



Formation mechanism of bulk nanocrystalline aluminium with multiply twinned grains by liquid quenching: A molecular dynamics simulation study



Zhaoyang Hou^{a,b,*}, Zean Tian^b, Ransu Liu^c, Kejun Dong^b, Aibing Yu^b

^a Department of Applied Physics, Chang'an University, Xi'an 710064, China

^b School of Materials Science and Engineering, University of New South Wales, Sydney, NSW 2052, Australia

^c School of Physics and Microelectronics Science, Hunan University, Changsha 410082, China

ARTICLE INFO

Article history:

Received 2 September 2014

Received in revised form 29 December 2014

Accepted 30 December 2014

Available online 19 January 2015

Keywords:

Liquid metal
Computer simulation
Solidification
Nanostructure

ABSTRACT

The formation mechanism of bulk nanocrystalline aluminium with multiply twinned grains has been investigated by a large-scale molecular dynamics simulation. The results show that bulk nanocrystalline aluminium can be obtained directly by quenching liquid at an appropriate cooling rate window. Most nanograins do not merge with each other in the coarsening stage due to the fast cooling rate, but are separated by high-angle grain boundaries. The nanograins exhibit a narrow grain-size range with an average diameter of 6.4 nm and random crystallographic orientations. These microstructure features are consistent with some of the bulk nanocrystalline alloys prepared by melt casting in experiments. The nanograins display various twinned morphologies, and they can be described by three twin elements of parallel, cross and fivefold twinning in varying amounts. The multiply twinned nanograins come from the successive formation of twin HCP planes during the layer-by-layer growth of FCC stacking blocks, and the growth kinetics plays a critical role in the grain morphology. This formation mechanism is different from that of fivefold deformation and annealing twins in the nanocrystalline metals.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Bulk nanocrystalline materials with twin structures usually exhibit an unusual combination of ultrahigh strength, good tensile ductility and fatigue resistance, comparing with twin-free nanocrystalline and ultrafine grained materials [1–4]. Among the twinned structures in the nanocrystalline metals, multiply twins have recently generated considerable interests due to their unique microstructures and formation mechanisms [5–11]. To explain the formation mechanism of fivefold deformation twins in the nanocrystalline metals, the sequential twinning mechanism was proposed by Zhu et al. [5] based on experimental observations, in which the high external stress and variation of external stress orientation are considered to be two critical factors. But molecular dynamics (MD) simulation predicted that the variation of external stress orientation is not necessary under some circumstances [6]. The formation of fivefold annealing twins in the nanocrystalline Cu was suggested to match the sequential twinning mechanism

too [7], but the experimental study showed that its dominant mechanism is grain boundary migration [8]. Furthermore, the sequential twinning mechanism cannot explain many multiply twinned structures observed in the nanocrystalline metals [9]. Up to now, the formation mechanism of multiply twinned structures in the nanocrystalline metals has not been well understood.

Ultrafine grains in nano-size can be obtained during the rapid solidification processes of liquid metals when the nuclei are restrained from growing [12], and some bulk nanocrystalline metals have been produced by one-step liquid quenching in experiments [13–16]. These bulk nanocrystalline metals usually present excellent structural features such as narrow grain-size distribution and free microvoid, but they were only realized in few alloys as strict solidification conditions are needed in their preparation processes. For example, ultraclean melts with few heterogeneous nuclei are usually required to obtain a high undercooling degree [16]. Appropriate cooling rate window is needed to produce fully single-phase nanocrystalline structure without other crystal phases or amorphous matrix [13].

MD method can simulate the liquid quenching process with a super-high cooling rate and ultraclean melt, which is crucial to produce the nanocrystalline structures. But amorphous or crystal

* Corresponding author at: Department of Applied Physics, Chang'an University, Xi'an 710064, China.

E-mail address: zhaoyanghou@163.com (Z. Hou).

structures, rather than the nanocrystalline structure, were usually obtained in a small-scale simulated system [17–22]. Recently, Stretitz et al. [23] found that the bulk nanocrystalline Ta can be obtained by simulating the solidification process of large-scale system. However, the detailed microstructure of nanograins and their formation mechanism were not presented. Furthermore, though the multiply twinned structures have been widely observed in the crystallization processes of metal nanoparticles [24–27] and some hard-sphere systems [28–32], they were seldom reported in the bulk nanocrystalline metals produced by liquid quenching.

In our previous work [33], we obtained the bulk nanocrystalline structure by means of a large-scale MD simulation on the rapid solidification process of liquid aluminium, and the microstructure of grain boundaries is investigated. In this work, we focus on the morphologies of the multiply twinned nanograins and their formation mechanisms on an atomic scale.

2. Computational methods

The large-scale MD simulations are performed for a system containing 1048576 Al atoms in a cubic box with periodic boundary conditions under an isothermal-isobaric (NPT) ensemble, by means of the LAMMPS codes [34]. The interaction potential adopted here is the embedded atoms method (EAM) potential proposed by Mendelev et al. [35]. The velocity-Verlet algorithm is used to integrate the motion equations with a time step of 2 fs. First, in order to obtain the equilibrium liquid, an ideal face-centred-cubic (FCC) configuration at 273 K is heated to 1273 K and then isothermally relaxed for 50 ps at 1273 K. Subsequently, the equilibrium liquid is quenched to 273 K at different cooling rates R varying from 1×10^{13} K/s to 1×10^{11} K/s. Then the local atomic configurations in the solidification processes are identified in terms of a newly developed method of the largest standard cluster analysis (LSCA) [36]. More detailed information on the simulation can be obtained in Ref. [33].

3. Results and discussion

Fig. 1 shows the change of total energy per atom during the solidification processes of aluminium at various cooling rates. At $R = 1 \times 10^{13}$ K/s, the energy decreases continuously with decreasing temperature and its slope changes slightly, which hints the formation of amorphous solid. The energy curves obtained at $R \leq 4 \times 10^{12}$ K/s deviate from that of $R = 1 \times 10^{13}$ K/s after 600 K, and the sudden changes of their slopes indicate the occurrence of

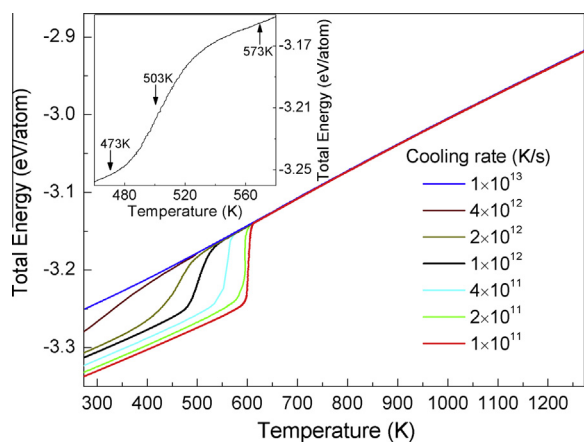


Fig. 1. Change of total energy per atom during the solidification processes of aluminium at different cooling rates. Inset: a segment of the energy curve at $R = 1 \times 10^{12}$ K/s.

crystallization. Furthermore, the onset temperature of crystallization where the energy begins to sharply fall, increases with the decrease of cooling rate. That is, the supercooling degree is enhanced by the increase of cooling rate.

From Fig. 2, it can be found that the crystal-like atoms are scarce in the amorphous solid at $R = 1 \times 10^{13}$ K/s, while there are few amorphous-like atoms in the FCC single crystal at $R = 1 \times 10^{11}$ K/s. At all other intermediate cooling rates (2×10^{11} K/s $\leq R \leq 4 \times 10^{12}$ K/s), bulk nanocrystals are formed in which the crystal-like atoms assemble into nanograins and are separated by the amorphous-like atoms. Since the glass-forming ability connected with the suppression of crystal nucleation in pure metal aluminium is much weaker than that in the multicomponent alloys, the cooling rate at which the bulk nanocrystals can be obtained in our simulations are much higher than that in experiments [13–16]. But the formation mechanisms of the bulk nanocrystalline structures are similar with each other. It can also be found that the average grain size in the bulk nanocrystalline aluminium increases with the decrease of cooling rate, while the number of grains in the system decreases. Furthermore, most nanograins consist of both FCC and HCP atoms, and the number of HCP atoms reaches maximum near $R = 1 \times 10^{12}$ K/s (see Fig. 2(b)). The fraction of cross twinning configuration in the nanograins increases with cooling rate, while that of fivefold twinning configuration decreases. This is due to that the crystallization process has finished before the cross twinning configuration grows into the fivefold twinning one under fast cooling rate. The number of amorphous-like atoms in the nanocrystalline structures increase with increasing cooling rate. The amorphous atoms have high energy than the FCC atoms, so the energy of the solidification structures obtained at fast cooling rate has high energy value (see Fig. 1).

To investigate the microstructure of the bulk nanocrystalline aluminium, each nanograin is distinguished by the clustering analysis adopted in Ref. [33]. As pointed out in Ref. [33], in the bulk nanocrystalline aluminium obtained at $R = 1 \times 10^{12}$ K/s, the size distribution of nanograins falls in a narrow range of 4–8 nm with an average diameter of 6.4 nm (see Fig. 3(b)), assuming a spherical shape of grains. The different grains have random crystallographic orientations, separated by high-angle grain boundaries. As shown in Fig. 3(c), the misorientation angle between $\{111\}$ planes of the adjacent grains marked with 1 and 2 (G1 and G2) is 67.3° . The microstructural features of bulk nanocrystalline aluminium in our simulations are different from that constructed by the Voronoi cell method [37–39], where the grain-size distribution is constrained to a normal distribution and the grain boundaries usually show certain structural coherencies. But our results are consistent with some bulk nanocrystalline alloys also prepared by melt casting in experiments [13–16], where the nanograins have a narrow grain-size distribution and are randomly oriented.

Most nanograins in the bulk nanocrystalline aluminium obtained at $R = 1 \times 10^{12}$ K/s display twinned structures rather than FCC (or HCP) single crystal, and most HCP atoms act as twin planes of FCC stacking. The different distributions of twin boundaries result in a variety of multiply twinned morphologies, but these twinned structures can be described by three twin elements: fivefold, parallel, and cross twinning in various amounts, as shown in Fig. 3(a) by three examples of G1–G3. G1 contains three fivefold twin axes labelled A, B and C which are composed of TDH atoms. The five dihedral angles around each twin axis by FCC twin planes are very close to $2\pi/5$, reflecting the fivefold rotational symmetry. Generally, the ideal angle between two $\{111\}$ twin planes is 70.53° , leaving an angular gap of $\sim 7.4^\circ$ in forming fivefold twinned structure [5], and the deviation between the maximum and the minimum angles in the fivefold deformation twinned structure can reach about 12° [5,6]. But the five dihedral angles around axis

Download English Version:

<https://daneshyari.com/en/article/1560452>

Download Persian Version:

<https://daneshyari.com/article/1560452>

[Daneshyari.com](https://daneshyari.com)