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MOLECULAR DYNAMICS STUDY OF DEFORMATION AND FRACTURE OF BI-SEGREGATED COPPER BICRYSTALS*

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ABSTRACT: The microprocesses of deformation and fracture of Bi-segregated copper bicrystals $\Sigma 33\ (\bar{3}\bar{4}5)\ 58.99^\circ$, $\Sigma 11\ (\bar{3}\bar{2}3)\ 50.48^\circ$ and $\Sigma 9\ (\bar{2}\bar{1}2)\ 38.94^\circ$ have been simulated by molecular dynamics in order to study the relationship between the grain boundary embrittlement (GBE) and grain boundary (GB) structure. It is shown that GBE is related to the segregated concentration and distribution of Bi atoms, while Bi segregation is related to the GB structure. Due to their different structures, the bicrystals $\Sigma 33$, $\Sigma 11$ and $\Sigma 9$ show an increasing propensity for Bi segregated concentration. So under the action of external force, $\Sigma 33$, $\Sigma 11$ and $\Sigma 9$ show transgranular ductile, intergranular tearing and intergranular brittle fracture modes, respectively.

KEY WORDS: molecular dynamics, grain boundary embrittlement, empirical *N*-body potential

I. INTRODUCTION

The grain boundary embrittlement (GBE) of metal copper caused by bismuth segregation has been extensively studied both experimentally and theoretically[1-11]. By using the orientation-controlled bicrystals, the strong dependence of Bi segregation and GBE upon grain boundary (GB) structures has been revealed[4, 7, 8]. Russel and Winter[6] observed that the fracture stress for the [100] tilt Cu-Bi bicrystal with CSL boundary is much higher than that with random boundary. The dependence of GBE upon GB structures for [110] tilt Cu-Bi bicrystals has been recently started by Wu et al.[7, 8] An interesting result was that the bicrystals with CSL boundaries show very different fracture behaviour, depending on both segregated concentration and distribution of Bi atoms in GB. The bicrystals display transgranular ductile, intergranular tearing and intergranular brittle fracture modes, respectively. Wu et al. [12] have studied the electronic aspect of GBE. Their results showed that the segregated bismuth atoms attract the electron charge from neighbouring copper atoms in GB onto themselves and weaken the bonds between those copper atoms.

Zhou et al. [9] have studied the atomistic aspect of GBE. Their results showed that with the high enrichment of Bi atoms in the GB core, the $\Sigma 33$ GB and even the $\Sigma 3$ twin GB exhibit brittle fracture, due to the break of the neighbouring weakened copper bonds induced by bismuth segregation. Only a monolayer of Bi atoms segregated in the core of GBs was considered there. The effect of selectivity of Bi segregation in GBs was not taken into account.

Based on studies made more recently by Zhou et al.[13] on the effect of selectivity of Bi segregation in GBs, the GBE for Cu-Bi system is further studied in this paper by molecular dynamics for three different [101] tilt Cu bicrystals.

II. COMPUTATIONAL PROCEDURE

As fracture is a volume-dependent process with the formation of new surfaces, in this paper we use the empirical *N*-body potential for Cu-Cu atoms constructed by Ackland et al.[14] and the approximate *N*-body potentials for Cu-Bi and Bi-Bi atoms constructed by Zhou et al.[13]

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The computational cell is chosen to be a bicrystal slab, similar to that in our previous work[9]. Periodic border conditions are used in the directions parallel to the GB plane. Along the tilt axis , two adjacent (202) planes are periodically repeated. In the direction perpendicular to the tilt axis, the repeat period of the cell is the length of the CSL vector of the corresponding GB or its multiplies, which is about $5a$ long (where a is the lattice constant of copper). In the direction normal to the GB plane, free surface border is employed in simulating fracture, which is different from that used in the previous study.[9]

In the computer simulation, the treatment of border is important and is much more difficult in the simulation of dynamic processes such as fracture than in the static study of matter properties, e. g. GB structure. Various methods have been used in the simulation of fracture, such as fixed border, flexible border and free surface border (for a review, see Yip and Wolf[10]). In our previous study on the fracture[9], the external load was instantaneously added by introducing a relative displacement between the atoms in the loading region and their neighboring atoms. Although it gave some insights to the mechanism of deformation and fracture of the bicrystal as well as the GB embrittlement, the method suffers from some deficiencies. For instance, the critical fracture stress could not be determined since this kind of load corresponds to an impulse load, which is so high that it always results in a rapid rupture of GB. A flexible loading border may reduce the effect of impediment of the border on the motion of dislocations, but it could not eliminated this effect, because the atoms in the loading region could only respond to the deformation of inner region in the tensile direction while the motion of atoms in the other two directions is confined. Therefore, in the present study, we use free surface border which allows the dislocation to glide freely onto surface. The external load is added up slowly. The simulation includes the following steps. At first, the GB structures with segregated Bi concentration are made to relax under the condition of free surface border with the fixed region removed, and the system is brought to a certain temperature. Then, the external forces are slowly applied to the atoms on the free surface normal to the GB plane and increase linearly step by step until the bicrystal fractures. The stress increment per time step (0.01ps) is taken to be 3.0×10^{-5} eV/A^3, which is low enough to minimize the effect of elastic waves on the results, as discussed by Baskes et al.[15] and Smith and Was[11].

III. THE MICROPROCESS OF DEFORMATION AND FRACTURE

3.1 Σ9 Bicrystal

Figs. 1(a)—(d) are the snapshots of the deformation and fracture of Σ9 bicrystal with Bi segregated concentration to be 66.7 atom % at the time steps 2704, 2750, 2773 and 2794,

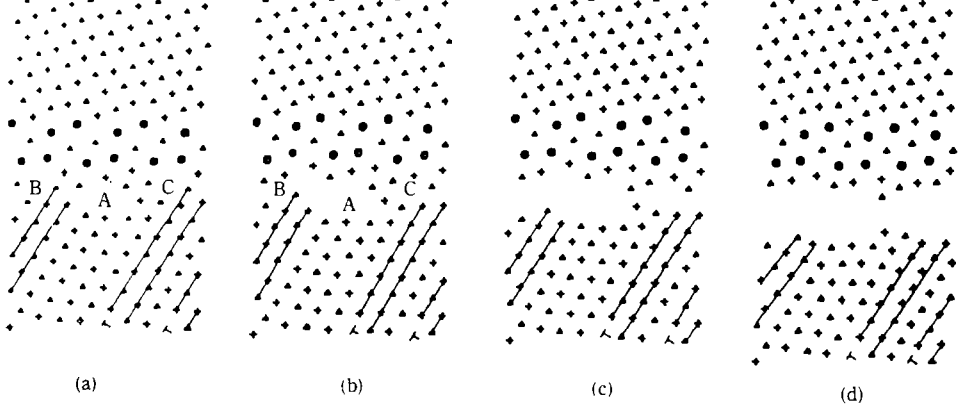

Fig. 1 Microprocess of brittle intergranular fracture of Bi-segregated bicrystal Σ9 at time steps (a) 2704, (b) 2750, (c) 2773 and (d) 2794.

respectively. The Bi atoms are mainly concentrated in the GB core, and Bi segregation leads to the upward migrating of GB plan[13]. Under the external load, a microcrack is formed due to the break of the weakened Cu-Cu bonds in the region A (as shown in Fig. 1(a)). The partial dislocation emission with accompanying stacking fault indicated by straight lines restrains the generation of microcracks in the neighboring regions B and C. Moreover, as the stress further increases, the weakened Cu-Cu bonds will break and lead to the formation of microcracks in those two regions (as shown in Fig. 1 (b)). The microcracks will grow and be connected, and finally result in the intergranular brittle fracture of the Σ9 bicrystal (see Figs. 1 (c) and (d)).

3.2 Σ11 Bicrystal

The snapshots of the microprocess of the deformation and fracture of Σ11 bicrystal with Bi segregated concentration to be 35.7 atom % are shown in Figs. 2(a)— (d) at the time steps 2754, 2776, 2812 and 2834 respectively. Since the distribution of the Bi atoms along the GB is quite inhomogeneous[13] near the site where the Bi segregated concentration is high, such as in A, the weakened Cu-Cu bonds will break leading to the formation of microcracks, but, in the neighboring region where the surrounding Bi concentration is low, the shear deformation appears due to the generation and emission of partial dislocations. Therefore, the fracture of the bicrystal Σ11 is intergranular one with some plasticity due to both the break of the weakened Cu-Cu bonds and shear deformation.

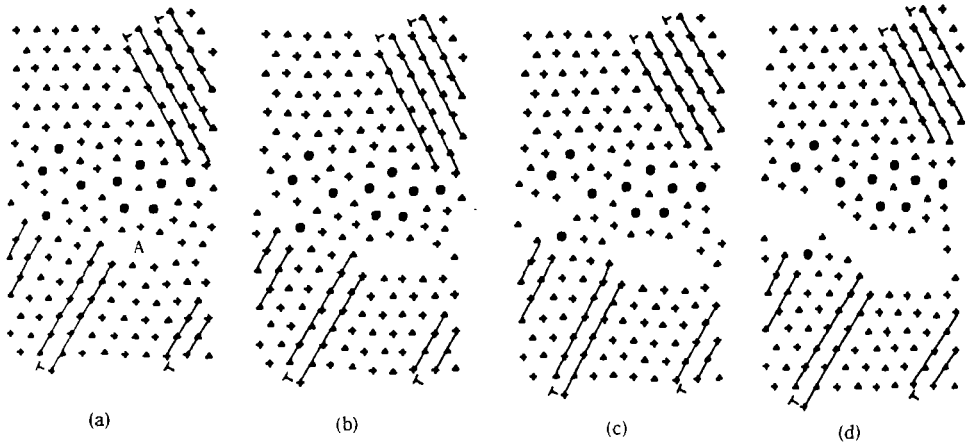

Fig. 2 Microprocess of intergranular shear fracture of Bi-segregated Σ11 at time steps (a) 2745, (b) 2776, (c) 2812 and (d) 2834.

3.3 Σ33 Bicrystal

The snapshots of the microprocess of deformation and fracture of Σ33 bicrystal with Bi segregated concentration to be 19.2 atom % are shown in Figs. 3 (a)— (d) at the time steps 3374, 3405, 3440 and 3467, respectively. The Bi segregated concentration is low and Bi atoms distribute dispersively.[13] Therefore, under the action of external stress, the microcrack is generated mainly due to the gliding of dislocations created in the grain, other than the break of the weakened Cu-Cu bonds (see Fig. 3 (a)). Above fact indicates that the fracture of Σ33 bicrystal is ductile and transgranular.

3.4 Stress-Strain Curves

The stress-strain curves for bicrystals Σ9 , Σ11 and Σ33 are shown in Fig. 4. The fluctuations of the curves are due to the molecular dynamics simulation on finite atoms where the lattice vibrations can be comparable to the change of bicrystal length. The stress corresponding to the point where strain increases rapidly is defined as the fracture stress. The calculated fracture stresses are 3.85, 4.05 and 4.55 eV/a^3 for bicrystals Σ9, Σ11 and Σ33, respectively, where a is the lattice constant of copper.

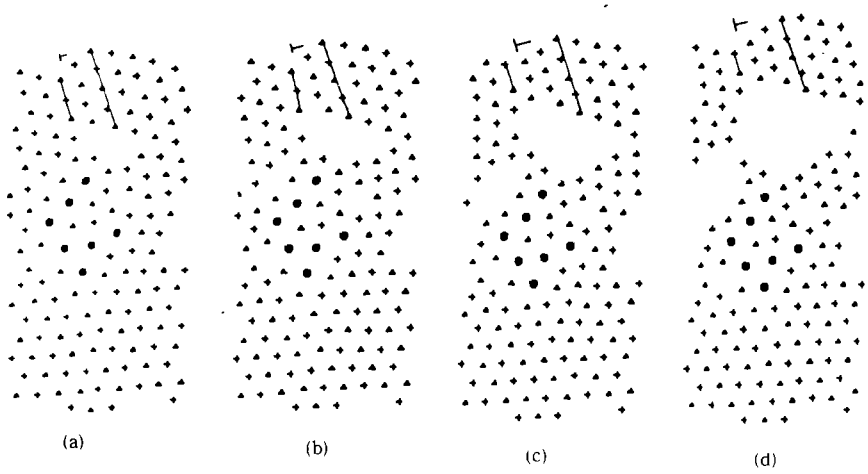

Fig.3 Microprocess of transgranular fracture of Bi-segregated bicrystal Σ33 at time steps (a) 3374, (b) 3405, (c) 3440 and (d) 3467.

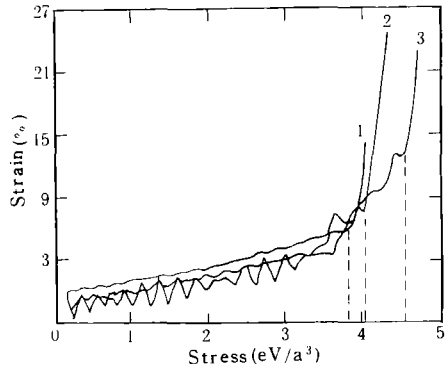

Fig. 4 Stress-strain curves for bicrystals Σ9 (curve 1), Σ11 (curve 2) and Σ33 (curve 3).

IV. DISCUSSION

The segregated concentration and distribution of Bi atoms determine the fracture behaviour of the bicrystals. Since Bi atoms are easy to segregate in the Σ9 GB and concentrate in the narrow region of the GB core, the Σ9 bicrystal exhibits a intergranular brittle fracture due to the break of weakened Cu-Cu bonds under the external stress. In the case of the Σ11 GB, Bi atoms distribute inhomogeneously along the GB plane. Under the external stress, in the region of high Bi segregated concentration microcracks will be formed due to the break of weakened Cu-Cu bonds, while in the region of low Bi segregated concentration shear deformation appears with the generation and emission of dislocations. Therefore, the fracture of the Σ11 bicrystal is intergranular one with shear deformation. In the case of the Σ33 GB, because of the low segregated concentration and dispersive distribution of Bi atoms, the fracture of the Σ33 bicrystal is transgranular and ductile.

The above results of molecular dynamics simulation agree qualitatively with the experimental results [7, 8].

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