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Super-plasticity via secondary twinning in magnesium nanowire revealed by molecular dynamics simulations

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ABSTRACT

We have explored the secondary twinning contribution to the ductility of the magnesium nanowire using molecular dynamics simulations. An ultrahigh 60% elongation is presented in $\langle 1\,1\,\bar{2}\,0\rangle$-oriented nanowires during tensile deformation as result of primary and sequential secondary twinning processes. Crystallographic and stress field analyses identify the dominant contribution from the formation and procreation of $\{\bar{1}\,\bar{1}\,2\,1\}$ mode secondary twin to the elongation. Our results provide new insight of improving structural alloy ductility through twining-induced plasticity at the nanoscale.

1. Introduction

Magnesium(Mg)-based alloys are promising light-weight structural materials while the limited plasticity is a great challenge to their application, which is common in Hexagonal Close-Packed (HCP) metals such as Titanium (Ti) and Zirconium (Zr) [1–8]. Increasing the plasticity of HCP metals by twinning can be an alternative way to overcome this limit when deformation twinning is the prevalent deformation mechanism. Such Twinning Induced Plasticity (TWIP) concept is widely adopted to designing advanced steels [9,10], and has been extended to Mg [4,5,11]. Two important but controversial issues related to deformation twinning in HCP structure should be studied in order that TWIP behavior is effectively applied in Mg: (1) selection of appropriate twinning mode to achieve higher plasticity, and (2) size effect of deformation twinning.

Various twinning modes have been discovered in HCP structures, while their contributions to plasticity are not the same. There are at least five different twinning systems reported in HCP structure [12–14] (i.e. $\{1\,\bar{1}\,0\,1\}|\langle 1\,\bar{1}\,0\,\bar{2}\rangle$,$\{1\,\bar{1}\,0\,2\}|\langle 1\,\bar{1}\,0\,\bar{1}\rangle$, $\{1\,\bar{1}\,0\,3\}|\langle 3\,\bar{3}\,0\,2\rangle$,$\{\bar{1}\,\bar{1}\,2\,1\}|\langle \bar{1}\,\bar{1}\,2\,\bar{6}\rangle$, and $\{\bar{1}\,\bar{1}\,2\,2\}|\langle \bar{1}\,\bar{1}\,2\,\bar{4}\rangle$). Among these twinning modes, the $\{1\,\bar{1}\,0\,1\}|\langle 1\,\bar{1}\,0\,\bar{2}\rangle$ and $\{1\bar{1}02\}|\langle 1\,\bar{1}\,0\,\bar{1}\rangle$ modes are dominant in Mg. $\{1\,\bar{1}\,0\,1\}$ twin is called compression (or contraction) twin since it is usually triggered by the compression along **c** axis of the HCP lattice, and $\{1\,\bar{1}\,0\,2\}$ twin is called tension twin in the same way [4,5,11,15]. TWIP behavior via $\{1\,\bar{1}\,0\,2\}$ twin is experimentally observed in both Mg single crystalline nanowires (NWs) [11] and micro-meter grained polycrystal [4]. On the contrary, contribution of $\{1\,\bar{1}\,0\,1\}$ twin is negligible to plasticity, since the formation of secondary $\{1\,\bar{1}\,0\,2\}$ twin in $\{1\,\bar{1}\,0\,1\}$ twin accounts for the generation of voids in the material [5].

It is worth to note that the secondary twin, though supports a further way for accommodating deformation strain after the first-step twinning, usually has negative effect to plasticity [5,16]. Hence an intriguing question is arisen: could secondary twin be beneficial to plasticity in some special conditions? Furthermore, even ternary twinning can be observed after secondary twinning [17], and could it promote plasticity? So far, most studies on secondary twinning mainly focus on the non-Schmid behavior [6,16] of twin variant selection, where only two types of secondary twin embryo with relatively small Schmid's factor are experimentally observed in $\{1\,\bar{1}\,0\,1\}$ twin. This phenomenon is well explained by the model based on dislocation reactions and corresponding critical shear stress [16], but the question of relationship between secondary twinning and plasticity remains.

Size effect of deformation twinning in HCP metals is more complex than that in wide-studied FCC metals. The trend also shows great difference between single crystalline [1,3,11] and poly-crystalline materials [7,8,18–21]. It is initially observed that deformation twinning is more favored in coarse-grained than fine-grained HCP materials and totally vanishes in nano-crystalline

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HCP materials [7,8,18,19]. Recently, deformation twin has been successfully discovered in nano-crystalline HCP Mg-based alloys. Nevertheless, it is unclear that if such deformation twin is resulted from the contribution of alloy element or ball-milling preparation process [22,23]. Due to such uncertainty, the studies of TWIP behavior are limited to micrometer grained Mg and Ti [4,24], and have not extended to nano-crystalline materials yet. With regard to HCP single crystalline nanowires (NWs) or microwires (MWs), the deformation mechanism goes through several transitions from tens of nanometers to several micrometers scale. Deformation twinning emerges in HCP NWs with a diameter from tens to hundreds nanometer or MWs thicker than several micrometers [2,11], while only slipping of basal or prismatic dislocation occurs in NWs with intermediate size [2,3,20,25]. Within even smaller diameter regime, deformation mechanism of HCP NWs has not been well studied by experiments.

When the size goes to less than tens of nanometers in diameter, ultra-thin NWs generally show abnormal structural and mechanical properties, and TWIP behavior has been discovered in FCC and BCC NWs both in experiments and computer simulations [26–28]. Since experimental and computer simulation results usually show consistency, it is meaningful to expand the study to ultra-thin HCP NWs by adopting preliminary simulations. Previous molecular dynamics simulations performed on the HCP metal NWs verified several deformation mechanisms such as $\{1\bar{1}02\}$ twinning [11,56,57], $\{1\bar{1}01\}$ twinning [11,13,30,57] and phase transformation [29–31] observed in experiments. Nonetheless, the formation of the secondary twinning and the corresponding mechanism in ultra-thin HCP NWs has not been revealed to our best knowledge.

In view of the aforementioned issues, we proposed to further study the deformation mechanism in ultra-thin Mg NWs, as well as the feasibility of TWIP via secondary twinning in primary $\{1\bar{1}01\}$ twin. Our hypothesis was that the NW first deformed via $\{1\bar{1}01\}$ twinning, following which secondary twinning occurred as a further way to accommodate strain and achieve super-plasticity. We carried out molecular dynamics (MD) simulation of the deformation in Mg NWs, since MD is a powerful tool in estimation and illustrating deformation mechanism of materials in atomic scale. The uni-axial tension processes of $\{\bar{1}\bar{1}20\}$ oriented Mg NWs were simulated and TWIP behavior was discovered in this work. Super-plasticity was successfully achieved via secondary twinning, while the twinning mode of secondary twin was the $\{\bar{1}\bar{1}21\}$ mode, a rarely discovered mode in Mg. In Section 2, we presented the details of the simulation conditions. The mechanical properties, structural evolution, crystallography and atomic motion were described in Section 3. The non-Schmid behavior, size dependence of deformation twinning and contribution of Secondary twinning to plasticity were discussed in Section 4.

2. Material and methods

The MD simulation here mainly included two parts of work: (1) uni-axial tension of $<\bar{1}\bar{1}20>$ oriented single-crystalline Mg NWs, and (2) shear process along the $\langle\bar{1}\bar{1}26\rangle$ direction of Mg single-crystal. The simulations were carried out by employing the LAMMPS code [32] and visualized with the Atomeye code [33]. Embedded Atomic Method (EAM) potential fit by Sun et al. [34] was chosen in this work since this potential can accurately describe the slipping of full or partial dislocations and is widely applied in the simulation of deformation in Mg [11,13,15,20].

2.1. Uni-axial tension of NWs

The configurations of the NWs for tensile simulation were initially $\langle\bar{1}\bar{1}20\rangle$ oriented with $\{0001\}$ basal plane and $\{\bar{1}100\}$ prismatic plane surfaces. Such configuration was designed for two purposes: (1) uni-axial tension along $[\bar{1}\bar{1}20]$ orientation will lead to compression along $[0001]$ direction that promotes $\{1\bar{1}01\}$ twinning. At the same time, the basal planar dislocations slipping were suppressed since loading direction was parallel to the basal plane. (2) Surface energies of $\{0001\}$ and $\{\bar{1}100\}$ planes are the first and second lowest calculated with the EAM potential (239 mJ/m^2 and 252 mJ/m^2 respectively). Thus such configuration was relatively stable than others in case of surface relaxation or surface induced structural transformation [29,30].

Cuboid samples of HCP Mg NWs were adopted with the orientations of $x//[\bar{1}\bar{1}20]$, $y//[\bar{1}100]$, and $z//[0001]$. The initial lengths of the NWs were $96\mathbf{a}$ ($[\bar{1}\bar{1}20]/3$ orientation, 30.57 nm), and the cross-section sizes range from $6\sqrt{3}\mathbf{a}$ ($[\bar{1}100]/2$ orientation, 3.31 nm) $\times$ 6c ($[0001]$ orientation, 3.11 nm) to $12\sqrt{3}\mathbf{a}$ (6.62 nm) $\times$ $12\mathbf{c}$ (6.22 nm), where $\mathbf{a}$ and $\mathbf{c}$ were lattice constants for HCP structure. Initial configuration with $12\sqrt{3}\mathbf{a} \times 12\mathbf{c}$ cross-section is exhibited in Fig. 1(a). Free surface condition was adopted for all the three dimensions of the system.

Uni-axial (along the x direction) tensile deformation at a strain rate of 4×10^7 s^{-1} was applied to the NWs under displacement controlled quasi-static schemes [30,35]. Several layers of atoms at the two tips were rigid and responsible for displacement control during the tension, while other atoms were allowed to relax, as shown in Fig. 1(a). During the whole process, Nosé–Hoover thermostat [36] was adopted to maintain the temperature of the movable atoms at 300 K.

2.2. Shear of single-crystal

The simulations of shear process were conducted for three purposes: (1) testing the probability of the formation of $\{\bar{1}\bar{1}21\}$ twin under shear strain; (2) analyzing the atomic motions of twinning; (3) evaluating the yield shear stress for nucleation of $\{\bar{1}\bar{1}21\}$ twinning.

Before creating the configuration of shear, we would first introduce the geometric characters of $\{\bar{1}\bar{1}21\}$ twinning mode. The twinning elements (illustrated in Fig. 1(b)) conventionally consist of: (1) twinning and conjugate (or reciprocal) twinning planes named $\mathbf{K}_1$ and $\mathbf{K}_2$ respectively; (2) twinning and conjugate (or reciprocal) twinning directions named $\boldsymbol{\eta}_1$ and $\boldsymbol{\eta}_2$; (3) normal vector of twinning plane $\mathbf{n}_1$; (4) shear plane $\mathbf{P}$ containing $\boldsymbol{\eta}_1$, $\boldsymbol{\eta}_2$ and $\mathbf{n}_1$; (5) normal vector $\mathbf{s}$ of shear plane. For $\{\bar{1}\bar{1}21\}$ twinning mode in HCP structure, $\mathbf{K}_1 = \{\bar{1}\bar{1}21\}$, $\mathbf{K}_2 = \{0001\}$, $\boldsymbol{\eta}_1 = \langle\bar{1}\bar{1}26\rangle$, $\boldsymbol{\eta}_2 = \langle\bar{1}\bar{1}20\rangle$ and $\mathbf{s} = \langle1\bar{1}00\rangle$, according some previous results [12,37,38].

In order to simulate shear induced $\{\bar{1}\bar{1}21\}$ twinning, the configurations were built in the following way: $y//\mathbf{s}$, $z//\boldsymbol{\eta}_1$ and $x//\mathbf{n}_1$, and y–z plane corresponded to $\mathbf{K}_1$. Atoms of the two $\{\bar{2}\bar{2}42\}$ planes near one tip of the system were kept rigid, and displacement along $\boldsymbol{\eta}_1$ was applied to atoms of two $\{\bar{2}\bar{2}42\}$ planes near the other tip of the system (marked 'displacement' in Fig. 1(c)), while the remained atoms were allowed to relax under thermostat [39]. Constant velocity is applied to control the shear strain rate to be 10^7 s^{-1}. Periodic boundary conditions is applied to z and y direction. Besides, some of the initial configurations with $\{10\bar{1}1\}$ and $\{0\bar{1}11\}$ surfaces were created without periodic boundary condition (the reasons for creating such configurations will be discussed in Sections 3.2 and 4.1), as shown in Fig. 1 (d). Nosé–Hoover thermostat [36] is adopted to maintain the temperature of the movable atoms at 300 K.

2.3. Basal plane vector and mis-orientation

Basal plane vector (BPV) analysis is an effective method to determine the twinning modes and different twin variants in