Computational Materials Science 142 (2018) 389–394

Contents lists available at ScienceDirect

Computational Materials Science

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

Molecular dynamics simulations of tensile deformation of gradient nano-grained copper film

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ARTICLE INFO

Article history:
Received 22 August 2017
Received in revised form 21 October 2017
Accepted 23 October 2017

Keywords:
Plastic deformation
Gradient nano-grained copper
Molecular dynamics simulation

ABSTRACT

Molecular dynamics simulations are performed to investigate the plastic deformation of a gradient nano-grained (GNG) copper film. An extra strengthening is observed in the GNG film which indicates there is synergetic interaction between different grain-size layers. The plastic deformation of the GNG film occurs first in small grains and then propagates into larger grains with increasing strain. This orderly plastic deformation process is attributed to the GNG structure and found independent of strain rate and temperature. Grain coarsening induced by the deformation is apparently suppressed in the GNG film due to the GNG structure.

1. Introduction

Nano-grained (NG) metals usually exhibit several times higher in strength than their coarse-grained counterparts but a very low tensile ductility [1,2]. The tensile brittleness of NG metals hinders their technological applications because of their immediate failure when the load exceeds their yield strength. Gradient microstructures, in which the grain size increases along the depth from nanoscale to micrometres, have been found to be an effective strategy to improve the ductility of nano-structured metals [3–8].

Many methods were used to produce gradient microstructures in metals, such as surface mechanical attrition treatment [9], surface mechanical grinding treatment (SMGT) [4] and platen friction sliding deformation [10]. A GNG copper surface layer was prepared by the SMGT on a coarse-grained (CG) copper substrate and showed a tensile plasticity comparable to that of the CG substrate [4]. The extraordinary ductility of the GNG surface layer was attributed to the effective suppression of strain localization by the gradient microstructure. Other observations [7,8] also indicated the GNG surface layer has an intrinsic tensile plasticity when the GNG surface layer is confined by the CG copper substrate with a gradient grain-size transition. The plastic deformation of a copper sample with a gradient microstructure was observed to occur orderly from coarse grains to small grains with increasing loads [7] by scanning electron microscope (SEM). This behavior suppresses the strain localization through the release of stress between neighboring grains of different sizes [3].

Strength-ductility synergy was also achieved in some engineering alloys with the GNG structures [5,11–13]. However, the mechanisms of the strength-ductility synergy of different engineering alloys were different, and they were also different to that of the GNG copper sample mentioned above [4]. In this work we focus our study on pure copper with GNG structure for simplicity.

In order to investigate the mechanical behavior of metals and alloys with the GNG structure on their surface, Li et al [14–16] developed dislocation-based theoretical models. The proposed theoretical models well captured the experimental results. Molecular dynamics (MD) simulations were also used to investigate the tensile deformation mechanism of Fe with the GNG structure [17] and the fracture behavior of precracked nanocrystalline Ni with grain size gradients [18]. However, these simulations were performed on a columnar grain structure with grain size gradients. MD simulations on a fully 3-dimensional grain structure may give more insight into the plastic deformation of metals with GNG structures, although in this case the grain size range which can be simulated is limited due to limited available computational resources.

Although the above-mentioned experimental observations [4,7] indicate the GNG layers may have an intrinsic tensile ductility comparable to the CG counterparts, the intrinsic tensile plasticity of free standing GNG films was still hardly observed experimentally because of the strain localization and early necking during deformation tests which induce cracking before the activation of plastic deformation mechanisms in the nanocrystalline films. MD simulations have been widely used to investigate the plastic deformation of nanocrystalline metals [19,20–24]. However, MD simulations on the plastic deformation of fully 3-dimensional GNG film models have not been reported until now.

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https://doi.org/10.1016/j.commatsci.2017.10.043
0927-0256/

In this work, we perform MD simulations to investigate the atomistic deformation mechanism of GNG copper film. The simulation results reveal a different plastic deformation behavior of the GNG film in comparison with the GNG layer adherent on a coarse-grained copper substrate. For the GNG film, the plastic deformation is observed gradually propagating from small grain-size layer to large grain-size layer with increasing strain. An extra strengthening induced by the GNG structure is also observed. Additionally, the influence of strain rates and temperature on the plastic deformation behavior of the GNG copper film is investigated.

2. Simulation details

MD simulations were carried out using the LAMMPS code [25]. An embedded-atom method (EAM) potential developed by Mishin et al. [26] was used to describe the interaction between copper atoms. Three fully 3-dimentional models, i.e., one GNG model and two homogeneous NG models, were constructed using the Voronoi tessellation technique [27,28] with random grain orientation containing no textures. To generate the homogeneous NG models, random grain centers were distributed in a simulation cell, and then Voronoi regions were generated to include the grain centers. These regions were filled with atoms in fcc lattice with random crystal orientations. The procedure for generating the GNG model is almost the same as that for generating the homogeneous NG models. The only difference is that the number of grain centers is distributed in a gradient form along the x direction.

In order to simulate the uniaxial tension of GNG or NG films, periodic boundary condition was applied along the y and z directions and non-periodic boundary condition was imposed in the x direction during the MD simulations. Energy minimizations using the conjugate gradient method were performed on three models first, and then they were relaxed at 300 K for at least 50 ps using the NPT ensemble [29], allowing unfavorable configurations in grain boundaries to relax. The relaxed atomic configurations of the three models are shown in Fig. 1, and the color coding is according to the adaptive common neighbor analysis (CNA) [30] performed in the OVITO code [31]. Green color represents perfect fcc atoms, red color represents perfect hcp atoms, and others represent the non-12-coordination atoms. The GNG model contains 1214708 atoms, with grain sizes increasing gradually from ~2.5 nm to ~10.5 nm (Fig. 1(a)). The two homogeneous NG models with mean grain sizes of 5.5 nm and 10.5 nm contain 674121 and 1027441 atoms, respectively. Uniaxial tension along the y direction was simulated with different strain rates and temperatures, meanwhile the overall pressures in the x and z direction were kept to zero using the NPT ensemble. At each time step, the sample length along the y direction was changed according to the given strain rate and the positions of atoms were rescaled.

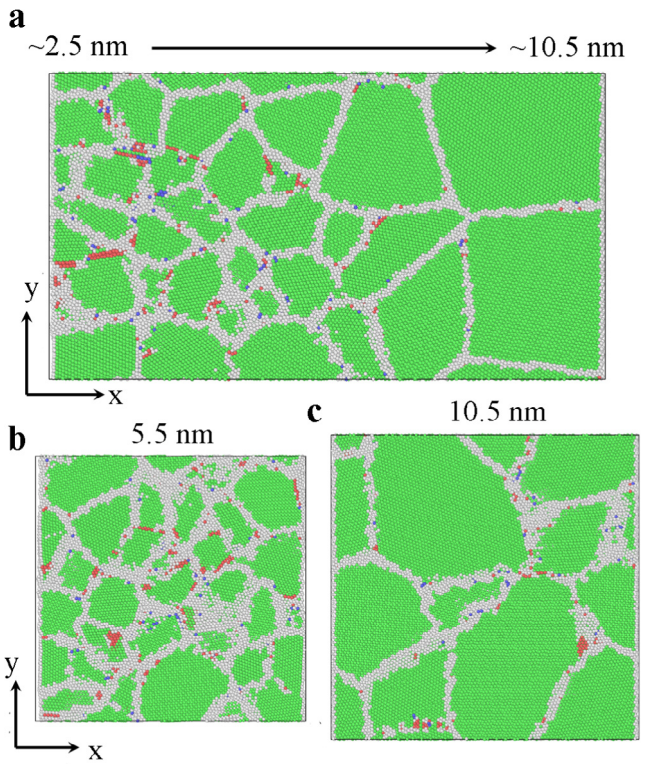

Fig. 1. The relaxed atomic configurations of the three models, i.e., the GNG film with grain sizes increasing from about 2.5 nm to 10.5 nm (a) and the NG films with mean grain sizes of 5.5 nm (b) and 10.5 nm (c). Non-periodic boundary condition is imposed along the x direction. Uniaxial tensile deformation is performed along the y direction.

3. Results and discussion

Fig. 2 presents the simulated stress-strain curves of the GNG film and the homogeneous NG films with mean grain sizes of 5.5 nm and 10.5 nm. The strength of the GNG film is very close to that of the homogeneous 10.5-nm-film and obviously larger than that of the homogeneous 5.5-nm-film. According to the inverse Hall-Petch relation, the strength of NG metals should decrease with decreasing grain size when the grain size is smaller than about 10 nm [21,22]. The largest grain size is about 10.5 nm in the GNG film. Therefore if we slice the GNG film into several independent layers perpendicular to the x direction, the strength of most layers will be smaller than that of the layer with the grain size of about 10.5 nm. And consequently the volume weighed sum of the strength of all independent layers will smaller than that of the homogeneous 10.5-nm-film. However, the simulation result shows the strength of the GNG film is nearly the same as that of the homogeneous 10.5-nm-film. This indicates that the grain size gradient induces an extra higher strength compared with the rule of mixture, i.e., the volume weighed sum of the strength of different layers of composite structure. The rule of mixture can be used to estimate the strength of the composite structure when the interaction between different components is weak [32]. But when there is a synergetic strengthening between different layers, the strength of the integrated sample will be higher than the strength

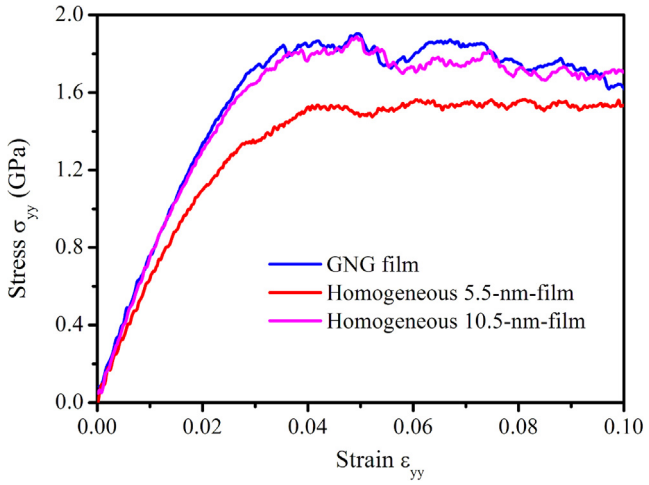

Fig. 2. The simulated stress-strain curves for the GNG film and the homogeneous NG films at a strain rate of 1×10^8 s^{-1} and 300 K.