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Atomistic modeling study of a strain-free stress driven grain boundary migration mechanism

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ABSTRACT

A recent experiment (Scripta Mater., 65:990, 2011) shows that the Σ7 {132}/{132} grain boundary in Al can migrate under external stress but produces no strain. Here, based on a bi-crystallographic analysis, an atomic shuffling path was identified as the feasible mechanism for this grain boundary migration. By a density functional theory calculation, it reveals that the enthalpy barrier of this atomic shuffling path increases by external shear stress applied with shear of the grain boundary along the tilt axis 〈111〉, which is in good agreement with experimentally measured shear-direction-dependence of activation enthalpy for this grain boundary migration.

For polycrystalline materials, grain boundary (GB) migration is the major structural transformation process that contributes to the grain growth phenomena [1,2]. Traditionally, GB migration is thought to occur only at medium or higher temperatures (>0.4 T_m, T_m is the melting temperature) by thermally assisted atomic shuffling motions in the GB zone [2]. Some efforts have been made to characterize the patterns of the motions of atoms involved, e.g., there are suggestions that a 'stringlike' motion of atoms [3] or rotation of cluster of atoms [4] in GB zone can be identified for migration of some particular GBs. It appears that the specific pattern of the atomic shuffling motions on migration of GB is a case-by-case basis because atomistic structure of the GBs are different one another, and different GBs can therefore display quite different temperature dependence of mobility [5]. Nevertheless, for a 'random' GB, this kind of atomic shuffling motions is generally random in nature as well: motions of atoms in the GB zone are less coordinated, and migration of the GB is thermally assisted without any transformational strain produced. However, in the past decade, it has been widely reported that, for small grained polycrystalline materials, GB migration can be induced by external stress at room temperature or even in cryogenic loading conditions [6–11]. Further investigations indicate that GB migration in these circumstances can be well accounted for by the shear coupled GB motions wherein the bi-crystallographic lattice structure of GB plays an important role [12]. These findings signify that, the stress driven GB migration behavior can be a typical characteristic of GBs, especially for GBs in small grained polycrystalline materials [12].

Compared with the thermally assisted migration of GB by random atomic shuffling motions in the GB zone, the shear coupled GB migration features a shear strain produced in the volume swept by the migration motion of the GB [12,13]. It is worth to mention that, a recent study shows that the basal/prismatic (B/P) boundary in Mg can migrate under uniaxial stress normal to the boundary [14]. Migration of the B/P boundary in this case is accomplished via a 'unit-cell-reconstruction' mechanism [15], and it produces a tetragonal strain by the migration of the boundary [14]. For both the shear coupled GB migration and the migration of the B/P boundary in Mg, atomic shuffling motions in the GB zone can be identified as a complementary process on migration of the GB [14,16,17]. In short, the stress driven GB migration is generally characterized by a transformational strain produced in the volume swept by the motion of GB together with complementary atomic shuffling motions in the volume. It is therefore quite similar to the martensitic phase transformation processes in materials [18,19].

However, an Al bicrystal experiment carried out recently by Molodov et al. [20] seems to provide an exceptional case. In their experiment, the Σ7 {132}/{132} symmetric tilt coincidence site lattice (CSL) boundary (hereafter termed as Σ7 {132} GB for short) in Al was

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shown to migrate under external stress at temperatures of 600–700 K. For external stress applied with shear of the GB along three different directions in the GB plane, no strain was measured in the GB migration processes, and the activation enthalpy measured for the GB migration shows a strong shear-direction-dependent characteristic. Although it has been proposed that a dislocation model of GB [13] can be used to interpret this GB migration phenomena [20], and also a two-step atomic shuffling process has been suggested [21], the following questions remain: (i) how the GB migration occurs on the atomistic level; (ii) why the GB migrates under external stress but produces no strain; (iii) why the activation enthalpy for the GB migration is shear direction dependent. It is the purpose of the present work to provide an atomistic level understanding of this mysterious GB migration phenomena and to answer these questions.

For the Σ7 {132} GB in Al, its bi-crystallographic structure can be analyzed first. Fig. 1a shows the CSL structure of this GB, with both the 'real sites' (spheres) of neighboring grains and the extrapolated 'virtual sites' (dashed circles) of the two grains displayed. It can be seen that the primitive cell of the CSL of this GB has exactly seven atoms, which conforms to the bi-crystallographic theory of GBs [1,22]. By selecting the boundary plane in the position as indicated by the black dashed line in Fig. 1a, the structure of the Σ7 {132} GB obtained can be illustrated by the blue lines sketched. To check whether the bi-crystallographic theory can describe the atomistic structure of this type of GB in Al or not, atomistic modeling of the structure of the GB in Al with an embedded atom method (EAM) potential [23] was performed by using LAMMPS [24]. A bicrystal model with the same lattice orientations of neighboring grains as in Fig. 1a was constructed. Periodic boundary condition (PBC) was applied to the dimensions parallel to the GB plane, while free surface boundary condition was used on the dimension perpendicular to the GB plane. A procedure the same as that of the references [16, 17] was adopted for exploration of the minimum energy structure of the GB.

Fig. 1b and c show the simulated atomistic structure of the GB in Al by the EAM potential. As can be demonstrated by the blue lines in Fig. 1b, the overall atomistic structure of the GB simulated agrees pretty well with the bi-crystallographic theory description as in Fig. 1a. On the other hand, the dashed ovals marked in Fig. 1b indicate that, the atoms in the layer closest to the boundary plane have a position biased from that of the bi-crystallographic lattice sites shown in Fig. 1a. Fig. 1c

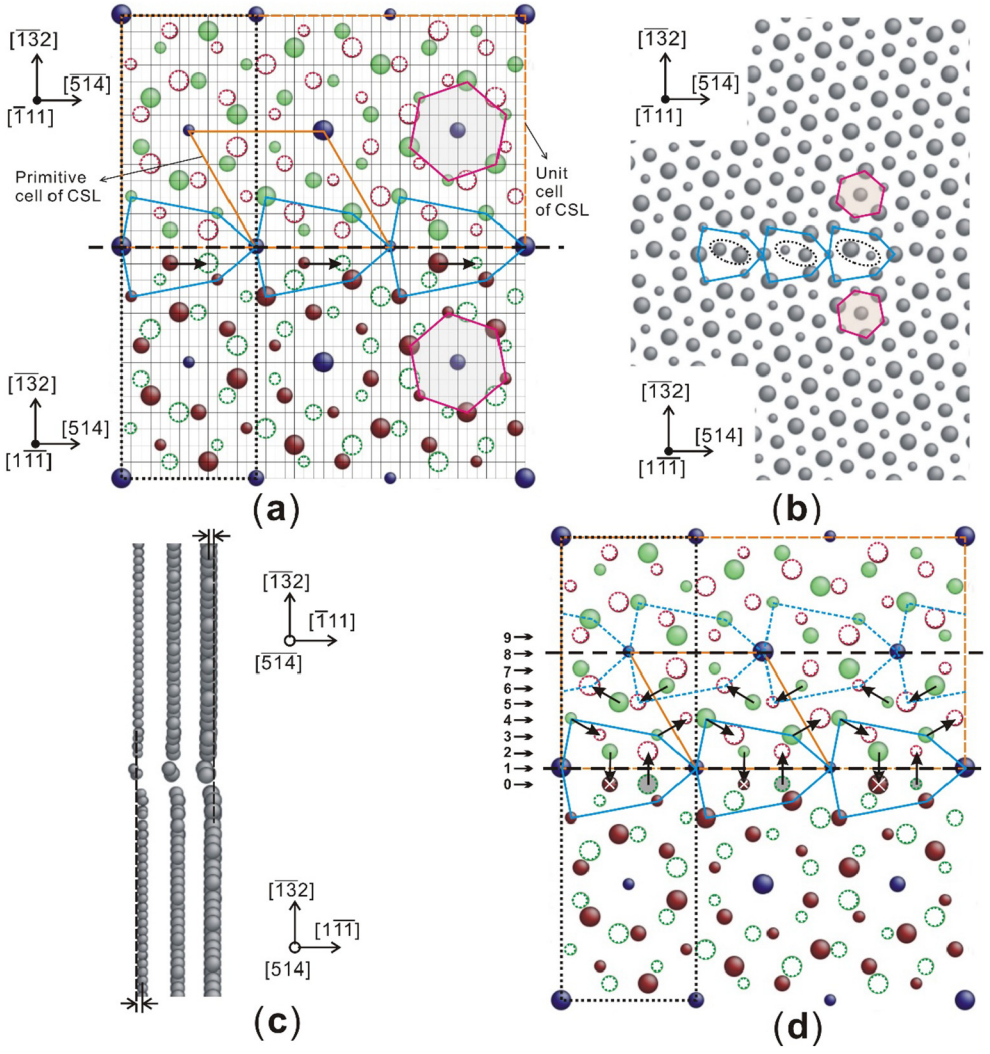

Fig. 1. Bi-crystallographic analysis of the Σ7 {132} GB in Al and the simulated GB structure. (a) is the CSL of the Σ7 {132} GB in FCC crystal viewed along the tilt axis < 111>. Green and dark red spheres represent lattice sites of the upper and lower grains ('real sites'), respectively. Green and red dashed circles represent the extrapolating of the lattices of the upper and lower grains to the other side of the boundary plane ('virtual sites'), respectively. The GB plane is indicated by the black dashed line. The dark blue spheres are the coincident sites. The fine grid is the displacement shift complete (DSC) lattice. Spheres/circles of three sizes distinguish the three different {111} lattice layers along the tilt axis < 111>, with the larger ones closer to the reader. (b) and (c) show the simulated atomistic structure of this type of GB in Al by EAM potential viewed along the tilt axis < 111> and perpendicular to the tilt axis, respectively. The size of spheres is also used to distinguish the three different {111} atom layers along the tilt axis < 111>. (d) is the CSL of the GB as in (a), which shows the atomic shuffling path for the GB migration. In (d), ten adjacent lattice planes (marked as 0–9) parallel to the boundary plane are marked.