## LACBED Study of a Σ3 Grain Boundary in Cu+6 at.% Si Alloy

Hwang Su Kim, Department of Physics, Kyungsung University, Pusan 608-736

A new application of the LACBED (Large Angle Convergent Beam Electron Diffraction) technique for the determination of the displacement vector **R** at a Σ3 grain Boundary in Cu+6at.% Si alloy is presented here. It is shown that in LACBED many high index reciprocal CSL reflections, $\mathbf{g}_c$, can be utilized to obtain the phase factor of $\mathbf{g}_c \cdot \mathbf{R}$, allowing a high accuracy for the determination of **R**. In this study the value of **R** at an asymmetric boundary of (121)/(525) in a $(\bar{1}2\bar{1})$ twin is accurately determined. This result indicates that there is no excess volume at this boundary.

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It has been generally known that the atomic structures at large angle grain boundaries (GBs) in metals and crystalline materials may be directly related to physical properties, such as segregation, interfacial corrosion, recrystallization and mechanical strength. A particular important factor in this regard is the excess volume that can occur in intergranular regions [1,2]. In this work, we have applied the LACBED (Large Angle Convergent Beam Electron Diffraction) technique to the study of a Σ3 GB in a Cu+6at.% Si alloy for obtaining an accuracy in the determination of the displacement vector **R**. The magnitude of any volume expansion at the GB is estimated from the component of **R** normal to the boundary.

**Observations and Simulations**: Foils of 75 $\mu m$ thick of Cu +6at.% Si alloy (fcc, with a = 0.362 nm) were examined by a Philips CM30 microscope having LACBED facilities. Fig. 1 shows the BF and DF LACBED pattern of the GB region of an asymmetric boundary of (121)/(525) in a $(\bar{1}2\bar{1})$ twin orientation. Fig. 2a and b show the calculated BF and DF LACBED patterns near $[311]_1$ orientation using formulations in [3], corresponding to Fig. 1a and b respectively. This computer simulations give us the phase factor of $\mathbf{h}_{\bar{2}20} \bullet \mathbf{R} = 0.15$. In this way other LACBED patterns of $\bar{1}\bar{1}5/\bar{3}33$ and $060/4\bar{2}4$ were also simulated with observations.The obtained phase factors associated with three independent diffracting vectors as summarized,

$$\mathbf{h}_{\bar{2}20} \bullet \mathbf{R} = 0.15 \pm 0.025 + n_1$$

$$\mathbf{h}_{4\bar{2}4} \bullet \mathbf{R} = 0.3 \pm 0.1 + n_2$$

$$\mathbf{h}_{\bar{3}33} \bullet \mathbf{R} = 0.8 \pm 0.1 + n_3$$

where $n_1$, $n_2$ and $n_3$ are unknown integers. The equations above give,

$$\mathbf{R} = 0.35\left[\frac{\bar{1}}{2}0\frac{1}{2}\right] - \frac{1}{60}[\bar{1}5\bar{1}].$$

*Clearly the component of **R** normal to the boundary plane $(525)_2$ is zero, which means no volume expansion.*

**The atomic structure in the grain boundary**: The atomic positions near the GB plane projected along the $[\bar{1}01]$ direction are plotted in Fig. 3 by analysing data above. In passing, it is worth noting that the displacement in the direction $[\bar{1}01]$ would not be detectable in HREM, which gives a 2-dimensional projection, for the orientation shown in Fig. 3.

**Conclusion**: This study has shown that the LACBED technique has distinct advantages as a TEM tool for the determination of rigid body displacement vectors, which are very important factors in the understanding of the macroscopic properties of metals and metal alloys in terms of the microscopic atomic scale structure of GBs. From the determination of **R** at the GB plane $(121)_1 / (525)_2$ of $\Sigma 3$ in a Cu +6at.% Si alloy under reasonable assumptions, it is concluded that this plane has no significant excess volume.

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[2] C. T. Forwood and L. M. Clarebrough, Electron Microscopy of Interfaces in Metals and Alloys, Adam Hilger, p74 (1991).

[3] H. S. Kim and S. S. Sheinin, phys. stat. sol. (a), **104**, 519-527 (1987).

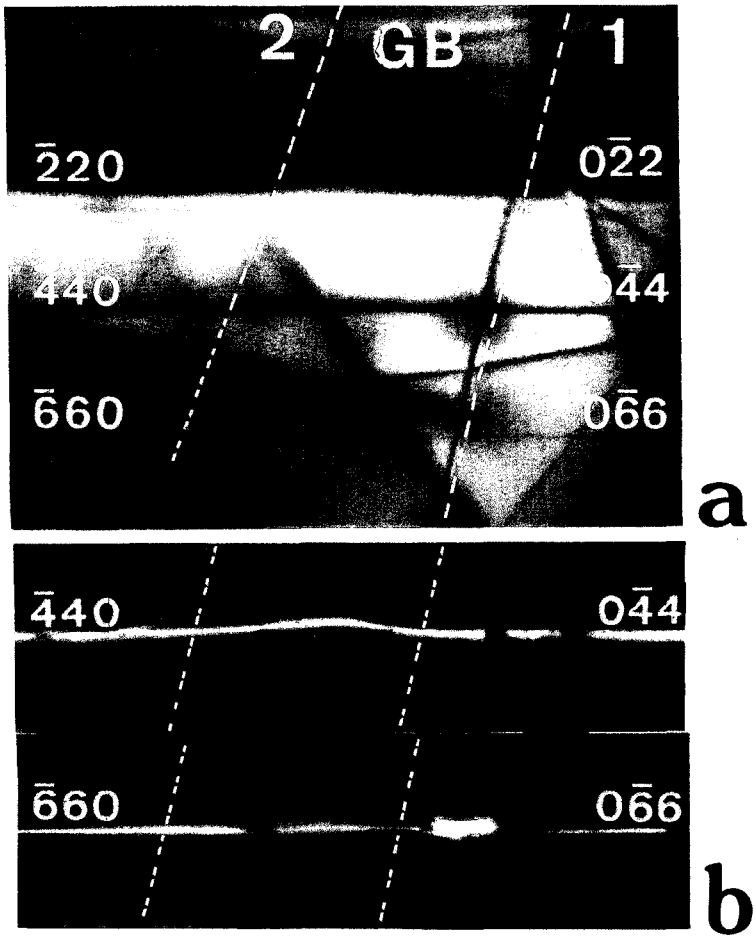


**Fig. 1** The a and b are for the BF and DF LACBED patterns near $[311]_1$ orientation. GB stands for Grain Boundary region bounded with dashed lines.1 and 2 denote grains 1 and 2 respectively.

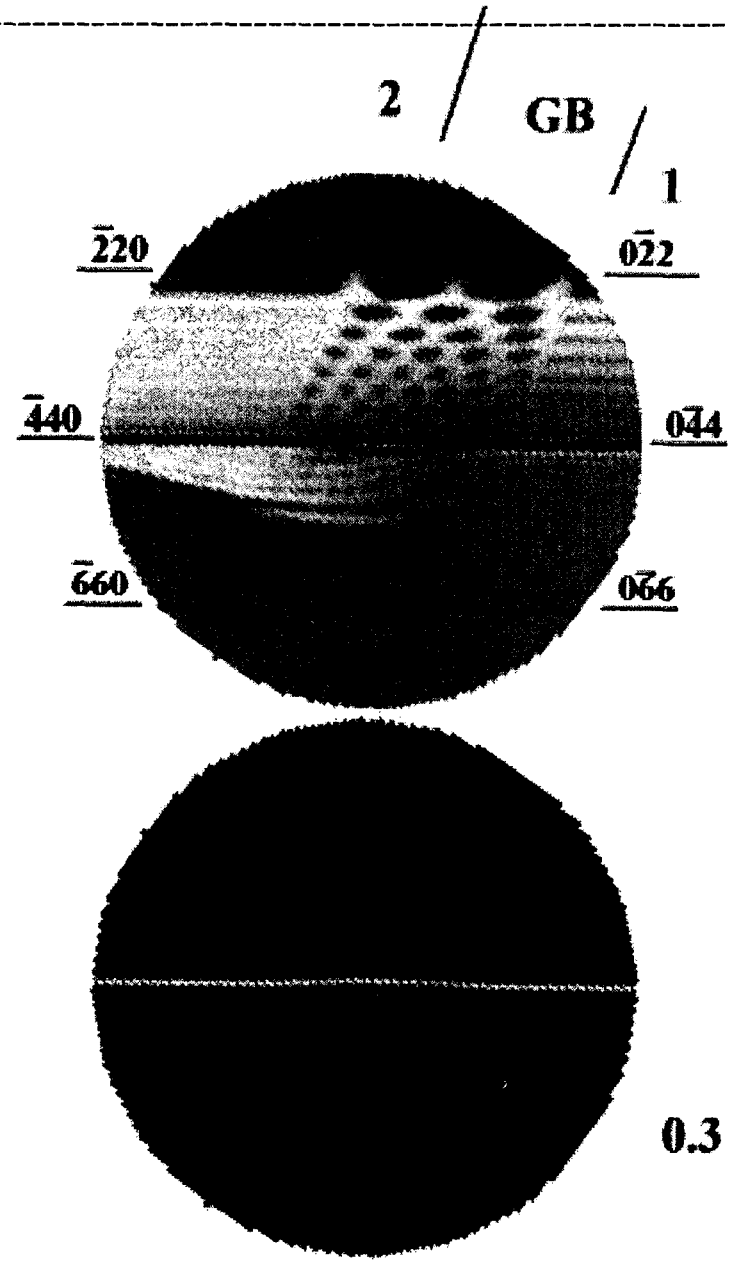


**Fig. 2** a is the calculated BF LACBED pattern corresponding to Fig. 1a. b is the calculated DF LACBED pattern corresponding to Fig. 1b with $0\bar{4}4/\bar{4}40$ diffraction line intensities only. 0.3 are the values of $\mathbf{h}_{\bar{4}40} \bullet \mathbf{R}$.

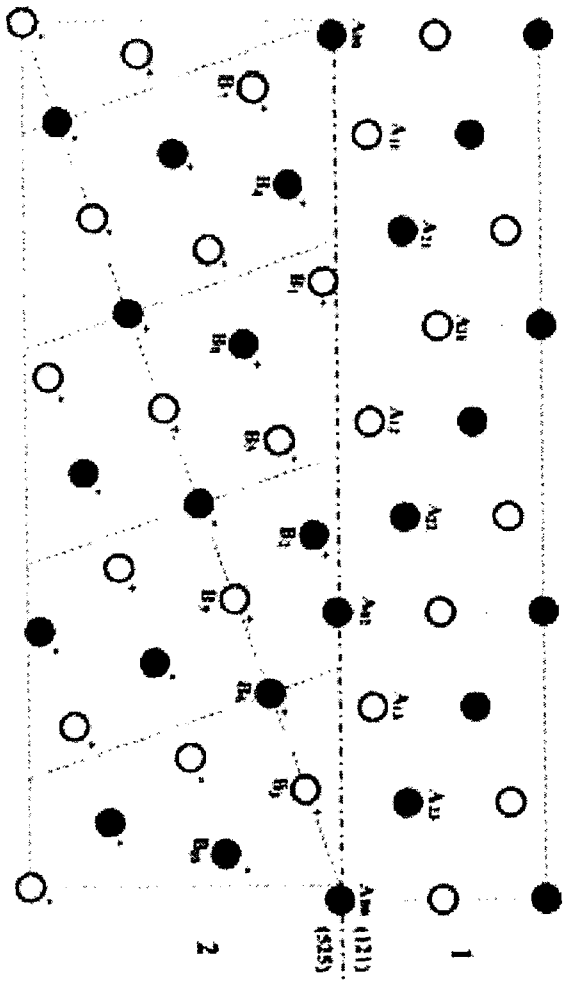

**Fig. 3** Diagram of atomic positions projected along $[\bar{1}01]$ in the grain boundary region with **R**. The solid dark circles represent atoms in the plane of paper and the white circles atoms are at $\pm\left[\frac{\bar{1}}{2}0\frac{1}{2}\right]$. The + sign in the grain 2 means the displacement of $0.35\left[\frac{\bar{1}}{2}0\frac{1}{2}\right]$.