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Molecular dynamics study of strain rate effects on tensile behavior of single crystal titanium nanowire

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ABSTRACT

Molecular dynamics simulations were performed to study the tensile behaviors of single crystal titanium nanowire along [0001] direction under different strain rates using the Finnis-Sinclair many-body potential. The applied strain rate is ranging from $10^8\ s^{-1}$ to $10^{11}\ s^{-1}$ ($0.0001–0.1\ ps^{-1}$). At strain rates below $0.01\ ps^{-1}$, the stress-strain curves can be divided into four distinct stages: initial linear stage, sharp drop stage, rapid rise stage and wavelike decrease stage. Structural analysis reveals that the growth of $\{10\bar{1}2\}$ tensile twin leads to the rapid rise stage in stress-strain curves. The evolution of twinning variants indicates that the number of nucleated twin variants increases with the applied strain rate and the overall twin volume fraction decreases with strain rate. At strain rates above $0.01\ ps^{-1}$, three distinct stages are observed in the stress-strain curves. At these strain rates, a rapid transformation to an amorphous state was observed leading to superplastic behavior of nanowire. Besides, deformation mechanism map was constructed for nanowire during tension process at different strain rates.

1. Introduction

Titanium and its alloys have been widely applied in various fields such as chemical equipment, medical machinery and aerospace sector due to their high strength, corrosion resistance and toughness [1]. Room temperature deformation of pure titanium may activate only four independent slip systems (two basal ⟨a⟩ and two prismatic ⟨a⟩ systems) [2]. To accommodate tensile or compression strains along the c axis, either pyramidal ⟨c + a⟩ slip or deformation twinning must be activated. In general, the pyramidal ⟨c + a⟩ slip system is difficult to operate as its associated higher critical resolved shear stress, thus twinning plays an important role in plastic deformation behavior of α titanium [3]. Up to now six types of twinning systems were found in HCP Ti [4], namely $\{10\bar{1}2\}$, $\{10\bar{2}1\}$, $\{11\bar{2}3\}$, $\{10\bar{1}1\}$, $\{11\bar{2}2\}$ and $\{11\bar{2}4\}$. $\{10\bar{1}2\}$, $\{11\bar{2}2\}$ and $\{11\bar{2}1\}$ deformation twinnings are frequently observed at room temperature and low temperature. $\{10\bar{1}1\}$ twins occur at relatively high temperature ($\geqslant$400 °C). $\{11\bar{2}3\}$and $\{11\bar{2}4\}$ twins occur under extremely harsh conditions such as shock loading [5]. The mechanical properties and deformation process of conventional coarse-grained titanium have been studied extensively [6–16]. Deformation twinning is affected by many factors, such as temperature, stress level [6,7], grain size [8,9], strain rate [10], loading direction [11–16] and so on. With the rapid development of material engineering technology, the research of nanowires has attracted significant attention due to their importance in fundamental low-dimensional physics and the potential applications in nanoscale materials and devices. The mechanical behavior and properties of nanowires are not well established due to the complexities involved in mechanical testing at the nanoscale level. Thus, molecular dynamics (MD) simulation has become an important tool for investigating the mechanical properties and deformation mechanisms of nanowires. At present, MD simulations are mainly focused on FCC and BCC metals, such as Cu [17–21], Ni [22], Ag [23,24], W [25], Fe [26–29] and Mo [30]. According to these studies, mechanical properties of nanowires are mainly dependent on deformation temperature and strain rate [17–22]. As strain rate increases or temperature decrease, both yield strength and fracture strain of nanowire increase. Also, mechanical properties of metal nanowires are considerable size-dependent, due to surface effect. It was found that FCC nanowires of size less than 2 nm can undergo phase transformation from FCC structure to a body-centered tetragonal (BCT) structure [31,32]. The deformation behavior of BCC nanowire was found to be strongly dependent on strain rate and strain induced phase transformation from BCC to FCC was observed [26–30]. The interactions between slip and twinning make the deformation mechanisms in

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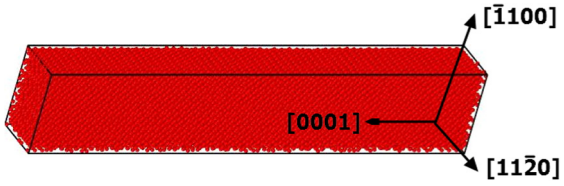

Fig. 1. Initial configuration of Ti nanowire after full relaxation.

HCP metals complex [33]. At present, there is few study on HCP nanowire, especially on its mechanical properties and deformation mechanisms. The dependence of deformation twinning on grain size shows that as grain size decreases, deformation twinning activated is considerable less [8,9]. In single crystal Mg, extensive twinning was observed under various modes of mechanical testing by experimental and simulation studies [34,35]. Nevertheless, MD simulation of nanocrystalline HCP Co found that mechanical twinning seldom took place and deformation was controlled by dislocation [36]. According to tensile and compression tests of coarse-grained titanium, its tensile behavior is controlled by dislocation slip [15,16]. However, compression deformation mechanism is primarily twinning [11–13]. MD simulations revealed a rare phase transformation from HCP to FCC phase in single crystal titanium orientated along [0001] during tension [37]. The pyramidal ⟨c + a⟩ slip was the main deformation mechanism for single crystal Ti nanopillars undercompression test in MD simulation [38]. These findings indicate that plastic behavior of Ti nanowire may be different from coarse-grained HCP metals. In this paper, MD simulations of tensile behavior of Ti nanowire under different strain rates were conducted to investigate plastic deformation mechanism of Ti nanowire.

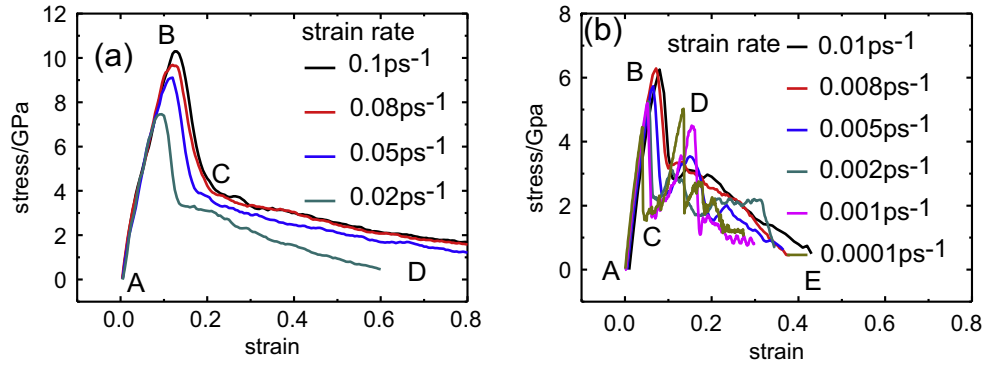

Fig. 2. Tensile stress-strain curves of Ti nanowire at different strain rates. (a) Three stages of stress-strain curves at 0.1–0.02 ps^{-1}: initial linear stage AB, sharp drop stage BC and gradual decline stage CD. (b) Four stages of stress-strain curves at 0.01–0.0001 ps^{-1}: initial linear stage AB, sharp drop stage BC, rise stage CD and wavelike decrease stage DE.

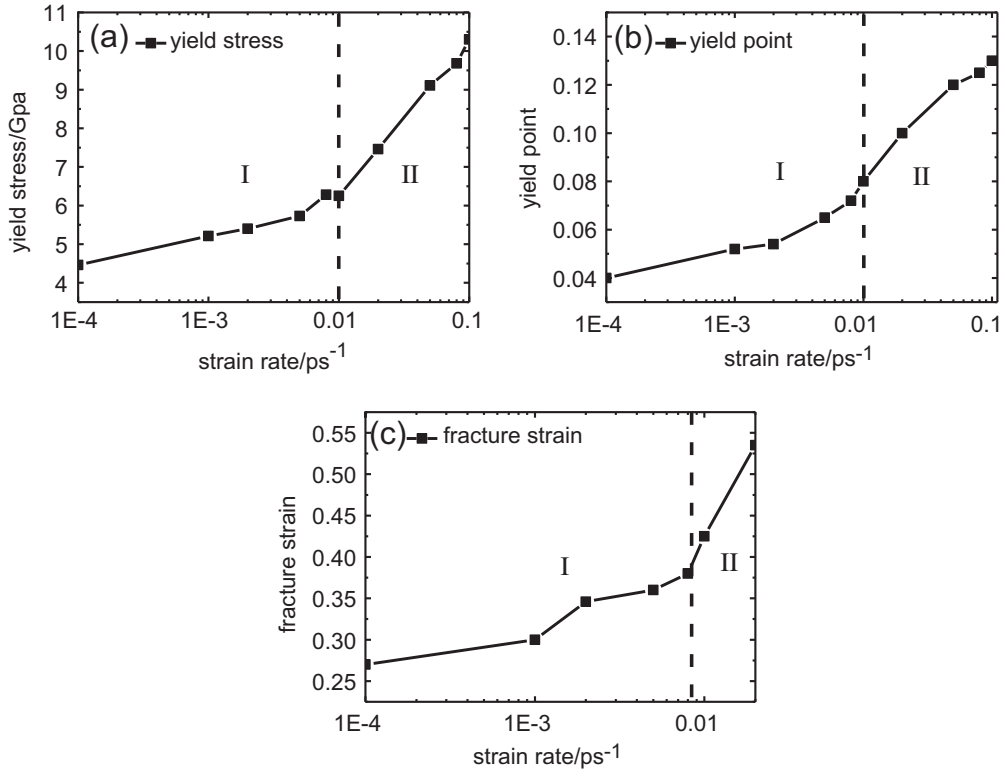

Fig. 3. Tensile properties of Ti nanowire under different strain rates: (a) yield stress; (b) yield point; (c) fracture strain.