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Size dependence of elastic mechanical properties of nanocrystalline aluminum

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ABSTRACT

The effect of grain size on the elastic mechanical properties of nanocrystalline pure metal Al is quantified by molecular dynamics simulation method. In this work, the largest nanocrystalline Al sample has a mean grain size of 29.6 nm and contains over 100 millions atoms in the modeling system. The simulation results show that the elastic properties including elastic modulus and ultimate tensile strength of nanocrystalline Al are relatively insensitive to the variation of mean grain size above 13 nm yet they become distinctly grain size dependent below 13 nm. Moreover, at a grain size < 13 nm, the elastic modulus decreases monotonically with decreasing grain size while the ultimate tensile strength of nanocrystalline Al initially decreases with the decrease of the grain size down to 9 nm and then increases with further reduction of grain size. The increase of ultimate tensile strength below 9 nm is believed to be a result of an extended elasticity in the ultrafine grain size nanocrystalline Al. This study can facilitate the prediction of varied mechanical properties for similar nanocrystalline materials and even guide testing and fabrication schemes of such materials.

1. Introduction

Nanocrystalline metals and alloys – with mean grain sizes < 100 nm – have strengths exceeding those of coarse-grained and even alloyed metals [1,2], and are thus expected to have many applications [3]. For example, pure nanocrystalline Al (with mean grain size of about 50 nm) has yield strength at the level of 500 – 600 MPa [4,5], which is over 10 times higher than that of the conventional coarse-grained polycrystalline Al (e.g. with mean grain size of about 40 μm) [5]. In general, it is observed that the yield strength increases with the decrease of the mean grain size larger than about 100 nm [6]. However, when the grain size is below about 20–10 nm, the yield strength instead decreases with decreasing the grain size. This is commonly known as the Hall–Petch breakdown [7,8]. Clearly, the mechanical properties and deformation of metals and alloys are strongly influenced by their grain sizes, especially at the nanometer scale [9,10].

In order to design nanocrystalline metals and alloys with optimum and/or tunable mechanical properties is it important to quantify their grain size dependence. The ability to completely characterize the grain size dependence of mechanical properties should also lead to the development of better materials-physics-based manufacturing and processing. However, it is not feasible in experiments to precisely control the grain size level in the synthesized nanocrystalline bulk samples. It is also challenging to fabricate ultrafine (< 5–10 nm) grain sized nanocrystalline bulk materials with densities close to theoretical levels using modern technologies. This is because of the existence of nanopores or nanovoids in the sintered nanocrystalline bulk materials resulted from various processing [11]. Therefore, a complete grain size dependence of mechanical properties cannot be easily obtained for nanocrystalline bulk materials using experimental techniques. However, computational materials modeling (especially atomistic simulations) is capable of providing robust and accurate measurements of the grain size dependence of mechanical properties for different nanocrystalline materials.

Aluminum, one of the most widely used lightweight metals, and its alloys are materials with promising continuing applications to meet the future challenge of pollution reduction and energy efficient transportations [12]. Thus, there is an urgent need to design and develop ultra-strong Al based alloys. Nanostructuring is considered as one of the most efficient ways to improve the mechanical properties of material systems [13]. In the literature, there are a number of scattered reports by both experiments and theoretical approaches to study the size effect of mechanical properties [4,5] and deformation mechanisms [14,15] in nanocrystalline pure metal Al, but no complete grain size dependence has been reported so far. In this work, we employ classical molecular dynamics (MD) simulations to quantify the grain size dependence of mechanical elastic properties of a range of samples of nanocrystalline pure metal Al. The complete knowledge of grain size dependence of

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mechanical properties of nanocrystalline pure metal Al will provide important fundamental basis for the design and development of Al based alloys with strong and/or tunable mechanical properties.

2. Simulation and analysis methods

2.1. Preparation of nanocrystalline samples

A set of 14 different 3-dimentional (3D) nanocrystalline atomic structures are generated using a Voronoi construction [16]. Each 3D nanocrystalline sample is cubic in shape and consists of 20 grains with a lognormal size distribution. As the side length of the cubic sample increases from 5 nm to 120 nm, the nanocrystalline sample increases in the number of atoms from 7.31×10^3 to 1.04×10^8. The mean grain size (d) is found to vary from 1.1 to 29.6 nm. In addition, a cubic sample of single crystal pure metal Al with side length as 40 nm (5.00×10^5 atoms) is also created and studied by MD for comparison purpose. In this study, MD simulations are performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) open-source code [17]. For the MD modeling, we use the embedded atom method (EAM) potential developed by Mishin et al. [18] established on the basis of experimental data and *ab initio* calculations.

All of the nanocrystalline and single crystal samples are relaxed to equilibrium configurations at 300 K with a pressure of 0 bar by using a Nose/Hoover type equation of motion sampled from isothermal-isobaric (NPT) ensemble. Simulation times of 50–100 ps (i.e. 50,000 – 100,000 steps with a time step of 0.001 ps) are found to be adequate for such relaxations. Periodic boundary conditions (PBC) are also employed. Fig. 1(a) and (b) show two representative nanocrystalline samples after relaxation containing mean grain sizes (d) of 2.2 nm (5.94×10^4 atoms) and 13.4 nm (1.30×10^7 atoms), respectively. Royal-blue atoms with FCC crystal arrangement possess coordination number of 12, the rest of the atoms (e.g. light blue, yellow, red, etc.) have non-12 coordination numbers and usually are located at the grain boundary regions. It is noticed the equiaxed (spherical like) shape grains in Fig. 1(a) change to polyhedral grains in the nanocrystalline sample when the mean grain size is increased from 2.2 to 13.4 nm. This is in agreement with various experimental observations (e.g. TEM characterization) on the grain morphology of nanocrystalline materials with varied mean grain sizes [3].

2.2. Structural analysis of nanocrystalline samples

The statistical structure parameters of nanocrystalline samples as a function of mean grain size are computed, including mass density, atomic fraction of GBs, and the average coordination number, as shown in Fig. 2(a), (b), and (c), respectively. First of all, all of these structural parameters show distinct size dependence with respect to the mean grain size. Especially, when the mean grain size is reduced to below 15–10 nm, the size dependence of each structural parameter becomes more significant. The computed mass density in the single crystal Al is 2.67 g/cm^3, this is in close agreement with the experimental density of Al – 2.70 g/cm^3 [19]. The mass densities of the nanocrystalline samples are overall smaller than that of the single crystal sample (see Fig. 2a). The relative densities of nanocrystalline samples with mean grain sizes of 20 nm and 10 nm are found to be 99.6% and 99.2%, respectively. These relative densities are generally higher than that of the experimental nanocrystalline samples with similar grain size levels. For example, the relative densities of nanocrystalline Se [20] and Ni [3] are 98.2% and 94.0% with mean grain size of 20 nm and 10 nm, respectively. This is probably due to the existence of nanopores or sub-nanoscale porosities in the experiments resulted from various processing of nanocrystalline samples [11]. When the mean grain size is below a few nanometers, the relative density in the nanocrystalline sample decreases significantly, it is calculated that the relative densities of nanocrystalline samples with mean grain sizes of 5 nm and 1 nm are 98.7% and 96.3%, respectively.

The reduced density in nanocrystalline samples is a direct consequence of the increased atomic fraction of grain boundary (GB) atoms [21,22]. As shown in Fig. 2(b), the atomic fraction of GB atoms in the nanocrystalline sample increases with the decrease of mean grain size. When the mean grain size is reduced to lower than 15–1 nm, more than 5–50% of atoms locate at the GB regions in the nanocrystalline sample. The large atomic fraction of GB atoms (or volume fraction of GBs) in the nanocrystalline samples possesses non-12 coordination numbers (the single crystal Al is of FCC structure with coordination number as 12) therefore has disordered atomic arrangement. As a result, the atomic density at the GB regions in the nanocrystalline sample is lower than that of in a perfect crystal. As shown in Fig. 2(c), the average coordination number of the nanocrystalline sample is less than that of a single crystal and it deceases significantly with decreasing the mean grain size. This distinct grain size dependence of the

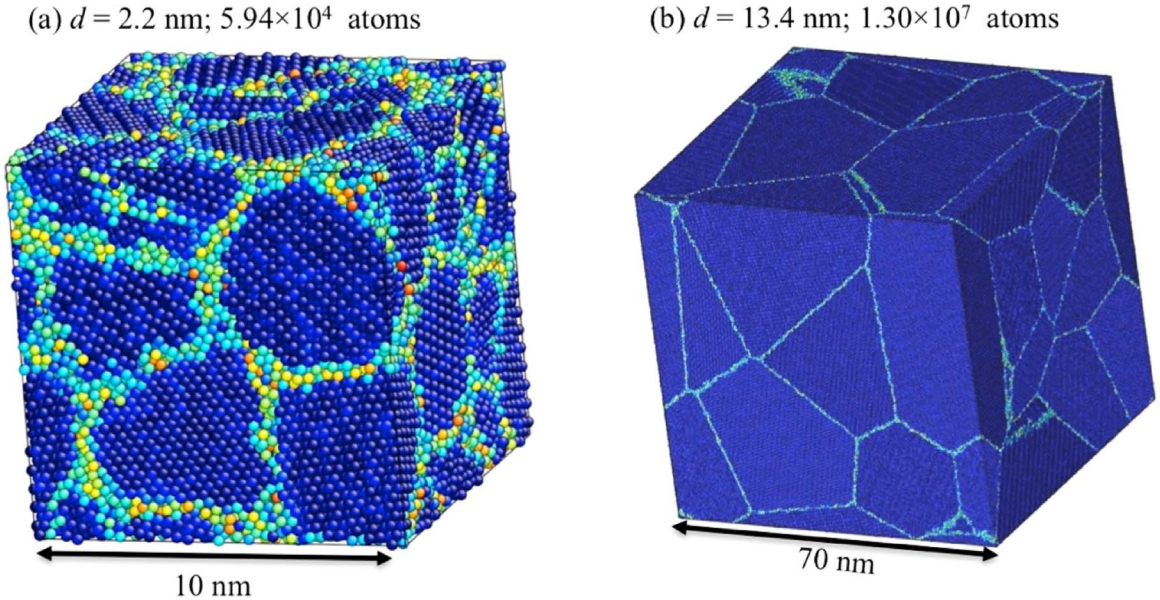

Fig. 1. Nanocrystalline Al bulk samples with representative different mean grain sizes d: (a) d =2.2 nm and (b) d =13.4 nm. Royal-blue atoms with FCC crystal arrangement possess coordination number of 12, the rest of the atoms (e.g. light blue, yellow, red, etc.) have non-12 coordination numbers and usually are found at grain boundary regions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)