Computational Materials Science 142 (2018) 135–144

Contents lists available at ScienceDirect

Computational Materials Science

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

Investigation on tensile properties of nanocrystalline titanium with ultra-small grain size

Le Chang, Chang-Yu Zhou *, Jian Li, Xiao-Hua He

School of Mechanical and Power Engineering, Nanjing Tech University, Nanjing 211816, China

ARTICLE INFO

Article history:
Received 28 August 2017
Received in revised form 6 October 2017
Accepted 7 October 2017

Keywords:
Molecular dynamics simulation
Nanocrystalline titanium
Size effect
Tensile deformation mechanism

ABSTRACT

Molecular dynamics was used to simulate tensile behavior of nanocrystalline titanium with ultra-small grain size ranging from 2.8 nm to 10.2 nm at the strain rate ranging from 10^8 s^{-1} to 10^{10} s^{-1}. Three dimensional samples with random oriented grains containing no textures were developed by Voronoi tessellation. For all the samples, the yielding is solely controlled by GB mediated process. The inverse Hall-Petch relation between grain size and flow stress was found. The strain rate sensitivity shows increase with the decrease of grain size due to the enhancement of grain boundary (GB) mediated process. Meanwhile, it increases with the applied strain rate due to the local disorder around GBs. Remakeable grain coarsening observed in the 2.8 nm sample causes the slight increase of flow stress. Both GB mediated process and partial dislocation slips play an important role in the plastic deformation of nanocrystalline Ti. With the increase of grain size, rare twins initiated from GBs can be observed. From the size dependent dislocation density analysis, it is concluded that with the increase of grain size, dislocation related deformation contributes more to the plastic strain.

1. Introduction

Nanocrystalline materials have attracted a great deal of attention in recent years, due to their excellent mechanical, physical and chemical properties, in comparison with conventional coarse-grained materials [1]. The mechanical properties of nanocrystalline materials are significantly influenced by their size. The well-known Hall-Petch relation describes that the increase in the flow stress and yield stress is inversely proportional to the square root of the grain size [2]. The deviation from the classic Hall-Petch relation occurs in the case of grains size in the range from hundreds of nanometers to tens of nanometers [3–6]. However, an inverse Hall-Petch relation is observed in nanocrystalline materials when grain size is below tens of nanometers. There have been many reports of the inverse Hall-Petch relation by both experiments [7–12] and molecular dynamics (MD) simulations [13–21]. This transition of strength-size effect as the size decreases is owing to the transition of plastic deformation mechanism from dislocation mediated hardening to the grain boundary (GB) mediated softening [21].

Previous studies were mainly focused on FCC nanocrystalline metals. In comparison with FCC metals, the plastic deformation in nanocrystalline HCP metals has received limited attention, due to the different slip systems and the complicated twinning behavior. Besides, according to the reports of the previous MD simulations [22–24], the simulated nanocrystalline HCP metals were mainly 2D structures with a columnar texture. For instance, MD simulations in [22] reveal the complex interactions between slip and twinning during plastic deformation process in $[11\bar{2}0]$-textured nanocrystalline Mg. MD simulations in [23] investigate the size and temperature dependent flow stress and tension deformation behavior of nanocrystalline Mg with $[11\bar{2}0]$ texture. MD simulations of columnar grain samples of nanocrystalline Zr with [0001] texture show the transition from dislocation-mediated deformation to grain boundary accommodation processes with decreasing sample size [24]. However, the simulated nanocrystalline structures with 2D textures used in these studies are much simpler than those in a real experiment. The fully dense 3D structure is more proper to be applied to reproduce the mechanical properties of nanocrystalline metals in experiments. Zheng et al. [25] investigated the deformation behavior of HCP nanocrystalline cobalt with 3D structure by MD simulation and found that deformation mechanism was partial dislocation slipping and stacking faults, however, deformation twinning was rarely observed. Besides, the atomistic simulation results [26] of HCP cobalt revealed that below 10 nm, the plastic flow of nanocrystalline cobalt was not controlled solely by the GB-mediated processes,

* Corresponding author.
E-mail address: changyu_zhou@163.com (C.-Y. Zhou).

https://doi.org/10.1016/j.commatsci.2017.10.017
0927-0256/

which is different from FCC nanocrystalline metals, as in this range of grain size, GB-mediated deformation mechanisms are believed to be dominant.

Though MD simulations have been extended to gain insight into the mechanical properties of HCP Mg (c/a = 1.624) [22,23], Zr (c/a = 1.593) [24] and Co (c/a = 1.623) [25,26], it is necessary to investigate mechanical properties of nanocrystalline Ti (c/a = 1.587). Nanostructured Ti were prepared by equal channel angular [27,28], pressing hydrostatic extrusion [29], surface mechanical attrition treatment [30], ball milling [31,32] and high energy shot peening [33,34] with grain size in the range from hundreds of nanometers to tens of nanometers. These experiments show that size dependent strength follows the Hall-Petch relation and the underlying deformation mechanism. For instance, nanoindentation hardness tests have shown the extremely small activation volume of $\sim 5b^3$ in nanocrystalline Ti with grain size about 76 nm and the underlying deformation mechanism for nanocrystalline Ti including the interactions between dislocation and grain boundary [27]. Liu and Li [33] investigated the deformation mechanisms of nanocrystalline α-Ti with different sizes. Their work implies that dislocation slip is the dominant deformation mechanism and twinning contributes much less to deformation. The occurrence of deformation twinning is attributed to the extremely high stress due to specific grain orientations and the large strain rate [34]. However, the mechanical properties and the underlying deformation mechanisms including GB mediated process, partial or full dislocation slip and deformation twinning of nanocrystalline Ti with grain size below 10 nm are unclear. Therefore, in this paper, 3D structures with randomly oriented grains were constructed to investigate tensile properties of nanocrystalline Ti and deformation mechanisms for the inverse Hall-Petch plasticity. Meanwhile, both the effects of grain size and strain rate were considered.

2. Simulation approach

In our simulation, three dimensional nanocrystalline titanium samples with different mean grain size from 2.8 nm to 10.2 nm were produced based on Voronoi construction [35]. Each cubic sample contains 100 defect-free and randomly oriented grains containing no textures. The number of atoms in the samples varies from about 4.5×10^5–7.1×10^6 according to the mean grain size of the samples.

MD simulations reported in this article were performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [36]. The Finnis-Sinclair many-body potential developed by Ackland [37] was adopted to describe the interatomic interactions, as the simulation results of previous MD simulations [38–41] using this potential show good agreement with the experimental results. Periodic boundary conditions were applied in three dimensions to mimic the situation that is deep within the bulk of a larger sample. Before loading, the samples were fully relaxed in NPT ensembles at 300 K for 100 ps to reach a equilibrium state with zero pressure. The time step used in the simulation was 1 fs. Then uniaxial tensile deformations along z-axis were conducted at strain rates of 10^8–10^{10} s^{-1} at 300 K. During the tensile simulations, again in NPT ensembles, the pressure of x-axis and y-axis was kept at zero to ensure the uniaxial loading condition. Visualization software OVITO [42] was used to visualize the tensile process. Atoms are rendered with common neighbor analysis (CNA): white, grey and green atoms respectively denote normal (HCP), disordered (non-HCP or FCC) and stacking faults (FCC). Fig. 1 shows a relaxed structure at 300 K with grain size of 7.5 nm.

3. Results and discussion

3.1. Stress-strain response of nanocrystalline Ti

Fig. 2 shows the true stress-strain curves of nanocrystalline Ti with different mean grain sizes at different strain rates. For each sample, below the strain rate of 10^9 s^{-1}, flow stress increases slowly with the applied strain rate, however, beyond this value, it increases rapidly with the strain rate, indicating the different strain rate sensitivities at different strain rates. Besides, Young's modulus increases with the applied strain rate for the smallest sample in Fig. 2(a), slight increase of flow stress with the applied plastic strain can be seen at the strain rate of 10^8 s^{-1}, which is absent at other all deformation conditions. At the strain rate ranging from 10^9 s^{-1} to 10^{10} s^{-1}, bumps can be observed at the strain beyond 6% in the true stress-strain curves. Besides, the ridgy shape in the stress-strain curves becomes significant with the increase of strain rate and grain size, which can be seen in Fig. 2(b)–(d), as for the simulated sample with large mean grain size, the burst of dislocation nucleation event is more significant.

3.2. Tensile mechanical properties

Due to the higher strain rate used in MD simulations, the peak stress in the stress-strain curves is amplified. After reaching the peak stress, the flow stress gradually decreases to a steady-state level. Therefore, in order to investigate the grain size dependent plastic deformation, it is more physically meaningful to compare the average flow stress over a certain strain interval [17,43]. To avoid the effects of crack formation, average flow stresses in the plastic strain 8–12% were selected for comparison. For all samples,

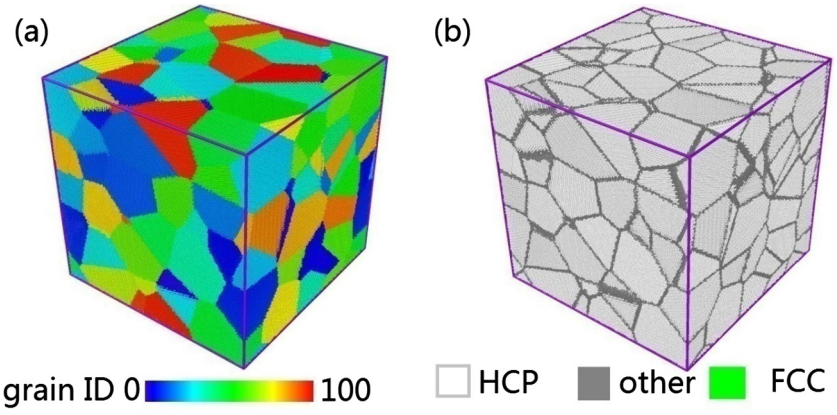

Fig. 1. The initial configuration of nanocrystalline Ti with an average grain size of 7.5 nm colored by (a) grain identity number and (b) common neighbor analysis.