Computational Materials Science 147 (2018) 272–281

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Atomistic simulation of tension-compression asymmetry and its mechanism in titanium single-crystal nanopillars oriented along the [1 1 $\bar{2}$ 0] direction

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ARTICLE INFO

Article history:
Received 22 November 2017
Received in revised form 9 February 2018
Accepted 10 February 2018
Available online 22 February 2018

Keywords:
α-titanium
Dislocation
Twinning
Stacking fault
Molecular dynamics

ABSTRACT

Molecular dynamics simulations were performed with a Finnis-Sinclair many-body potential to investigate the mechanical properties and deformation mechanisms under applied uniaxial tensile and compressive loads in α-titanium (Ti) single-crystal nanopillars oriented along the ⟨1 1 $\bar{2}$ 0⟩ direction. The results indicate that the mechanical properties and plastic deformation mechanism display tension–compression asymmetry. The non-linear elastic behavior is attributed to the difference in friction between the neighboring atomic planes at the elastic deformation stage under push and pull loading conditions. Increasing the friction leads to hardening with compression. Decreasing the friction leads to softening with tension. Increasing the friction may also lead to higher yield stress with compression compared with tension. Perfect nanopillars are yielded via the nucleation and propagation of {$\bar{1}$ 0 1 0} ⟨1 $\bar{2}$ 1 0⟩ dislocations on the surface and corners of the nanopillars. Prismatic slip is the dominant mode of plastic deformation in the Ti nanopillars under compressive loading. However, {1 0 $\bar{1}$ 1} ⟨1 0 $\bar{1}$ $\bar{2}$⟩ twinning is the dominant plastic deformation mechanism together with prismatic slip under tensile loading. Two typical intrinsic stacking faults (SFs) with different propensities exist in the nanopillars. The microstructural evolution of the SFs was also simulated.

1. Introduction

As technology progresses to smaller and smaller scales, the distinct and fascinating mechanical properties of nanopillars, first discovered by performing nanomechanical experiments [1], distinguishes them from their bulk counterparts. Recently, a great deal of research has focused on the deformation mechanisms of nanopillars, such as hexagonal-close-packed (hcp) α-Ti. As the favored materials of the aerospace industry, titanium and its alloys have captured extensive interest around the world due to their high strength and toughness, excellent resistance to fatigue and corrosion, high temperature performance, and low thermal conductivity [2].

To date, available literature mainly focuses on the mechanical properties and deformation mechanisms of face-centered-cubic (fcc) and body-centered-cubic (bcc) metal nanowires. Although there are fewer studies on hcp crystals than fcc and bcc crystals, the mechanical properties and deformation mechanisms of hcp crystals have also been the subject of a number of experimental and theoretical studies; for example, the deformation mechanisms of Mg and Ti micro- and nanopillars and micro-cantilevers using a variety of loading modes, such as compression, tension and bending, have been investigated in detail [3–11]. It is well established that the critical resolved shear stresses are sensitive to the size of the specimens, and the flow stress approaches the ideal strength of the material as the specimen size decreases. In our previous experiments, the strength of 300 nm pillars reached 16% of the theoretical strength of α-Ti loaded along the [1 1 $\bar{2}$ 0] direction [5]. Experimental and simulation results have confirmed that prismatic ⟨α⟩ slip and pyramidal ⟨c + a⟩ slip are the main deformation mechanisms in [1 1 $\bar{2}$ 0]-and [0 0 0 1]-oriented nanopillars under compression loading [12,13]. No deformation twins were observed during compression along the [0 0 0 1] c-axis. The twinning stress significantly increased with a decrease in sample size for Ti–5Al single-crystalline pillars compressed along the [0 0 0 1] direction, including a transition from twinning to ordinary slip-dominated processes when the sample size was reduced to below 1 μm [3].

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https://doi.org/10.1016/j.commatsci.2018.02.029
0927-0256/

In contrast, twinning is the primary deformation mechanism in bulk single crystals during c-axis compression [14]. Moreover, Yu et al. [4] observed $\{1\,0\,\bar{1}\,2\}$ twinning in tensile-deformed magnesium single crystals and $\{1\,0\,\bar{1}\,1\}$ twinning during compressive deformation.

Dislocation slip significantly contributes to plastic deformation; in comparison, deformation twinning is much more complex and plays an important role in maintaining the homogeneous plastic deformation of hcp materials [15–19]. There are six major twinning systems in hcp Ti [20]: the tensile twinning of $\{1\,1\,\bar{2}\,1\}$, $\{1\,0\,\bar{1}\,2\}$, and $\{1\,1\,\bar{2}\,3\}$ and the compressive twinning of $\{1\,0\,\bar{1}\,1\}$, $\{1\,1\,\bar{2}\,2\}$, and $\{1\,1\,\bar{2}\,4\}$. The activation of deformation twinning systems strongly depends on the testing temperature [21], stress level [22,23], grain size [24,25], strain rate [26], and loading direction [27–32]. The plastic deformation behavior of α-Ti nanopillars may be different from that of coarse-grained α-Ti. Our previous MD simulation results revealed a rare phase transformation from the hcp to fcc phase in single-crystal Ti oriented along the [0 0 0 1] direction during tension [33]. Instead of compression twinning along $\{1\,0\,\bar{1}\,1\}$, the pyramidal ⟨c + a⟩ slip was the main deformation mechanism in single-crystal Ti nanopillars during c-axis compression [13].

Although the mechanical properties and deformation mechanism of Ti at the nanoscale have been studied extensively [34–37], the deformation mechanisms of Ti and its alloys at the nanoscale still need to be explored. To obtain further understanding of the mechanical properties and deformation mechanism in single-crystal Ti, MD simulations were carried out in the present work to investigate the compressive and tensile deformation behavior at the nanoscale. The tension-compression asymmetry of plastic deformation is explained based on the observation of the deformation mechanisms. Meanwhile, the formation mechanism of the two types of SF observed during tensile and compressive deformation is discussed.

2. Simulation model and methodology

In this study, MD simulations are used to investigate the mechanical behavior and deformation substructure of Ti nanopillars with $[1\,1\,\bar{2}\,0]$ orientation under compressive and tensile loadings by using the interatomic potential for Ti within the Finnis-Sinclair many-body potential of Ackland [38]. The Finnis-Sinclair many-body potential equation for the energy of an atom can be expressed by

$$E_i = \frac{1}{2}\sum_j V(r_{ij}) - \rho_i^{1/2} \tag{1}$$

where V is a pairwise function between neighboring atoms i and j.

The potential, ρ_i, is equal to

$$\rho_i = \sum_j \phi(r_{i_j}) \tag{2}$$

where ϕ is the electronic density function and r_{ij} is the distance between atom i and neighboring atom j. The calculated values of the elastic constants are in accordance with the experimental data [39]. This potential has been used extensively in various MD studies, including those for Ti single crystals [12,13,33–36] and nanocrystals [40]. The calculated plastic deformation mechanism of the Ti single crystal is consistent with the experimentally observed mechanism [5]. The Finnis-Sinclair many-body potential is suitable for describing defect evolution in Ti single crystals during loading.

The nanopillar orientations utilized in the present study are schematically shown in Fig. 1. The MD simulation first generated

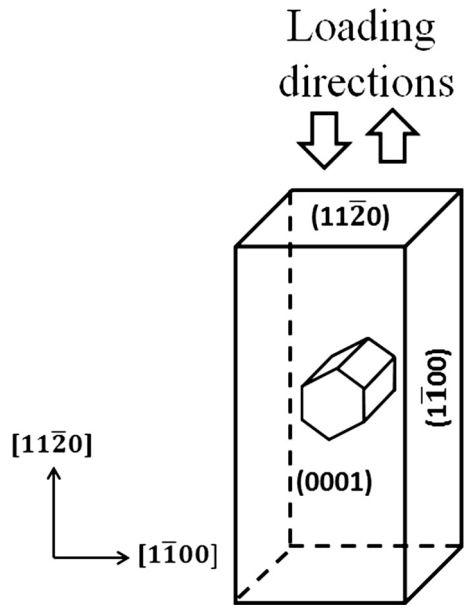

Fig. 1. Schematic of the nanopillar crystallographic orientations and loading directions considered in this paper.

a simulation cell with hcp atoms of orientation $[1\,1\,\bar{2}\,0]$ in the x-direction, $[1\,\bar{1}\,0\,0]$ in the y-direction, and $[0\,0\,0\,1]$ in the z-direction, and free boundary conditions (non-periodic and shrink-wrapped) were applied in all three directions. The height-to-width ratio of all nanopillars considered in the simulations was 2:1, and the dimension of width varied from 12 nm to 15 nm. All MD simulations were performed with a time step of 1.0 fs. Single-crystal nanopillars were loaded along the $[1\,1\,\bar{2}\,0]$ orientation for double prismatic slips. Molecular static calculations by means of the conjugate gradient method were used for energy minimization to obtain equilibrium configurations before uniaxial tensile (or compressive) loading. The nanopillars were then thermally equilibrated at 300 K for 500 ps using a Nosé–Hoover thermostat [41,42]. The canonical ensemble, i.e., constant atom number, volume, and temperature (NVT), was applied to keep the system temperature at a constant 300 K. The relaxed nanopillars were then loaded along the x-direction, with the atoms at the ends fixed to play the role of loading grips. The compressive or tensile strain was applied by a ramp velocity profile to give the minimum strain at one fixed end and the maximum at the other. The strain rate during loading was 1×10^8 s^{-1}. Common neighbor analysis (CNA) [43] was used to distinguish atoms in the (fcc-like) SF from the hcp-coordinated atoms. MD calculations were carried out using the large-scale parallel molecular dynamics program LAMMPS [44] and visualized with the visualization program AtomEye [45]. The compression and tension stress of the nanopillars were calculated as the virial stress, i.e., the average value of all atoms in the system, and the maximum stress is defined as the yield stress. The strain was evaluated as $\varepsilon = \frac{|l_0 - l|}{l_0}$, where l_0 is the initial length of the nanopillars and l is the length of the nanopillars after compression or tension loading.

3. Results and discussion

3.1. Tension-compression asymmetry and size effect

The stress–strain curve of a Ti nanopillar oriented in the $[1\,1\,\bar{2}\,0]$ direction subjected to tension-compression is shown in Fig. 2. The yield stress at the onset of plastic deformation is defined as