Computational Materials Science 108 (2015) 177–182

Contents lists available at ScienceDirect

Computational Materials Science

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

Atomic dynamics of grain boundaries in bulk nanocrystalline aluminium: A molecular dynamics simulation study

Z.Y. Hou [a,*], Z.A. Tian [b], Y.F. Mo [b], R.S. Liu [b], J.G. Wang [a], X.M. Shuai [a], K.J. Dong [c]

[a] Department of Applied Physics, Chang'an University, Xi'an 710064, China
[b] School of Physics and Microelectronics Science, Hunan University, Changsha 410082, China
[c] Institute for Infrastructure Engineering, University of Western Sydney, Penrith, NSW 2751, Australia

ARTICLE INFO

Article history:
Received 9 March 2015
Received in revised form 12 June 2015
Accepted 26 June 2015
Available online 7 July 2015

Keywords:
Atomic dynamics
Grain boundaries
Bulk nanocrystalline aluminium
Molecular dynamics simulation

ABSTRACT

Dynamics of grain boundary (GB) atoms in the bulk nanocrystalline aluminium is investigated by means of a large-scale molecular dynamics simulation. It is found that the GB atoms in the nanocrystalline aluminium display the glassy dynamics. Their dynamic features are, on one hand, similar to those in the glass systems and bicrystal GBs, in terms of the time-correlation functions of mean-square displacement (MSD) and non-Gaussian parameter (NGP). But on the other hand, these GB atoms also demonstrate some different dynamic behaviors due to the more complicated microstructure. In particular, the immobile GB atoms are localized into their equilibrium positions due to the strong cage effect, and they are mainly at the surfaces of grains, especially the large grains, while the mobile GB atoms are active and can easily hop away from the cage around them. These mobile GB atoms gather together at the surfaces of small grains and the triple junction regions of GBs, and they form some abnormally big clusters. The size distribution of these clusters significantly deviates from the power law.

1. Introduction

Bulk nanocrystalline materials have been a subject of extensive research in recent decades, due to their unique physical and chemical properties [1]. This class of materials is distinguished by a significant volume of grain boundaries (GBs). The dynamic behaviors of GB atoms, such as diffusion, migration, and sliding, play a pivotal role in the deformation and grain growth of bulk nanocrystalline metals [2–5]. Many studies [3–8] have been performed to elucidate the spatiotemporal evolution of GBs in the bulk nanocrystalline metals, but our understanding of GB dynamics at atomic level is still limited owing to the disparities in the length and time scales associated with its experimental observation [9]. The width of GBs in the bulk nanocrystalline structure usually is about 2–4 atomic layers, so it is difficult to experimentally probe its microstructure and dynamic evolution at the atom level [10].

Molecular dynamics (MD) simulation is an effective tool to study the microstructure and dynamics of bulk nanocrystalline materials, as a very useful extension of experimental and analytical investigations. Some simulation studies [11–13] showed that the microstructure of GBs in bulk nanocrystalline metals is disordered, quite similar to the glass systems. Other simulations [14–16] also suggested the similarities between the bicrystal GBs and the glass systems in dynamics, evidenced by the dynamic heterogeneous and the string-like cooperative atomic motion. And the glassy dynamics of GBs has been experimentally confirmed in some colloidal systems [17,18].

However, previous dynamic studies of GBs focused on the bicrystal GBs which comprise only two grains and their interfacial regions, while the atomic dynamics of GBs in the bulk nanocrystalline metals was seldom reported. The microstructure and dynamics of GBs in the realistic bulk nanocrystalline metals are more complex than those in the bicrystal GBs. For example, the GBs in the bulk nanocrystalline structure contain lots of triple junction (TJ) regions which usually have particular kinetic and thermodynamic properties [19–22]. As the nanograins in the bulk nanocrystalline structure have different sizes and random crystallographic orientation, the GB dynamics were found to vary with the misorientation angle between adjacent grains [17]. Furthermore, recent studies [23–25] demonstrated that a large percentage of GB atoms are in the regions with significant crystalline order, while the disordered amorphous-like atoms mainly locate at the TJ regions.

In our previous work [25,26], the bulk nanocrystalline aluminium was produced by means of a large-scale MD simulation of the rapid solidification process of liquid, and the microstructure of GBs is investigated in detail. It was found that the

* Corresponding author.
E-mail address: zhaoyanghou@163.com (Z.Y. Hou).

http://dx.doi.org/10.1016/j.commatsci.2015.06.039
0927-0256/

microstructure features of grains and GBs obtained in our simulations are consistent with those produced in some experiments and geometrically constructed by the Voronoi cell method. In this work, we further investigate the atomic dynamics of these GBs. It is found that the GB atoms display the dynamics similar to those in the glass systems and bicrystal GBs in some aspects, but also exhibit some different dynamic features from the latter.

2. Computational methods

2.1. Molecular dynamics simulation

The rapid solidification process of liquid aluminium is simulated using the LAMMPS codes [27] for a system containing 1,048,576 atoms in a cubic box with periodic boundary conditions. The interaction potential adopted here is the embedded atoms method (EAM) potential proposed by Mendelev et al. [28]. As shown in Refs. [25,26], the bulk nanocrystalline aluminium is obtained below the temperature 473 K, when the liquid Al is quenched from 1273 K at a cooling rate of 1×10^{12} K/s. The local atomic clusters in the system are identified in terms of a recently developed method of largest standard cluster analysis (LSCA) [29], in which the neighbor of an atom are identified with a parameter-free topological criterion rather than a fixed cut-off distance r_c. The method of identified grain and GB atoms are described in Refs. [25,26]. In the nanocrystalline structure, as shown in Refs. [25,26], the nanograins with an average size of 6.4 nm are separated by high-angle GBs. The GB regions neighboring the grains display FCC-like short-to-long range order. The TJ regions of GB are not disordered like liquid, but present icosahedral- and BCC-like short-range order. To investigate the dynamic properties of GB atoms, the nanocrystalline structures at different temperatures, every 100 K from 473 K to 273 K, are respectively relaxed 500 ps under an isothermal–isochoric (NVT) ensemble. More detailed information on the simulation methods can be obtained in Refs. [25,26].

2.2. Characterization of dynamics

The mean-square displacement (MSD) [30] is usually used to study the dynamic motion of atoms, which is defined as

$$\langle r^2(t)\rangle = \frac{1}{N}\sum_{i=1}^{N}\left\langle |r_i(t) - r_i(0)|^2 \right\rangle, \quad (1)$$

where N is the number of atoms in the system, $r_i(t)$ is the position vectors of the ith atom at time t.

The non-Gaussian parameter (NGP) [31] is frequently used to quantify the dynamic heterogeneity of supercooled liquids, and is defined as:

$$\alpha_2(t) = \frac{3\langle r^4(t)\rangle}{5\langle r^2(t)\rangle^2} - 1, \quad (2)$$

where $\langle r^4(t)\rangle$ is the mean quartic displacement. The heterogeneity of the atom motion can thus be inferred from the time evolution of α_2, which is zero for a Gaussian distribution, and $\alpha_2 > 0$ for non-Gaussian behavior. The α_2 reaches a maximum for a characteristic time named t^*.

3. Results and discussion

3.1. Dynamics of grain boundaries

Fig. 1 shows the time dependence of MSD for the GB atoms in the bulk nanocrystalline aluminium at different temperatures. In

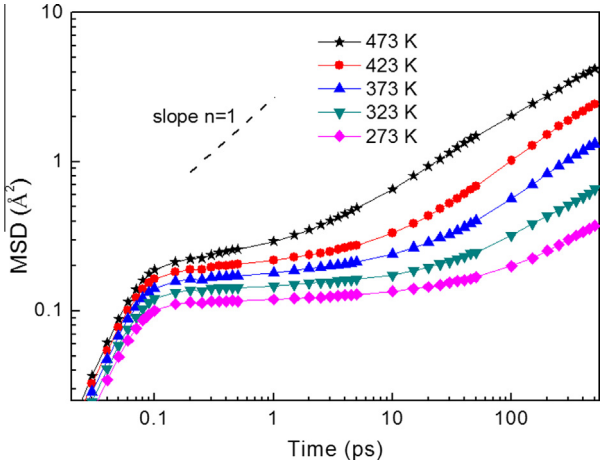

Fig. 1. Time dependence of MSD for the GB atoms in the bulk nanocrystalline aluminium at different temperatures.

the short time from the beginning ($t < 0.1$ ps), all curves show a power-law behavior which indicates the ballistic motion of atoms. At the intermediate time, the atoms are trapped in the transient cages formed by their neighbor atoms, and the trapped atoms need some time to escape from the cages. So a plateau appears on the MSD curve due to the cage effect, and it becomes pronounced with the decrease of temperature. At the final time, the curves increase with the slope $n < 1$, indicating the onset of cage-breaking rearrangement. The time window correlated with the cage effect is usually called the β-relaxation regime and the following time window is the α-relaxation regime [30].

To further assess the dynamics of GB atoms in the bulk nanocrystalline aluminium, its dynamic heterogeneity is investigated by means of the NGP. As shown in Fig. 2, when $t < 0.1$ ps, all NGPs at different temperatures are close to zero, indicating the Gaussian distribution of the vibration displacements of GB atoms. During the following β-relaxation window, all NGP curves rise monotonically to a maximum value, and the position of maximum shifts toward the longer time as the temperature decreases. This suggests that the GB atoms in the bulk nanocrystalline aluminium exhibit dynamic heterogeneity in the β-relaxation window, and such heterogeneity increases with the enhancement of cage effect.

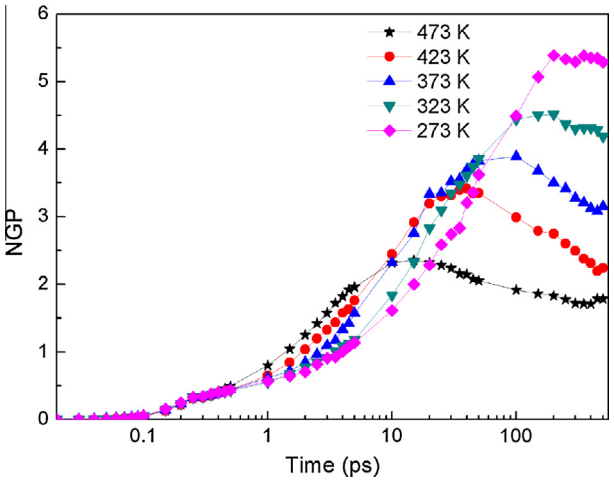

Fig. 2. Time dependence of non-Gaussian parameter (NGP) for GB atoms in the bulk nanocrystalline aluminium at different temperatures.