Atomistic Simulation Study on the Tensile Deformation Behaviour of Nanocrystalline Ni

Wenbin Li[a], Fuping Yuan[b] and Xiaolei Wu[c]

State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

[a]liwenbin0115@163.com, [b]fpyuan@lnm.imech.ac.cn, [c]xlwu@imech.ac.cn

Keywords: Nanocrystalline materials, Molecular dynamics simulations, Plastic deformation, Stress states.

Abstract. Using molecular dynamics simulations, the influence of transverse tensile stresses on the plastic deformation behaviour of nanocrystalline (NC) Ni under tension has been investigated. The sample with an average grain size of 20 nm was created using a Voronoi construction, and two different tensile tests of the sample were performed at a constant strain rate. The simulation results revealed that more partials were emitted from the grain boundaries and propagate into the grain interiors after adding the transverse tensile stress, enhancing the dislocation density in the grain interiors. This increased dislocation density can cause additional strain hardening observed in the stress strain curve. Meanwhile, it was observed from microstructures that nanovoids are easier to form and coalesce into cracks under the biaxial stress state, causing strain softening. The two competing effects of the transverse tensile stress on the plastic deformation behaviour of NC Ni resulted in the flow stresses from 4% to 10% strain in the biaxial stress state slightly larger than those in the uniaxial stress state.

Introduction

Because of their remarkable mechanical properties, nanocrystalline (NC) metals have been the focus of much research in recent years. Extensive investigations over the past decades have indicated that freestanding NC metals usually exhibit a significantly high strength and a very limited tensile ductility [1, 2]. The brittleness is believed to be the heel of Achilles of NC metals, which is often attributed to strain localization originating from the lack of an effective hardening mechanism under uniaxial tensile deformation [3]. However, a good tensile plasticity can be achieved in the NC Cu film when confined by a coarse-grained Cu substrate [4]. Unlike a freestanding NC metal film, the substrate-supported NC metal film can effectively suppress strain localization under tension, but the deformation mechanism is still not fully understood.

Previous studies [5, 6] have shown that the necessity for strain compatibility in the thin film–substrate composite system would cause transverse stresses to be induced, giving rise to non-negligible biaxial stress states in the thin film. Numerous experiments and molecular dynamics (MD) simulations have revealed that mechanical properties and plastic behavior of nano-structured materials are closely related to the loading direction and stress states [7-9]. These results raise a question: What effects of transverse stresses appearing in a certain deformation stage on the plastic behavior?

In this regard, the plastic deformation behaviours of NC Ni with an average grain size of 20 nm under both uniaxial and biaxial stress states have been investigated using MD simulations in the present study. The results and findings should have implications for understanding the plastic deformation behaviour of the substrate-supported NC metals.

Simulation techniques

The simulations are performed on a three-dimensional polycrystal sample with an average grain size of 20 nm. The sample containing 16 grains is generated using a Voronoi construction and all the grains in the sample are randomly oriented.

Before starting a simulation, the simulated system was first subjected to energy minimization by the conjugate gradient method, then gradually heated up to the desired temperature in a step-wise fashion, and finally relaxed in the Nose/Hoover isothermal-isobaric (NPT) ensemble under both the pressure 0 bar and the temperature 300 K for 100 picoseconds. The relaxed system is shown in Figure 1. The Ni system is simulated using embedded atom method potential developed by Mishin *et al.* [10]. Periodic boundary conditions are imposed in all three directions during loading. The local atomic arrangement of the deformed configuration is visualized using the common neighbor analysis (CNA) method, in which black or blue color represents perfect fcc atoms, cyan color represents atoms in stacking faults and green or red color represents atoms in grain boundaries (GBs) and dislocation cores.

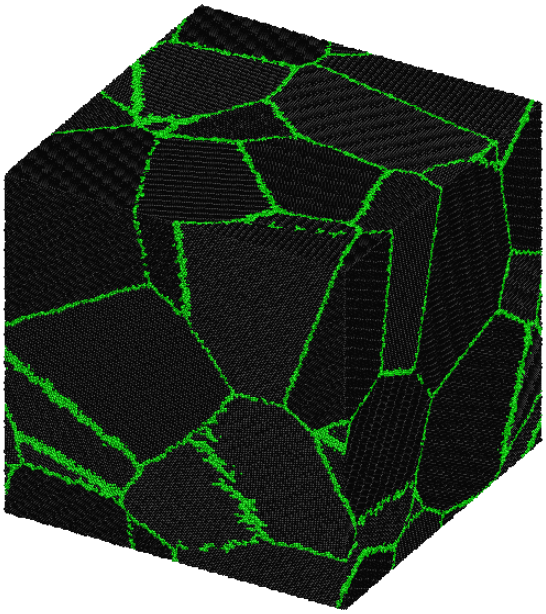

Fig. 1. The initial configuration of NC Ni system with an average grain size of 20 nm. The simulation box contains 16 grains having different lattice orientations, and periodic boundary conditions are applied in all three spatial directions. Atoms in the grain boundaries have been marked with a green color.

During a simulation, the sample is stretched along x direction with a constant strain rate of 5×10^8 /s. Two simulations are performed under different stress states in order to investigate the effects of transverse stresses on the plastic behaviour. The first simulation is performed under a tensile deformation along x direction with zero pressure in two other directions orthogonal to the tensile axis. Then, according to the first simulation, a strain ε_m corresponding to the peak stress σ_m is identified in the stress–strain curve. Then the second simulation is performed under the same tensile deformation along x direction as the previous case, except that the stresses in y direction are set to a certain value (approximately two-tenth of σ_m) at and after tensile strain ε_m. During the first tensile deformation, the system is in uniaxial stress states, while in the second tensile test, transverse tensile stresses are imposed in the plastic stage, causing stress states changing from uniaxial stress states to biaxial stress states.

Results and discussion

To investigate the effect of transverse tensile stresses appearing in the plastic stage on the plastic behavior, stress–strain curves and detailed microstructures of the two different tensile tests are compared. Figure 2 shows the stress–strain behavior of the system.

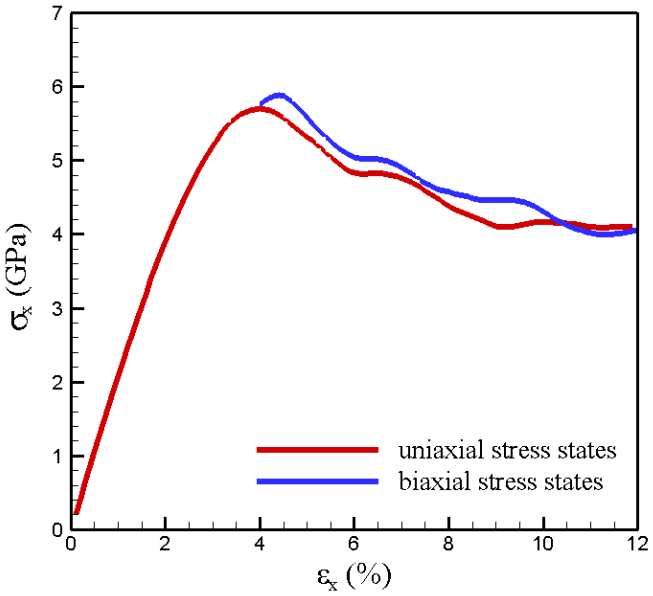

Fig. 2. Stress–strain curves obtained for the tensile deformation along x direction in the uniaxial stress state and the biaxial stress state. The constant strain rate is 5×10^{8} /s along x direction.

Due to the fast strain rate, the values of the flow stress obtained from MD simulations are high compared to experiments. From the curve of uniaxial stress states, a plastic deformation starts at approximately 3.4% strain, just before the maximum stress is reached, according to a recent experimental investigation [11]. Tensile stress increases with strain up to 5.7 GPa corresponding to 4% strain, before gradually decreasing to a steady value. When stresses in the y direction are set to 1.0 GPa (approximately two-tenth of 5.7 GPa) at and after 4% strain, we can obtain a stress–strain curve under the biaxial stress state, as shown in Figure 2. Under the biaxial stress state, tensile stress increases to 5.9 GPa at 4.4% strain, then decreases to a steady value similar to that of under the uniaxial stress state. The drop of tensile stresses in the two stress–strain curves is due to the high strain rates generally employed in MD simulations. After changing the stress states, the tensile behavior does not show significant difference. However, the flow stresses from 4% to 10% in the biaxial stress state are slightly higher than those in the uniaxial stress state. Here we focus on the deformation processes on this region. The results are investigated in the following.

As for NC Ni with a mean grain size of 20 nm, plastic deformation is dominated by partial dislocations [12, 13]. Leading partials are nucleated from and absorbed by the GBs without the emission of trailing partials in the same slip plane, creating substantial stacking faults in the grain interiors. Instead of the emission of a trailing partial in the same plane, a twinning partial in an adjacent slip plane is possibly emitted from some GBs after the emission of a leading partial. In this case, a deformation twin forms. Both leading partials and twinning partials are Shockley partials with the same (a/6) <112> type of Burgers vector, but they play different roles in plastic deformation. The former carries conventional dislocation slip, while the latter takes part in twinning or de-twinning.

From a slip vector analysis [14] and detailed atom inspection of several different cross sections, total partials and twinning partials densities in the grain interiors are measured, as shown in Figure 3. The total partial dislocation density consists mainly of leading partials and twinning partials densities in the grain interiors. Figure 3 shows that densities of total partials from 5% to 9% strain in the biaxial stress state are higher than those of in the uniaxial stress state. The measured total partial density reaches to 31.7×10^{10} cm^{-2} in the biaxial stress state at 6% tensile strain, including the twinning partial density of 8.3×10^{10} cm^{-2}. The corresponding total partial and twinning partial density are 27.5×10^{10} cm^{-2} and 3.8×10^{10} cm^{-2} respectively in the uniaxial stress state. The increased dislocation density after changing stress states is largely attributed to the increased twinning partial density. It is demonstrated that compared to uniaxial stress states, different slip systems can be activated to form different microstructures with the help of transverse stresses, as shown in Figure 4.

From the pictures in Figure 4 showing a section of the three dimensional system, it is found that the GBs react differently under the uniaxial and the biaxial stress state.

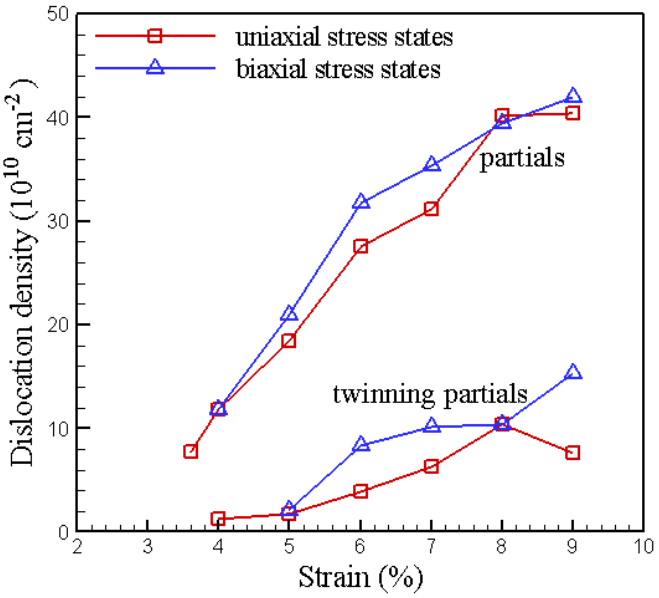

Fig. 3 Partials and twinning partials densities in the grain interiors during tensile deformation processes under the uniaxial stress state and the biaxial stress state. Partials mainly consist of leading partials and twinning partials.

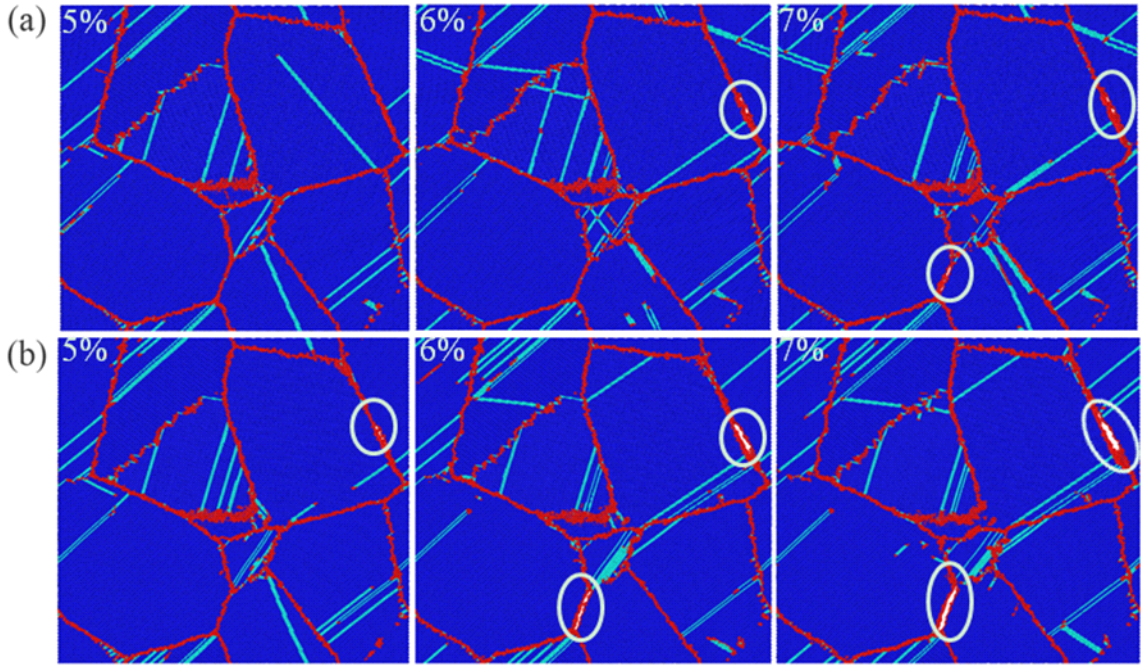

Fig. 4 Three snapshots showing microstructures of a section at 5, 6, 7% tensile strain under (a) the uniaxial stress state and (b) the biaxial stress state. The atoms are colored according to their CAN values, where the red colored atoms represent grain boundaries and dislocation cores, the cyan colored atoms represent stacking faults, and the blue colored atoms represent fcc.

The pictures in Figure 4 show a sequence of tensile deformation at 5, 6, and 7% tensile strain under the uniaxial and the biaxial stress state. Cracks are observed in the inter-granular regions, such as GBs and triple junctions, during deformation. As for NC Ni, crack formation during tensile tests could be another reason of reduced flow stress, in addition to the stress relaxation caused by fast strain rates in MD simulations. In the uniaxial stress state, as shown in Figure 4 (a), nanovoids are not observed up to 6% strain. However, under the biaxial stress state, as shown in Figure 4 (b),

nanovoids begin to form at 5% tensile strain and coalesce into cracks at 7% strain. Significant cracks are observed at 7% strain in the biaxial stress state but not in the uniaxial stress state. The result reveals that cracks are easier to form under the biaxial stress state than under the uniaxial stress state.

Conclusions

The effect of transverse stresses on the plastic behavior of NC Ni has been investigated using MD simulations, and the following conclusions can be drawn:

(1) More partials, especially twinning partials are nucleated from GBs and propagate into the grain interiors after adding the transverse tensile stress in a certain deformation stage. The increased partials in the grain interiors under the biaxial stress state can inhibit the dislocation motion, causing strain hardening.

(2) Nanovoids are easier to initiate and coalesce into cracks in the biaxial stress state, causing strain softening.

(3) There exist two competing effects of the transverse stress on the plastic deformation behaviour of NC Ni. From 4% to 10% strain, the effect of transverse stresses is dominated by partials increasing, resulting in the corresponding flow stresses larger than those in the uniaxial stress state.

Acknowledgements

The authors would like to acknowledge the financial support of 973 Program of China (Nos. 2012CB932203 and 2012CB937500) and NSFC (Grant Nos. 11002151 and 11072243).

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