Materials Letters 76 (2012) 32–35

Contents lists available at SciVerse ScienceDirect

Materials Letters

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

Effect of grain boundary structures on grain boundary sliding in magnesium

Hidetoshi Somekawa [a,*], Toshiji Mukai [b]

[a] Research Center for Strategic Materials, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan
[b] Department of Mechanical Engineering, Kobe University, 1-1 Rokkodai, Kobe, 657-8501, Japan

ARTICLE INFO

Article history:
Received 12 January 2012
Accepted 4 February 2012
Available online 16 February 2012

Keywords:
Magnesium
Grain boundary sliding
Nanoindentation creep
Grain boundary structure
Grain boundary energy

ABSTRACT

The effect of grain boundary structures on the deformation behavior at the grain boundaries in magnesium was examined by the nanoindentation creep test. The results of the nanoindentation creep test showed that the dominant deformation mechanism around the grain boundary was grain boundary sliding; however, the occurrence of grain boundary sliding was closely related to the grain boundary energy. The grain boundary with high energy showed high strain rate sensitivity, which was the same tendency as that of the other metallic materials. Furthermore, the addition of aluminum atoms into magnesium tended to prevent the grain boundary sliding due to the decrease in grain boundary energy.

1. Introduction

Understanding the characteristics and the deformation responses of the grain boundary in metallic materials is important, since the grain boundaries affect the mechanical properties such as strength and ductility. The effect of the grain boundary structures on the grain boundary strengthening [1,2] and the grain boundary migration [3,4] has been examined through various experiments, and the grain boundary energies [5,6] have also been obtained for many kinds of bicrystals with different boundary structures. The deformation behavior near the grain boundaries in magnesium and its alloys is quite unique compared to that of the other metallic materials. For example, the major slip system in magnesium at room temperature is only basal dislocation; however, not only basal—but also non-basal dislocations are activated at the grain boundaries during the plastic deformation due to the operation of a compatibility stress/strain at the grain boundary [7]. These activations can be observed near the grain boundaries in the deformed samples [7]. The grain boundary sliding has also occurred even at room temperature [8] because of the higher diffusion rate of the grain boundary in magnesium [9]. The polycrystalline magnesium with fine-grain structures showed a large strain rate dependence behavior at room temperature [10,11]. On the other hand, most of these results for magnesium and its alloys showed the deformation response not at the individual—but at all the grain boundaries.

Our recent paper showed that a grain boundary was confirmed to obtain high strain rate sensitivity by the nanoindentation creep test [12]. However, there are no sufficient results to comprehend the deformation behavior at each of the grain boundaries in magnesium like that in other materials. Thus, the effect of the grain boundary structures on the deformation mechanism at the grain boundaries in magnesium is examined using the nanoindentation creep test, which is widely used for the investigation of mechanical properties and deformation behavior in small volumes of materials, in this study. The grain boundary energy is evaluated using the molecular dynamic (MD) simulation. The impact of additional elements, i.e., a conventional alloying element such as aluminum, will also be discussed.

2. Experimental procedure

2.1. Nanoindentation creep

Pure magnesium with a purity of 99.94% and a Mg–1.0 at.%Al alloy were prepared by casting, and then they were extruded in this study. The extruded alloys were annealed to reduce the dislocation density and to produce coarse-grained structures with an average grain size of about 50 μm. The nanoindentation creep tests were carried out to investigate the deformation behavior at the specific grain boundaries. An indentation load of 500 μN, a constant loading- and unloading-rate of 50 μN/s, and a holding period of 0.5 ks were used in all the nanoindentation creep tests using the Berkovich tip. Since the region around the grain boundary in magnesium had high strain rate sensitivity [12], the tip was indented about 1.0 μm away from the grain boundary, which consisted of misorientation angles of 23°, 44° and 78° in pure magnesium and 78° in the Mg–Al alloy. The indented grain interior had a Schmid factor of 0.25. A typical example of an indentation area observed by the electron back scatter diffraction method is shown in

* Corresponding author. Tel.: +81 29 859 2473; fax: +81 29 859 2601.
E-mail address: SOMEKAWA.Hidetoshi@nims.go.jp (H. Somekawa).

0167-577X/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.matlet.2012.02.010

Fig. 1. The creep behaviors were measured at 20 or more points for each condition. The details of the experimental conditions in the nanoindentation creep test and the sample preparation for magnesium are reported elsewhere [12].

2.2. MD simulation

Magnesium bicrystals with three types of [1–100] symmetric tilt boundaries, which were Σ25 with the tilt angle of θ = 23°, Σ14 with θ = 44° and Σ10 with θ = 78° (hereafter denoted as, 23°-, 44°- and 78°-tilted boundaries, respectively), were modeled in this study. A typical tilt boundary model is shown in Fig. 1(d). The grain boundary energy, γ_{gb}, in the present models was evaluated at a temperature of 1 K with a NTP ensemble using the generalized EAM potential, which enables calculations for alloys containing magnesium and aluminum atoms. The grain boundary energy was obtained using the following equation:

$$\gamma_{gb} = \frac{U_{gb} - U_{bulk}}{2A_{gb}} \quad (1)$$

where U_{gb} and U_{bulk} are the internal energies with and without the grain boundary, respectively, and A_{gb} is the grain boundary area. Magnesium atoms existing at the interfaces were also replaced by aluminum atoms, consisting of 4 atoms in each space, in the 78°-tilted boundary model (inset in Fig. 1(d)) to investigate the effect of the alloying element on the grain boundary energy.

3. Results and discussion

The variation of indentation depth as a function of the time is shown in Fig. 2. This figure shows that the depth increases with the load holding segment, and the nanoindentation creep behavior affects the grain boundary structures. The maximum depth was obtained with a misorientation angle of 23°. The relationship between the stress, σ, (hardness; H) and the strain rate, $\dot{\varepsilon}$, using the classical Tabor relationship during the creep behavior is given as follows;

$$\dot{\varepsilon} = A\sigma^n = A\left(\frac{H}{\alpha}\right)^n \quad (2)$$

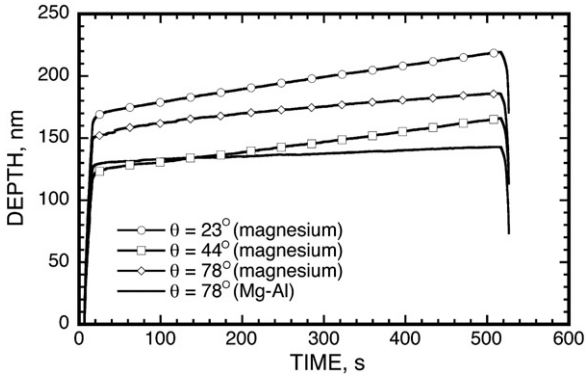

Fig. 2. The variation of indentation depth as a function of time in magnesium and Mg–Al alloy.

where A is a constant, α is the Tabor factor (= 3.3 [13]) and n is the stress exponent (= 1/m; m is the strain rate sensitivity exponent). The strain rate is defined as the instantaneous descent rate of the indenter divided by the displacement at a particular point in time, and the actual effective strain rate during the indentation, $\dot{\varepsilon}_{eff}$, is expressed as [14]:

$$\dot{\varepsilon}_{eff} = C \times \dot{\varepsilon} = C \times \left(\frac{1}{h}\right)\left(\frac{dh}{dt}\right) \quad (3)$$

where C is a constant of 0.1 [15,16]. A typical example for the variation of stress as a function of effective strain rate in nanoindentation creep is shown in Fig. 3. The m-value corresponded to the slope, and was obtained by the least square method from the stress (or hardness) and the strain rate curves of each indentation test. The average m-values for the grain boundary misorientation angles are listed in Table 1. The m-values of more than 0.3 were obtained in this study, and these values indicate that the dominant deformation mechanism around the grain boundaries is assumed to be grain boundary sliding. The present strain rate is found to be in a similar range as that for the initiation of grain boundary sliding, which was obtained from the uniaxial tensile tests [10]. On the other hand, the m-values are influenced by the grain boundary structures; the m-value for the

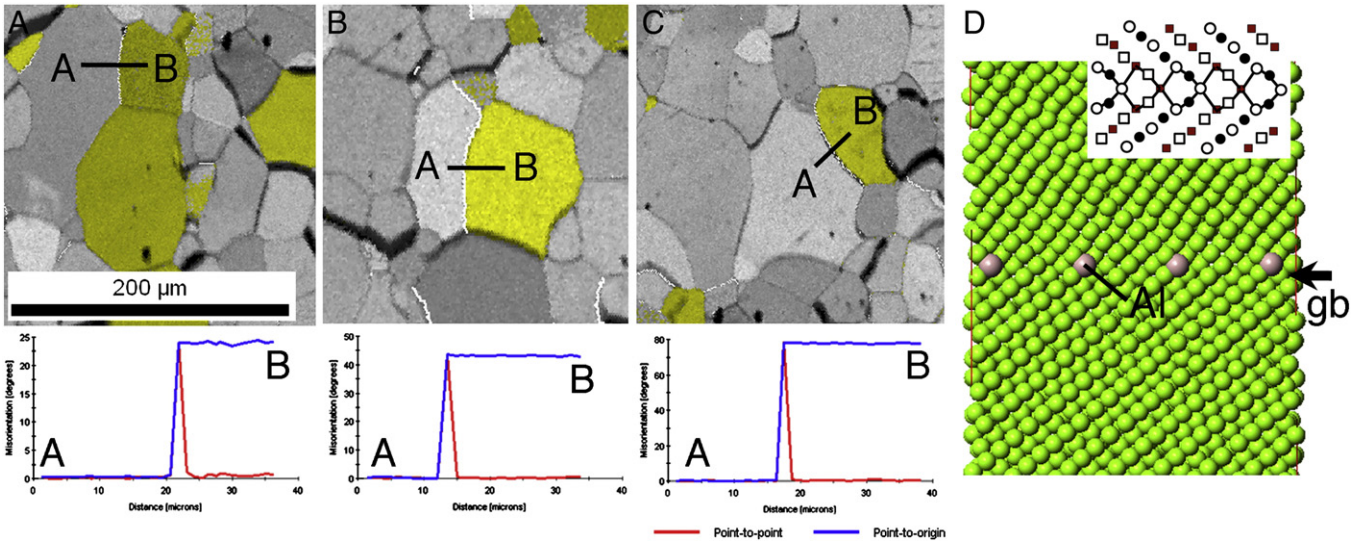

Fig. 1. Indentation area observed by the electron back scatter diffraction method and the grain boundary model in MD simulation; (A) misorientation angle of 23°, (B) 44°, (C) 78°, (D) [1–100] symmetric tilt boundary with the angle of 78°. Where the grain with the yellow color is a Schmid factor of 0.25, and the grain boundary with the white color is a specific misorientation angle of 23°, 44° or 78° in (A)–(C), respectively.