the mechanism of the formation of the non-equilibrium basal SF in HCP metals, we performed molecular dynamics (MD) simulations of deformation of pure Mg. An embedded atom method (EAM) [37,38] interatomic potential for Mg developed by Liu et al. [39] was used in our simulations. This well-developed EAM potential has been used to simulate the deformation behavior of Mg alloys in numerous studies [23,40], and the results obtained in the simulations were satisfactory.

3. Results

3.1. TEM observations

Fig. 1a shows a TEM micrograph of a deformation $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin in pure Mg. Inside the twin, straight lines (indicated by the arrows) can be seen. These lines are perfectly aligned with the trace of the basal plane. The lines seem to be emanated from one side of the TBs, but terminate inside the twin. Fig. 1b shows a high resolution TEM (HRTEM) micrograph of the lines in Fig. 1a. It can be clearly seen that the lines are parallel to the basal plane and indeed are basal SFs. Notably, the width of these basal SFs (measured by the length of the lines) can reach as large as 1.0–1.5 μm, two to three orders of magnitude wider than the equilibrium width (1–3 nm) of the basal SFs.

Wide basal SFs were ubiquitously observed in all the deformed specimens. Fig. 2a shows the basal SFs that cross the whole twin in the deformed AZ31 Mg alloy. Note that the TBs are serrated and highly incoherent. The SFs and the incoherent TB can be better viewed in the HRTEM micrograph in Fig. 2b. The SFs are all parallel to the basal plane.

Fig. 3a shows basal SFs inside a $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin in deformed Co. Near the center of Fig. 3a, in the circled region, traces of interaction can be observed between the ends of the two basal SFs. The magnified view of the circled region is shown in the inset of Fig. 3b. The lattice fringes of the basal planes were disrupted, indicating that a dislocation or another SF was present and was interacting with the two basal SFs.

Wide basal SFs that cross a whole $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin in the deformed Ti were also observed, as shown in Fig. 4a. Again, the TBs are highly incoherent. The