An Analysis of $\Sigma 9$ Grain Boundaries in a Cu+6 at.% Si Alloy

Hwang Su Kim

Department of Physics, Kyungsung University, Pusan 608-736

Introduction: It is very important to know the atomic structure of grain boundaries(GBs) formed usually in metals or alloys because of the marked effect of these interfaces on many physical and chemical properties, such as segregation, interfacial corrosion, re-crystallization and material strength[1, 2]. In this work, the author present an electron microscopy study on a typical type of $\Sigma 9$ GBs followed from $\Sigma 3$ {111} coherent twin boundaries and their atomic structures in a Cu-Si alloy

Observations and Analysis: Foils of a Cu-Si alloy (fcc, with a=0.362 nm) were thinned and then examined in a J100CX electron microscope. Fig.1 shows the bright field image of three grains A, B and C and their triple junction boundaries. The zone axis of each GB plane is turned out to be commonly {110}. And the A-C and the A-B boundaries are $\Sigma 3$ GBs with coherent (1 -1 1) and (1 -1 -1) twin planes, respectively. Naturally the B-C must be formed by $\Sigma 9$ GBs with (-2 2 1) twin plane, and the boundaries are identified as (-1 1 1)/(-1 1 5) and (-7 7 10)/(-1 1 14) planes which are obviously incoherent GBs.

The atomic positions near the GB plans projected along the [110] direction are given with (-1 1)/(-1 1 5) interfaces in Fig.2. The atomic positions of the interface of (-7 7 10)/(-1 1 14) are given in Fig.3.

Discussion: One of the compressed pair atoms at the a site in Fig.2 and at the a, b, c and d sites in Fig.3, can be removed to maintain the same atomic density as in the grains. Then one can see locally compressed atoms as seen the pair atoms at b sites in Fig.2 and relaxed atoms at removed atom sites appeared periodically. One might consider overall relaxations of the compressed atoms by a grain body displacement. However the displacement of the grain of $\Sigma 9$ GBs make the energy of $\Sigma 3$ GBs drastically increased, because the coherent twins of $\Sigma 3$ GBs have the most minimum boundary energy. Therefore any significant body displacement of the grain B to the C would be unlikely arisen.

[1] K.L. Merkle, Microsc. Microanal. 3, 339-351 (1997).
[2] V. Randle, M. Caul and J. Fiedler, Microsc. Microanal. 3, 224-233 (1997).

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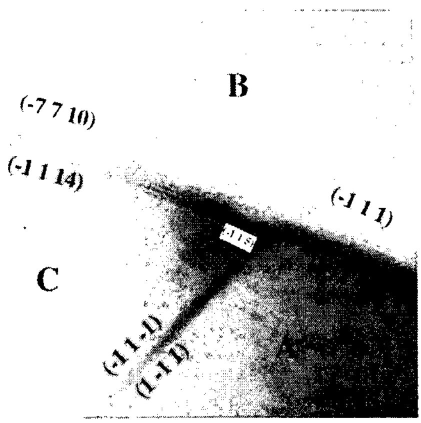

Fig. 1. The bright field image of showing grains A, B and C. The magnification is 26K× 3. The thickness was estimated as ~540 nm(the right side) to ~300 nm (the left side). The angle between (-1 1 1) and (-7 7 10) planes is about 10° . The boundary inclination of (-1 1 1)/(1 -1 -1) is about 80° , but the inclination of (-1 1 -1)/(1 -1 1) is ~ 90° with respect to the incident beam direction.

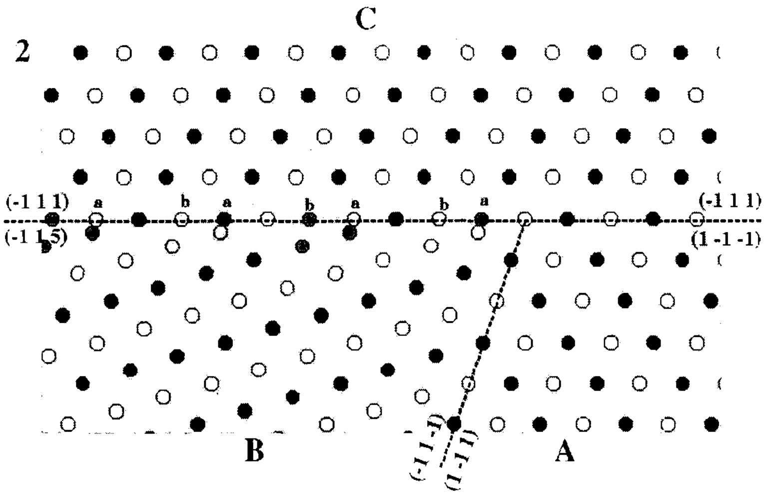

Fig. 2 is a diagram of atomic positions projected along [110] direction in the A, B and C grain regions. The ●'s represent atoms in the plane of paper and the ○ atoms are at ± [½ ½ 0]. It can be seen that the atoms at the a and b sites are compressed.

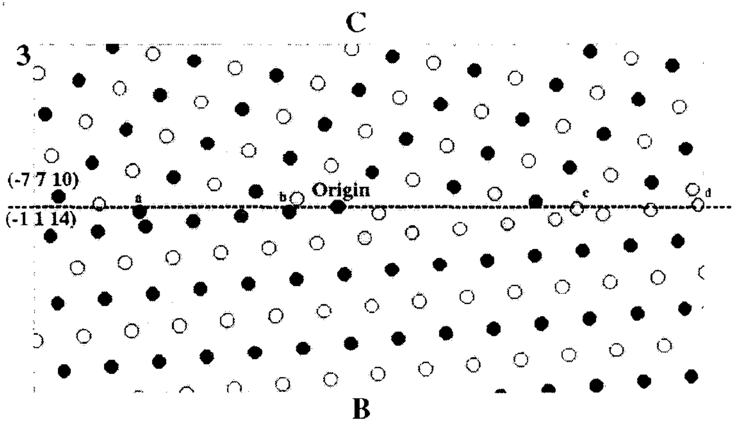

Fig. 3 is for the atomic positions in the grain B and C with (-7 7 10)/(-1 1 14) incoherent GB. The common origin of crystallographic unit cells of the B and C grainsis is denoted as "Origin". The atoms at a, b, c and d sites are seen to be compressed.