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Twin boundary migration creating zero shear strain: In-situ TEM observations and atomistic simulations

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Abstract

Atomistic simulations were conducted to study the migration of $\{10\bar{1}2\}<10\bar{1}\bar{1}>$ twin boundary. A bi-crystal that satisfies the twin orientation relationship was constructed and a tensile strain was applied in parallel to the <*c*> axis of one crystal. Under the tensile strain, the twin boundary starts to migrate but the migration (twin growth) does not produce any observable shear strain on the bi-crystal. In-situ transmission electron microscopy (TEM) observations of a single crystal Mg under tension and compression confirm that during twinning and detwinning, no shear strain is produced. The specimen uniformly elongates and narrows during twinning, and widens across the width during detwinning.

Introduction

Twinning plays a vital role in metals with hexagonal close-packed (hcp) crystal structures. It accommodates plastic strain along the <*c*>-[0001] direction during deformation [1-3]. Compared with twinning in metals with cubic crystal structures, where twin nucleation and twin growth are mediated by well-defined partial dislocation at the twin/matrix interface, i.e., twin boundaries (TBs) [4-5], twinning in hcp metals is much more complicated in the following aspects:

(1) In cubic metals, twinning can be accomplished by a homogeneous shear mediated by slip of Shockley partials. However, in hcp metals, for most of the twinning modes, a homogeneous shear is unable to complete the twinning process and atomic shuffling is required to achieve correct twin orientation relationship [6]. Shuffling is usually considered having negligible effect on twinning but recent studies show that this is not the case [7]. In fact, the relative magnitude of elementary twinning dislocation and atomic shuffling determines the configuration of twinning dislocations, which in turn determines the migration of TBs.

(2) Multiple twinning modes can take place. There are four major twinning modes with $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ mode being the predominant in all hcp metals. The properties of individual twinning modes vastly differ from one mode to another. For example, the $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ mode presents reversibility or pseudoelasticity [8-10], non-Schmid effect [11], penetration of twin variants through grain boundaries [12], zero shear strain [13], and extremely incoherent TBs [14]. These properties cannot be accounted for by any model of twinning dislocations [15-16]. Recently, Li and Ma [7] proposed that this particular twining mode is dominated by atomic shuffling and no twinning dislocations are involved. This theory properly resolves the puzzles regarding the mechanism of the predominant twinning mode in hcp metals. As to $\{10\bar{1}1\}\langle10\bar{1}\bar{2}\rangle$ twinning, shear dominates and minor shuffles are involved, and zonal twinning dislocations can be well defined at TBs [17].

In this work, we performed in-situ transmission electron microscopy and atomistic simulations on twinning and detwinning in single crystal Mg. The results obtained show that indeed, $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning produces zero shear strain during reversible twinning.

Methods

Tension specimens were fabricated from a single crystal Mg by a FEI Helios 600 Dual Beam Focused Ion Beam (FIB) with rectangular cross sectional area and an aspect ratio 4:1. The dimensions of the specimens are shown in Figure 1a, with a thickness 125 nm and a width 420 nm. The c-axis of the specimen is exactly in the axial direction. A uniaxial tension was first carried out along the c-axis. After twinning, one end of the specimen was removed by FIB, and the load was reversed to compression. In-situ mechanical experiments were performed with a Hysitron PicoIndenter inside a JEOL 2100 TEM operating at 200 keV. All tension and compression tests are run in displacement control mode.

Atomistic simulations were conducted by applying a tensile strain to a bi-crystal in which the two individual crystals satisfy $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twin orientation relationship. The loading axis was parallel to the *c*-axis of one crystal. After twinning, the tensile load was reversed to compressive.

Results and discussions

A tensile load was first applied along the c-axis, i.e. [0002] direction. $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning was favored and activated during tension. Figure 1a and b shows the sample geometry before and after tension. The entire gauge length was twinned, as confirmed by the selected area diffraction (SAD) analysis. The *c*-axis was reoriented by ~90 degrees, typical of $\{10\bar{1}2\}\langle10\bar{1}\bar{1}\rangle$ twinning. Since the electron beam is parallel to the $\{10\bar{1}2\}$ twinning plane and the $<1\bar{2}10>$ zone axis, any shear deformation in the single crystal can be readily captured. Surprisingly, during and after twinning, the specimen uniformly elongated along the loading direction and narrowed across the width, leaving no observable traces of shear offset on the sample surface.

A high resolution transmission electron microscopy (HRTEM) image was acquired and the structure of the twin boundary is shown in Figure 2. In the atomic scale, the twin boundary is extremely incoherent and far off the $\{10\bar{1}2\}$ twinning plane. Such a huge deviation between the twinning plane and the twin boundary violates the requirement that a twin boundary should

match the twinning plane if the twinning is controlled by twinning dislocations.

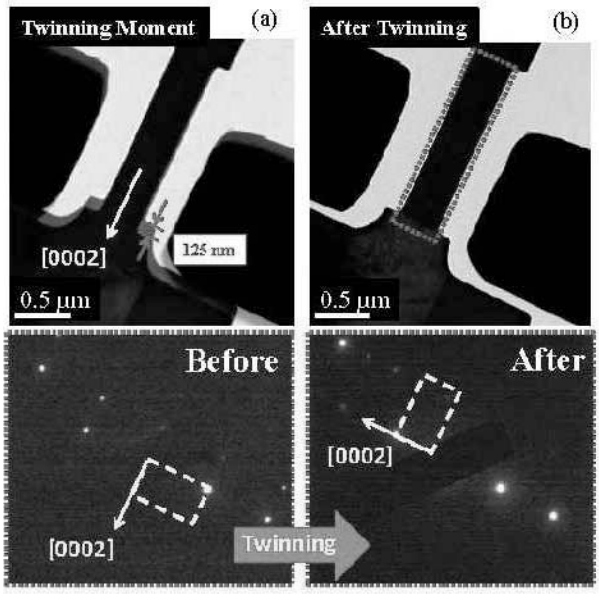

Figure 1. (a) Specimen geometry before tensile loading. (b) After loading along the c-axis, twinning occurred but the specimen uniformly elongated without observable shear offset. The diffraction patterns show that after twinning, the orientation of the twin is ~90 ° with the parent.

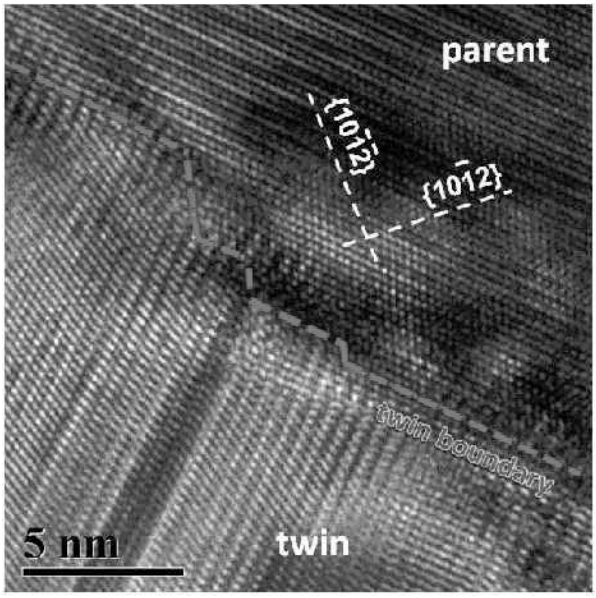

Figure 2. High resolution TEM shows the lattice fringes of the twin and the parent. The twin boundary is extremely incoherent and hugely deviates from the two possible twinning planes $\{10\bar{1}2\}$ and $\{10\bar{1}\bar{2}\}$.

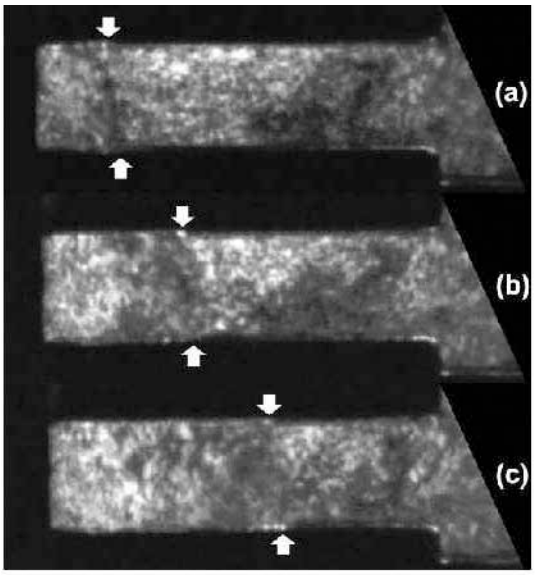

Figure 3. After twinning, the tensile load was reversed to compression and detwinning occurred. The specimen uniformly widens across the width, leaving no shear offset on the specimen as well.

It has been extensively observed that $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning is reversible. If an external load is removed or reversed, deformation twins shrink or completely disappear [8-10]. Indeed, detwinning was observed in our *in-situ* TEM observations. Figure 3 shows in time sequence the geometry evolution when the tensile load was reversed to compressive. The specimen uniformly widens toward both sides. SAD analysis confirms that the *c*-axis of the twinned region is reversed to the original orientation before twinning.

To understand the mechanism of the astonishing *in-situ* TEM observations, we also conducted atomistic simulations. The results of twinning under tension and detwinning under compression are shown in Figure 4 and 5. In Figure 4a-c, during tension, the incoherent twin boundary migrates toward left. The twinned region uniformly narrows. After the twin boundary moved close to the left end, the tensile load was reversed to compression. The migration of the twin boundary is shown in Figure 5a-c. The twin boundary reverses its moving direction while detwinning occurs. A perfect match between our experiments and simulations can be seen. During twinning and detwinning, no measurable shear strain was produced while the sample surfaces remained atomically flat after the twin boundary traverses, but the sample uniformly narrows during twinning and widens during detwinning.

Theoretically, the twinning shear s for $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ equals $(\gamma^2-3)/(\sqrt{3}\cdot\gamma)$. For Mg, s = –0.129. Hence, a considerable shear strain should be generated during twinning. But in our *in-situ* TEM observations and atomistic simulations, no shear strain was produced. On the other hand, a reversible twinning should invoke a coherent, elastic interface free of dislocations because

dislocation slip is irreversible once the dislocations reach free surfaces. Our results strongly suggest that this particular twinning mode involves no twinning dislocations and results in zero shear strain.

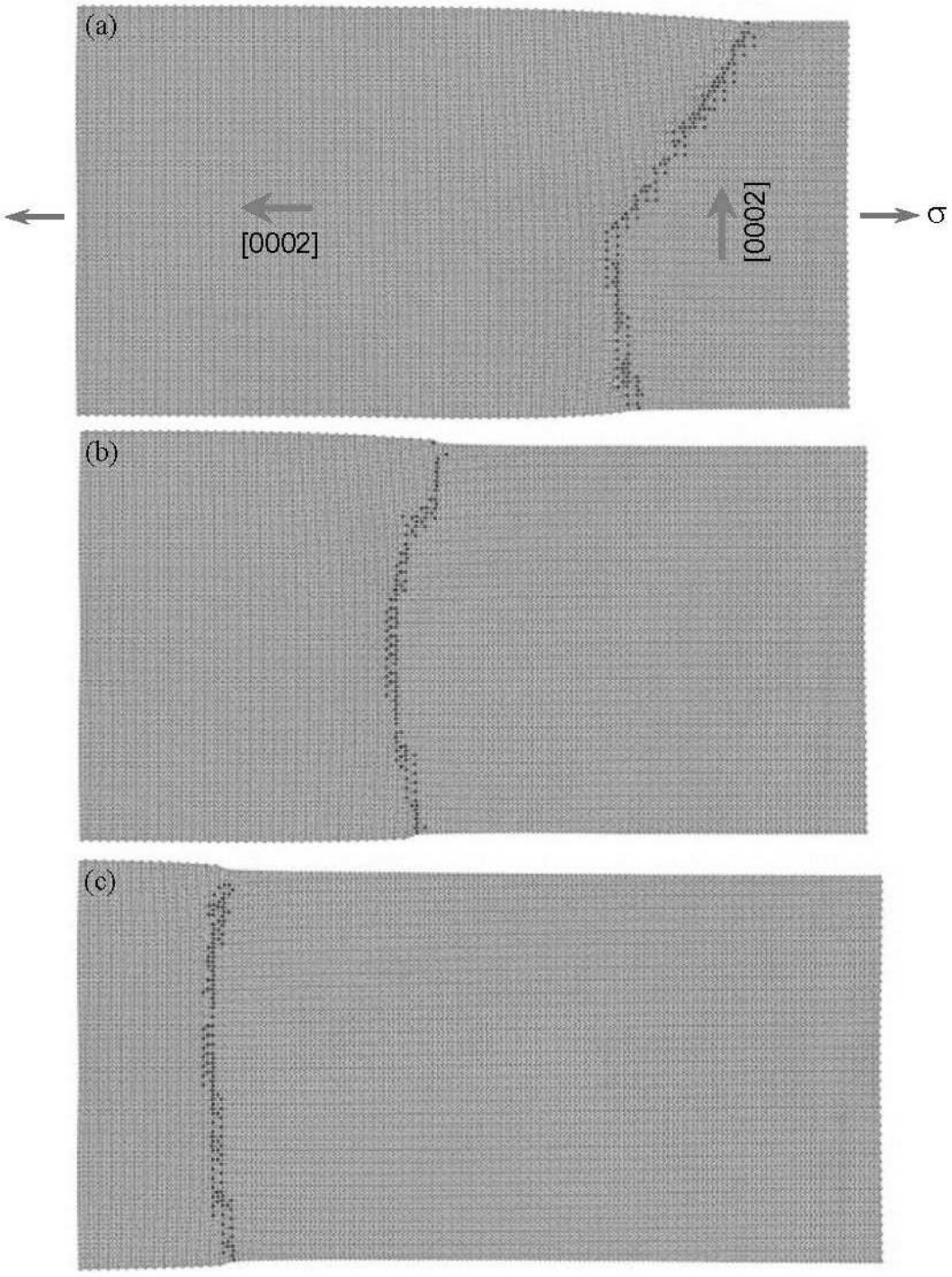

Figure 4. Molecular dynamics simulations of twin boundary migration under a tensile load. The twin boundary migrates toward left and the twin boundary hugely deviates from the twinning plane. The twinned region uniformly narrows without being sheared.

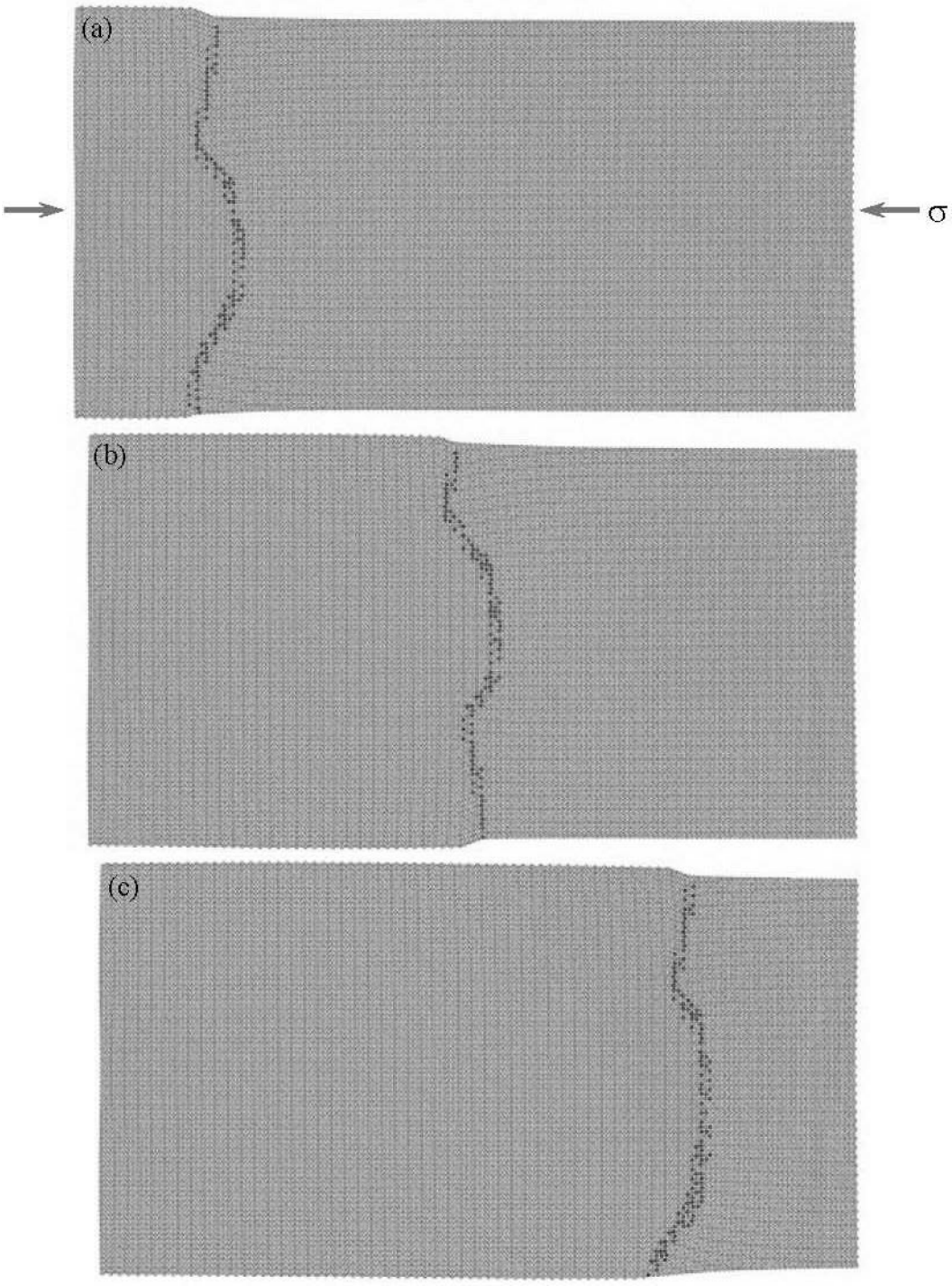

Figure 5. After the twin boundary approaches the left end, the tensile load is reversed to compression. The twin boundary reverses its moving direction and detwinning occurs. During detwinning, the specimen widens uniformly on both sides, different from a shear deformation.

For the predominant twinning mode in hcp materials, i.e., $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$, the theoretical Burgers vector of the twinning dislocation equals $(a(3-\gamma^2))/(2\sqrt{3+\gamma^2})$, where a is the lattice parameter and γ the c/a ratio [3]. For magnesium (Mg), the Burgers vector equals 0.024 nm, which is exceptionally small. Such a small Burgers vector indicates that atomic shuffling should dominate $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning [7].

The tiny, theoretical Burgers vector of the twinning dislocation (0.024 nm for Mg) indicates that, structurally, the twin lattice almost exists in the parent lattice before a homogeneous shear is activated. Li and Ma [7] demonstrated how a twin lattice can be directly reconstructed from a parent hcp lattice without involving any twinning dislocation. In their model, only atomic shuffling is required to accomplish $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twinning. Through concerted shuffles, the correct hcp stacking and c/a ratio are achieved. Immediately, the reversible twinning is well explained: because no twinning dislocations are involved, the twinning process is reversible, and the twin boundary does not have to coincide with the twinning plane, resulting in the huge deviations observed in Figure 2 and in the atomistic simulations.

Conclusions

We performed in-situ TEM observations on uniaxial tension and compression of a Mg single crystal. During extension twinning, the specimen uniformly elongated without being sheared; whereas during compression, detwinning occurred and the specimen uniformly widened across the width without observable shear offset. These observations were supported by our atomistic simulations in which both twinning and detwinning were accomplished by atomic shuffling.

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