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Strain rate dependence of tension and compression behavior in nano-polycrystalline vanadium nitride

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ABSTRACT

We performed molecular dynamics (MD) uniaxial tension and compression simulations of nano-polycrystalline (npc) vanadium nitride (VN) with different strain rates to investigate strain rate effects and tension-compression asymmetry in npc VN. The Zener's familiar anisotropy index *A* of the polycrystalline VN model is 0.957, very closed to 1.0, demonstrating its elastic isotropy. The Young's modulus increases with the increase of strain rate. The yield strain, yield stress and flow stress increase in power form with the increase of strain rate. As the strain rate varies in the range between 5E8 and 1E9 s^{-1}, strain rate effect becomes insignificant, and the corresponding loading can be regarded as quasistatic or low strain rate loading. Tension-compression asymmetry was observed and analyzed systematically. The elastic tension-compression asymmetry should be ascribed to the higher friction in compression, the asymmetry of interatomic potential, and the effect of cutoff distance in a MD simulation. While the plastic tension-compression asymmetry should mainly result from the different kinds of atomic interaction, intergranular fracture and dislocation glide. No distinct grain boundary sliding was found.

1. Introduction

Grain boundaries (GBs) have been acknowledged to play an important role in the mechanical properties of bulk materials due to that they can react with incoming defects and serve as dislocation source and dislocation storage. The well-known Hall-Petch relation [1,2] was proposed to describe the dependence of grain size on strength, specifically, the strength increases with the decrease of grain size. Therefore, grain refinement is thought as an effective way to enhance the mechanical properties of materials. However, it was found that there is a critical grain size, below which the strength would decrease with the further decrease of grain size, known as inverse Hall-Petch relation [3].

Molecular dynamics (MD) simulation, as a powerful means, has been widely used to understand the mechanical response of nano-polycrystalline (npc) metals under various loading conditions [4]. Swygenhoven et al. [5] analyzed in details the nucleation and propagation of dislocations from the grain boundaries in npc Aluminum. Schiotz et al. [6] performed MD simulations for tension of npc Cu samples with various grain sizes, and found that the flow stress reaches a maximum as the grain size decreases to a critical value, then the flow stress falls if the grain size further decreases, which was attributed to the transition from dislocation-mediated plastic deformation to grain-boundary-associated mechanisms [7]. Li et al. [8] simulated the tension of twinned nanocrystalline Cu samples with different twin thicknesses λ and found that there is a critical λ, below which the flow stress decreases with the decrease of λ. However, Zhou et al. [9] and Zhu et al. [10] found that, when subjected to an external stress parallel to the twin planes, the strength of nano-twinned Cu may keep increasing even though λ falls to a sufficiently small value, which is different from that reported by Li et al. [8]. So far most work about the grain size effects on strengthening/softening behavior focused mainly on metals [4], less progress about grain size effect has been achieved in transition metal nitrides (TMNs). TMNs, such as vanadium nitride (VN) and titanium nitride (TiN), have attracted a great deal of interest in recent years due to their excellent physical and mechanical properties, such as high hardness and extraordinary resistance against wear [11–13]. However, at the present stage, studies were mainly focused on single crystalline TMNs. For examples,

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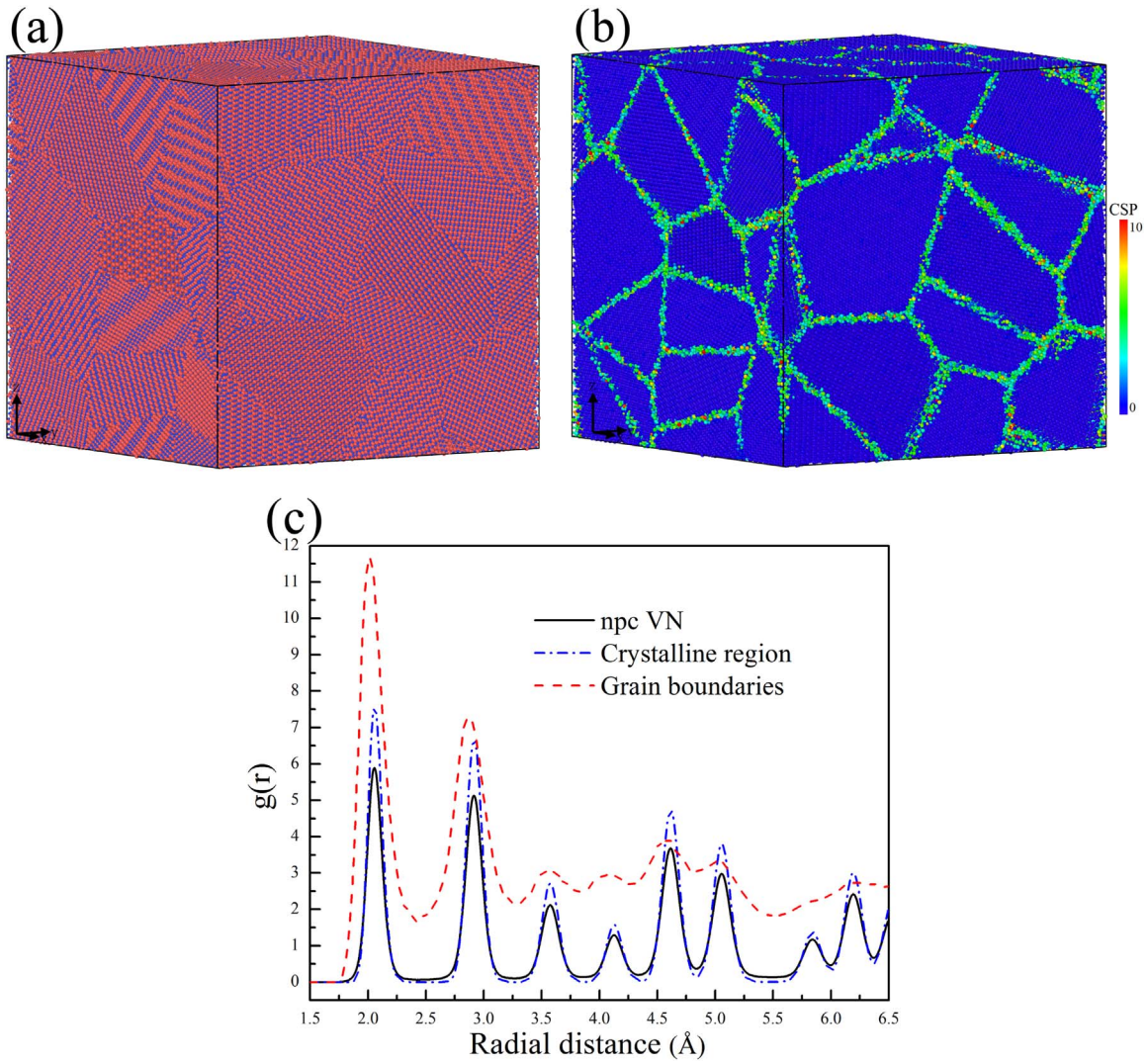

Fig. 1. Atomic configuration of a npc VN model with mean grain size of 7.0 nm after relaxation at 300 K. (a) Colored with atomic type and (b) colored with *CSP*. (c) RDF distributions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

for single crystalline VN, break of bonds was thought as the dominant failure mechanism in tension [14], while dislocation glide and twinning were considered as the main deformation mechanisms during the nanoindentation on its (001) [15] and (111) [16] surfaces using a cylindrical indenter. Deformation mechanisms are closely related to the state of stress, which may account for that they are quite different under tension and under compression. Fu et al. performed MD simulations for the nanoindentation VN (001) with a spherical indenter [13] to investigate the primary plasticity and the formation mechanisms of four kinds of dislocation loops. Yang et al. [17] explored the deformation mechanisms in Ti/TiN multilayer under compressive loading using MD simulation, where the in-plane grain size effects have not yet been taken into account. GBs were usually observed in bulk TMNs [11,12,18,19], metal/TMNs ceramic multilayers [20,21] and TMNs ceramic multilayers [22,23] in experiments. Therefore, it is necessary to explore the mechanical properties of polycrystalline TMNs, especially, whether the tension-compression asymmetry exists in nc TMNs and what the underlying mechanisms are. On the other hand, the time scale in MD simulations is small, thus the strain rate in MD simulations is much larger than that in experiments. To find a suitable strain rate, which is comparable with that in experiments, is significant for the investigation of the size-dependence of mechanical responses using MD simulations.

In this article, we performed MD uniaxial tension and compression simulations of npc VN with average grain size of 7 nm at different strain rates to investigate the strain rate effects and tension-compression asymmetry of VN at nanoscale.

2. Simulation details

The modified embedded atom method (MEAM) potential [24–26] is adopted to describe the interatomic interaction of the V-N system. The detailed parameters of the MEAM potential for the two single elements, V and N, and the binary V-N system have already been given by Baskes et al. [27], Lee et al. [28] and Fu et al. [14], respectively. These potential parameters can reproduce the physical and mechanical properties of VN [14] and have been widely used in the simulations of the mechanical behaviors of VN subjected to uniaxial tension [14] and nanoindentation [15,16,29].

A three dimensional polycrystalline model with average grain size of 7 nm is built based on the Voronoi construction with 27 random "seeds", and the size of the model in each direction is 21.0 nm. Before relaxation, the overlapped atoms, defined as those in the pairs of atoms whose separation distance are less than 1.0 Å, are removed to avoid abnormally high local stress. The number of the atoms in the model is about 1.055×10^6 after removing the overlapped atoms. Subsequently, the model is optimized using the conjugate gradient algorithm to achieve a minimum equilibrium energy state. Before tension and compression, the polycrystalline model is relaxed at 300 K for 200 ps