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Mechanical behaviour of rapidly solidified aluminium with multiple twinned nanograins: A molecular dynamics simulation study

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ABSTRACT

The mechanical behaviour of rapidly solidified aluminium with multiple twinned nanograins is investigated by a large-scale molecular dynamics simulation. The nanocrystalline structures with mean grain sizes ranging from 3.1 nm to 24.4 nm are prepared by quenching liquid at appropriate cooling rates. It is found that the mechanical properties of rapidly solidified aluminium with multiple twinned nanograins are dependent on its grain size. The flow stress displays inverse Hall-Petch relationship in the present grain-size range. The multiple twinned nanocrystalline aluminium with large and small grain sizes respectively displays different deformation mechanisms during the uniaxial tensile processes. For that with large grain size, the dominated deformation mechanism is twin boundary migration, though co-existing with dislocation activities. And the morphologies of multiple twinned nanograins remain nearly unchanged during the deformation process. For that with small grain size, the deformation is governed by the softening mechanisms of grain growth and detwinning. The grain boundary migration and grain rotation are found in the grain growth process. And the morphologies of multiple twinned nanograins gradually transform into parallel twins or monocrystal.

1. Introduction

Grain refinement is an efficient approach to improve the mechanical properties of solidification solids [1]. As the grain size reduces from microscale to nanoscale, the yield strength increases with the decrease of mean grain size (i.e. Hall-Petch relationship [2,3]), then decreases below a critical grain size d_c (*i.e.* inverse Hall-Petch relationship [4]). Some reports have shown that the critical grain size is around 10–30 nm for different nanocrystalline metals [4–10]. In general, for conventional coarse-grained metals with an average grain size larger than 100 nm, the primary deformation mechanism is dislocation nucleation from intragrains or grain boundaries (GBs) and its propagation. When the grain size decreases to less than 100 nm, the intragranular dislocation nucleation is restricted, and the Hall-Petch relationship weakens. In particular, when the grain size is reduced to less than d_c, the dislocation nucleation becomes limited and the GB associated behaviours such as GB migration and GB rotation become the dominant deformation mechanism. Obviously, the mechanical properties and deformation mechanisms of metals are strongly influenced by their grain sizes, especially at nanoscale.

Nanocrystalline metals possess excellent strength comparing with their coarse-grained counterparts, but they usually exhibit fragility. It was found that the nanocrystalline metals can simultaneously possess high strength and good ductility by introducing twin boundaries (TBs) inside nanograins [11–15]. More interestingly, Lu [16] displayed that the strength of nanocrystalline Cu with twin lamellae first increases as the TB spacing λ decreases, reaching a maximal strength at a critical λ_c, then decreases as λ is further reduced. Some reports [17–21] have shown that the strengthening of nano-twinned metals as $\lambda > \lambda c$ is resulted from the dislocation pile-ups at TBs; the softening as $\lambda < \lambda c$ is due to TB migrations. These researches suggest that the mechanical properties and deformation mechanisms of nano-twinned metals are strongly influenced by their twin morphologies.

Many researches have been performed to investigate the mechanical behaviour of nano-twinned metals, but most of them focused on the effect of TB spacing on the mechanical behaviour of the nanocrystalline Cu with parallel twin morphology. However, the nanocrystalline structures with multiple twinned nanograins were seldom involved,

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while the multiple twinned nanograins are popular in producing nano-twinned structure [22–26]. The effect of grain size on the mechanism behaviour of nanocrystalline metals without twinned structure has been well studied, but its knowledge on the nano-twinned metals is still limited [18]. Especially for aluminium, it is still difficult to obtain the nanocrystalline structure with uniform twinned nanograins in experiment as its high stacking-fault energy [27–29].

At present, computer simulation is a powerful tool to study the mechanical behaviour of nano-twinned metals, due to the difficulty in preparing high-quality samples. Most initial nanocrystalline samples in computer simulations are geometrically constructed by the Voronoi cell method [7,18,19]. The initial defects inside nanograins such as vacancy, dislocation, and stacking fault usually does not allow in these samples, which deviate from the realistic experiments more or less.

In this work, the mechanical behaviour of nanocrystalline aluminium with multiple twinned nanograins is investigated by a large-scale molecular dynamics (MD) simulation. The initial multiple nano-twinned samples are prepared by quenching liquid at appropriate cooling rates. Their deformation mechanisms are analysed in terms of the cluster description method of largest standard cluster analysis (LSCA) proposed by us [30–32].

2. Computational methods

MD simulations are performed using the large-scale atomistic/molecular massively parallel simulator (LAMMPS) [33]. The embedded atoms method (EAM) potential proposed by Mendelev et al. [34] is used to calculate the interactions among atoms. The velocity-Verlet algorithm is used to integrate the motion equation with a time step of 2 fs.

For the initial samples, the rapidly solidified aluminium with multiple twinned nanograins obtained in our previous work is used here [32]. As shown in Ref. [32], when the liquid aluminium is rapidly quenched at appropriate cooling rates, the nanocrystalline structures with multiple twinned grains can be achieved as the grain growth in the supercooling liquid is restricted (see Fig. 1). It can also be found that the mean grain size increases with the decrease of cooling rate, while the grain number and twin density both decrease [see Fig. 1(f)]. Bulk nanocrystalline metals have been experimentally prepared in some multicomponent alloys by one-step liquid quenching [35–37]. Though the cooling rate in these experiments is much lower than that in our computer simulations, the formation mechanisms of nanocrystalline structures in them are similar with each other.

The five nanocrystalline structures shown in Fig. 1(a)–(e) are axially loaded by applying a constant strain rate of $1.0 \times 10^8\,s^{-1}$ along the z axis at 273 K. During the uniaxial tensile process, the Berendsen barostat and Nose-Hoover thermostat are employed to keep the normal stress components along the x and y directions at zero and maintain the system temperature at 273 K. Periodic boundary conditions were employed along three coordinate axes.

The local atomic clusters in the system are identified in terms of a recently developed method of largest standard cluster analysis (LSCA) [30–32], in which the neighbor of an atom are identified with a parameter-free topological criterion rather than a fixed cut-off distance r_c.

3. Results and discussion

3.1. Mechanical properties of multiple twinned nanocrystalline aluminium

The relationship of stress-strain during the deformation process can reflect the basic mechanical properties of materials. From the stress-strain curves of the multiple twinned nanocrystalline aluminium with different mean grain sizes, as shown in Fig. 2, it can be found that their slopes in the elastic deformation stage are different. This indicates that the elastic moduli changes with the grain size. As shown in Fig. 3, the elastic moduli decreases with decreasing grain size d, and this reduction accelerates when $d \leq 6.4$ nm. This is mainly due to the rapid increase of disordered GB atoms when $d \leq 6.4$ nm [see Fig. 1(f)], which will cause lower elastic stiffness. The elastic moduli of the multiple twinned nanocrystalline aluminium with mean grain size of 11.4 nm is 61.0 GPa,

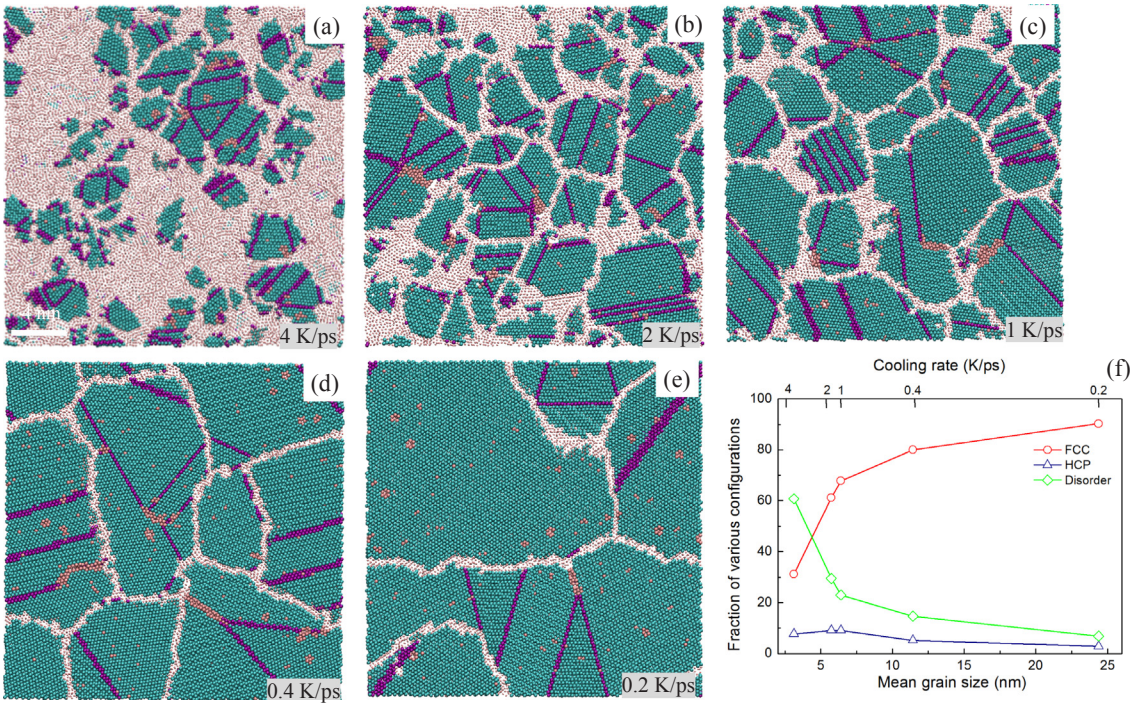

Fig. 1. Atomic configurations of solidification structure of aluminium at 273 K under different cooling rates: (a) 4 K/ps, (b) 2 K/ps, (c) 1 K/ps (d) 0.4 K/ps, (e) 0.2 K/ps,. Cyan, purple, and pink spheres correspond to FCC, HCP and disordered atoms. Radii of disordered GB atoms are reduced for better visualization. Nanocrystalline structures with multiple twinned grains are formed. (f) Fraction of various configurations in the nanocrystalline structures as a function of mean grain size. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)