Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 74 (2014) 39–48

Acta MATERIALIA

www.elsevier.com/locate/actamat

A comprehensive molecular dynamics study of low-angle grain boundary mobility in a pure aluminum system

M.J. Rahman *, H.S. Zurob, J.J. Hoyt

Department of Materials Science and Engineering, McMaster University, Canada

Received 9 September 2013; received in revised form 18 March 2014; accepted 29 March 2014

Abstract

Molecular dynamics (MD) simulations have been utilized to determine the low-angle grain boundary (LAGB) mobility of [1 1 2] tilt boundaries in pure aluminum. The mobility data were extracted from two different MD techniques as a function of temperature and misorientation. The artificial driving force method (ADF) and the random walk method were analyzed critically and a detailed comparison of the two techniques was conducted. Within numerical uncertainties, both techniques provide the same magnitude of mobility at 300 K for a grain boundary with low misorientation in Al and the two techniques also agree at 700 K for the highest misorientation studied. For other misorientations, however, there are considerable discrepancies between the two techniques and reasons for the differing results are presented. The results indicate that considerable care must be taken in applying the ADF method to the case of low-angle boundaries. The temperature dependence of LAGB mobility is studied and, consistent with previous MD studies, the activation energy is found to be approximately 10 times lower than the experimental observations.

Keywords: Low-angle grain boundary (LAGB); Mobility; Aluminum; Molecular dynamics (MD); Artificial driving force (ADF)

1. Introduction

The mechanical properties of a material are mainly governed by its microstructure. Strength is often achieved through grain refinement by means of thermomechanical processing. The key microstructure evolution events taking place during thermomechanical processing are recovery, recrystallization and grain growth. The mobility of high- and low-angle boundaries has a very strong effect on these processes. Therefore, an improved understanding of the thermodynamic driving forces and the mobility of grain boundaries is critical to the development of accurate microstructural evolution models useful for a wide range of processing applications.

The mobility of a grain boundary is the constant of proportionality between the applied driving force and the interface velocity. Grain boundary mobility strongly depends on the crystallographic misorientations between the neighbouring crystals. In general, grain boundaries can be divided into two different categories, namely low-angle grain boundaries (LAGB) and high-angle grain boundaries (HAGB). HAGBs are important in normal grain growth processes, whereas LAGB mobility plays a central role in the kinetics of recovery and nucleation of recrystallization. In many alloys, such as high stacking fault energy materials, plastic deformation leads to the creation of a microstructure characterized by subgrains with low misorientations at their interface. Several models [1–6] have tried to capture the evolution of these subgrains into viable recrystallization nuclei. The mobility of low-angle boundaries is therefore an essential input for these models.

* Corresponding author. Tel.: +1 9055314504.
E-mail address: rahmanmj@mcmaster.ca (M.J. Rahman).

http://dx.doi.org/10.1016/j.actamat.2014.03.063
1359-6454/

Due to the importance of grain boundary kinetics in the prediction of microstructural evolution, there exists a vast literature on the determination of grain boundary mobility. Traditionally, experimental measurements of grain growth in polycrystalline metals have been used to extract such data. However, simple growth experiments yield only an average mobility, and therefore cannot distinguish the important role of misorientation on the rate of grain boundary motion. Over the past few decades, a number of experimental methods have been developed to measure the mobility for specific boundaries of known orientation. In the early 1970s Sun and Bauer [7] introduced a sample geometry consisting of initially straight boundaries intersecting free surfaces, which then migrate to form minimum energy hyperbolic shapes. The Sun–Bauer geometry was subsequently used to study the mobility as a function of misorientation in Cu [8], Al [9] and Fe–3.5% Si [10]. Molodov et al. [11] employed bicrystals containing grain boundary loops to determine the mobility and the technique was used to investigate the effect of impurities on GB motion in Al [12]. In addition to a capillary driving force, grain boundary mobility has been measured through the application of a magnetic field [13,14] and stress [15,16]. By monitoring the position of triple junctions during the annealing process, Yang et al. [17] were able to obtain the energy and mobility vs. misorientation for a large number of grains in Al. The Yang results showed very different behavior for low and high angle grain boundaries. In an experiment utilizing a shear stress driving force, Winning et al. [18] used X-ray diffraction techniques to monitor the motion of [1 1 2], [1 1 1] and [1 0 0] tilt boundaries in pure Al. The authors noted a roughly two orders of magnitude increase in the mobility as the misorientation angle increased from below ~10° to above ~15°. The dramatic jump in mobility was explained in terms of the interaction of the boundaries with network dislocations. For LAGBs, which can be viewed as a periodic array of distinct edge dislocations, the motion can be pinned by other network dislocations. For HAGBs, on the other hand, network dislocations are absorbed by the migrating boundary. This explanation is consistent with an earlier proposal by Viswanathan and Bauer [8], who observed an activation energy for the LAGB in Cu that is consistent with dislocation climb and a much lower activation energy for the case of HAGBs.

In addition to requiring sophisticated sample preparation methods, experimental studies of grain boundary mobility are complicated by the presence of impurities, which, even in very small concentrations, can have a dramatic effect on the mobility. Therefore, in recent years, molecular dynamics (MD) simulations have been employed to determine the intrinsic grain boundary mobility in several metal and model systems. In pioneering work by Schonfelder et al. [19] planar asymmetric boundaries in MD-generated bicrystals were driven through the application of an applied biaxial strain. The technique relies on the elastic anisotropy of the crystal to establish an unbalanced elastic energy in the two crystals. Zhang et al. [20] have used elastically driven boundary migration to study the mobility vs. temperature for an embedded atom method (EAM) description of Ni, and Schonfelder et al. [21] studied both the diffusivity and mobility of [0 0 1] twist boundaries in Cu. As an alternative to elastic driving forces, Zhang [22] et al. employed MD bicrystals in the half loop geometry to study [1 1 1] tilt GB motion in EAM Al. The curvature driven technique can be compared directly to experiments [23]; however, only the product of mobility times boundary stiffness, and not the bare mobility itself, is obtained with this MD method. Janssens et al. [24] developed an MD scheme where a tunable increase in energy can be applied to just one crystal of a bicrystal geometry. The so-called artificial driving force (ADF) method was then used in a comprehensive study of the mobility of 388 boundaries in EAM Ni [25,26]. In MD techniques that utilize the application of a driving force to induce boundary motion, the magnitude of the force is typically quite high. Two fluctuation based methods have been introduced that have the distinct advantage of extracting the GB mobility in the limit of zero driving force. Trautt et al. [27] (see also Hoyt et al. [28]) demonstrated that the average displacement of a planar GB undergoes a random walk (RW) and a plot of the mean squared displacement vs. time yields a "diffusion coefficient" directly related to the mobility. Foiles and Hoyt [29] investigated the entire fluctuation spectrum of an asymmetric tilt boundary in EAM Ni and were able to determine both the mobility and stiffness. In 2006, Cahn et al. [30] demonstrated that some grain boundaries are coupled in the sense that shear deformation parallel to the boundary plane induces motion normal to the boundary. Karma et al. [31] then showed that the capillary fluctuation spectrum has a different wavenumber dependence for coupled boundaries than for uncoupled ones. Of particular relevance to the present work, the Karma et al. study compared three different MD techniques – fluctuations, RW and stress-driven motion – and observed GB mobility dependence as a function of misorientation in LAGBs. The authors concluded that mobility increases with decreasing misorientation at 1200 K in the pure Cu system.

The majority of MD studies of grain boundary motion have concentrated on HAGBs and relatively little attention has been paid to the case of small misorientations. In a recent MD study, Toda et al. [32] simulated the motion of LAGB in a body-centered cubic alloy, which illustrated a migration mechanism in terms of the glissile dislocation movement in LAGB. In the present work, we have employed MD simulations to examine the grain boundary mobility as a function of temperature and misorientation in [1 1 2] tilt LAGBs in an EAM description of pure Al [33]. Two techniques were chosen – the ADF method [24] and the RW method [27] – and particular attention is paid to comparing the two results. The variation of mobility with misorientation at different temperature is also addressed. The next section describes the simulation cell geometries