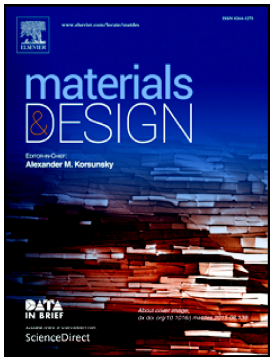

Size-dependent deformation mechanism transition in titanium nanowires under high strain rate tension

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Size-dependent deformation mechanism transition in titanium nanowires under high strain rate tension

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Abstract

Tensile deformation of single crystal titanium nanowires (NWs) with size ranging from 3nm to 20nm along [0001] orientation is investigated by molecular dynamics (MD) simulations. For all NWs, the initial yielding at different strain rates is induced by the nucleation of $\{10\bar{1}2\}$ twinning. Following the saturation of twin volume fraction, the size dependent transition of deformation mechanisms in twinned regions is observed. At the strain rate from 10^8s^{-1} to 10^9s^{-1}, following the deformation twinning, the phase transformation from HCP to FCC dominates the plastic deformation of Ti NWs. By increasing sample size to 20nm, phase transformation can be replaced by prismatic dislocation slip. At the strain rate from 10^9s^{-1} to $10^{10}s^{-1}$, the critical size for the transition from phase transformation to full dislocation slip decreases with the applied strain rate. With further increasing sample size, after the saturation of $\{10\bar{1}2\}$ twins, the initial single crystal NW transforms to nanocrystalline NW. Subsequent plastic deformation mechanism in the nanocrystalline Ti NW with large size is transferred from grain boundary dominate deformation to the cooperation of grain boundary deformation and dislocation activity. Furthermore, deformation mechanism map is proposed to provide a deep understanding of the plastic deformation of Ti NWs.

Key words: molecular dynamics simulation; titanium nanowire; size effect; tensile deformation mechanism

1. Introduction

One-dimensional metal NWs have garnered much attention in recent years due to their unique properties, structures and the potential as the fundamental building blocks of the nanotechnological applications [1-2]. The mechanical behavior and properties of NWs are not well established due to the complex mechanical testing at the nanoscale level. Thus, molecular dynamics (MD) simulations have been performed extensively to obtain material properties at the nanoscale. The atoms on NWs surfaces have fewer neighbors than atoms in the interior. The surface effects have a great effect on the properties of NWs, as the high surface to volume ratio. With the increase of the structure dimensions of NWs, the surface effects become negligible. The surface stress induced phase transformation and pseudo-elastic and shape memory effect have been studied extensively [3-6]. For example, MD simulations have shown that the phase transformation from FCC structure to a BCT structure can be driven by surface stress in FCC NWs [3-4]. MD simulations on BCC NWs show that the strain induced solid-solid phase transitions in iron NWs and the transition temperature was dependent on the wire diameter [7]. Also, plastic deformation mechanism is strongly dependent on the size of NWs [8-13]. MD simulations in [8] demonstrate the size-dependent transition, from super-plastic deformation mediated by twin propagation to the rupture by localized slips in deformed region as the Au nanowire diameter decreases. Iron NWs up to 11.42nm size can undergo twinning mediated