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ATOMIC STRUCTURE OF A 6°[001]/(110) TILT GRAIN BOUNDARY IN ALUMINUM BY HREM

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Introduction

A knowledge of the atomic structure of grain boundaries is central to a better understanding of the properties of polycrystalline materials. Attempts to predict grain boundary structure have so far led to the development of various geometrical models for grain boundaries. The concepts of coincident site lattice (CSL) (1), displacement shift complete (DSC) lattice (2,3,4) and the 0-lattice model (2), based on geometrical constructions of adjoining crystals forming boundaries, have been found useful in characterizing the structure of ideal grain boundaries. These models give suggestions regarding the atomic relaxation that occurs at the core of the boundary in the form of dislocations. The 0-lattice model is particularly useful in describing the primary dislocation content of low angle grain boundaries.

With the recent development of intermediate voltage electron microscopes (300-400 kV), it is possible to obtain atomic resolution images of grain boundaries in most metals (5). The atomic structure of a few simple grain boundaries in FCC metals has been investigated (6,7). For example, attention has been focused on (110) aluminum grain boundaries such as $\Sigma 3$[110] tilt (8), $\Sigma 9$[110] tilt (9) and 90°[110] tilt (10). In most of these cases, the ideal CSL, DSC lattice and the 0-lattice geometrical models have been used advantageously for structural characterization. For low angle tilt grain boundaries in FCC metals HREM studies have been performed mainly on (110) tilt orientations (11). For these interfaces, good agreement between the primary dislocation content predicted by the 0-lattice model and the experimentally observed dislocation content is achieved. Examples of HREM studies of [001] tilt low angle grain boundaries in FCC metals are very rare. To our knowledge, only a 16°[001] tilt boundary in gold has been investigated (12). However, due to a 10° inclination of the interface to the electron beam, and the resolution limit for the 200kV high resolution microscope used in the study, the core structure of this particular boundary was not resolved. The only visible features were the displacement fields of the primary dislocations. The spacings of the dislocations was found to be in agreement with the 0-lattice theory.

In this paper we present a high resolution electron microscopy investigation of the core structure of a 6°[001] symmetical tilt grain boundary in aluminum. For the first time the atomic structure of such a grain boundary in an FCC metal is resolved. The boundary structure obtained from the HREM images is compared to the corresponding structure predicted by the 0-lattice model and found to be in excellent agreement.

Experimental Procedure

The aluminum bicrystal used in this study was prepared by cross-rolling and annealing method described in detail elsewhere (13). The thin foil of 3 mm diameter containing the boundary was obtained by spark cutting followed by electropolishing in 73% methanol, 25% nitric acid and 2% hydrochloric acid at a voltage of 50 V at room temperature. The thin foil was examined in a 120 kV Hitachi electron microscope to determine the angle/axis orientation of the boundary. High resolution electron microscopy was performed with a JEM 4000EX electron microscope operated at 400 kV. All images were obtained and recorded near the optimum defocus,

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typically at a magnification of 500,000 times. Under these experimental conditions atomic columns appear black and the atomic structure of the boundary was resolved unambiguously.

Results and Discussion

The investigated boundary is a [001] 6° low angle tilt boundary with a twist character of only 0.1°. Electron microscope observation shows that most of the grain boundary appears straight and roughly parallel to the median of the (110) planes of both crystals. Figure 1 shows an HREM micrograph of a straight portion of the boundary. The boundary can be described in terms of regular arrays of dislocations separated by nearly perfect lattice. A Burgers circuit drawn around one of these dislocations, as shown in Fig. 2, gives a Burgers vector of magnitude a/2 $[\bar{1}10]$, which is common to $(\bar{1}11)$ and $(1\bar{1}1)$ planes. For a pure edge dislocation, such line vector is normal to an extra half plane on either of the {111} planes. In [001] projection, the trace of these extra half planes will also appear along two mutually perpendicular <100> directions. In the HREM micrograph of Fig. 2, extra half planes can be observed along [100] and [010] directions. This implies that pure edge dislocations with Burgers vector a/2 $[\bar{1}10]$ only exist at this portion of the boundary.

Figure 3 shows a two-dimensional representation of the dichromatic pattern with superimposed 0-lattice for the 6°[001] misorientation. In this plane the coordinates of the 0-lattice vectors referred to the lattice of crystal 1 (represented by circles in Fig. 3) are determined in the limit of a small rotation angle θ as:

$$\vec{X}_a^{(0)} = \begin{bmatrix} 1/\theta \\ 1/2 \\ 0 \end{bmatrix} \qquad \vec{X}_b^{(0)} = \begin{bmatrix} -1/2 \\ 1/\theta \\ 0 \end{bmatrix}$$

In the third dimension, the 0-lattice runs parallel to the common rotation axis. The 0-lattice vector in this direction is:

$$\vec{X}_c^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1/2 \end{bmatrix}$$

The observed grain boundary plane runs parallel to a vector $\vec{X}^{(0)} = \vec{X}_a^{(0)} + \vec{X}_b^{(0)}$, which corresponds to a line of maximum fit between the two misoriented crystals. However, in order to accommodate for the small angle misorientation, 1/2<110> lattice edge dislocations form, the trace of which is indicated at the location marked "⊥" on Fig. 3. These locations are the region of poorest fit between the two crystal lattices. A grain boundary parallel to $\vec{X}^{(0)}$ will therefore be constituted of perfectly crystalline patches spaced by lattice dislocations at the positions of maximum misfit as can be seen in the HREM image (Fig. 1). The spacing, D, between primary dislocations constituting the grain boundary is given in the small angle limit by the formula $D = a/\theta$, where a is the lattice spacing on the (110) plane. A calculated D of 2.9 nm is in excellent agreement with the dislocation spacing measured on the HREM image of Fig. 1.

Conclusion

We have presented for the first time the atomic structure of the core of a 6°[001] low angle tilt grain boundary in an FCC metal as resolved by HREM. The primary dislocation content of the 6°[001]/(110) low angle tilt grain boundary in aluminum observed by HREM is in excellent agreement with the grain boundary predicted by the 0-lattice geometrical model. The grain boundary plane is located along the median of the [110] direction of both crystals. This boundary orientation possesses the lowest primary dislocation density, which may correspond to a minimum energy configuration.

Acknowledgements

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References

1. M. L. Kronberg and F. M. Wilson, Trans A.I.M.E., 85, 26 (1964).
2. W. Bollmann, Crystal Defects and Crystalline Interfaces, Stringer, New York (1970).
3. R. W. Balluffi, in Interfacial Segregation, A.S.M., Metals Park, Ohio (1977).
4. D. A. Smith and R. C. Pond, Intern. Metals Reviews, 205, 61 (1976).
5. A. Bourret and J. M. Penisson, JEOL News, 25E, 1 (1987).
6. J. M. Penisson, J. de Physics, CS49, 87 (1988).
7. F. Cosandey, Siu-Wai Chan, and P. Stadelmann, Scripta Metall., 22, 1093 (1988).
8. M. Shamsuzzoha, P. A. Deymier, and David J. Smith, Phil. Mag., submitted.
9. M. J. Mills, G. J. Thomas, M. S. Daw, and F. Cosandey, MRS Proceedings, Fall Meeting, Boston (1989).
10. U. Dahmen and K. H. Westmactott, Scripta Metall., 22, 1673 (1988).
11. M. J. Mills, Phil. Mag., A66, 355 (1989).
12. W. Krakow and D. A. Smith, Ultramicroscopy, 22, 47 (1987).
13. M. Shamsuzzoha and P. A. Deymier, Scripta Metall., accepted for publication (1990).

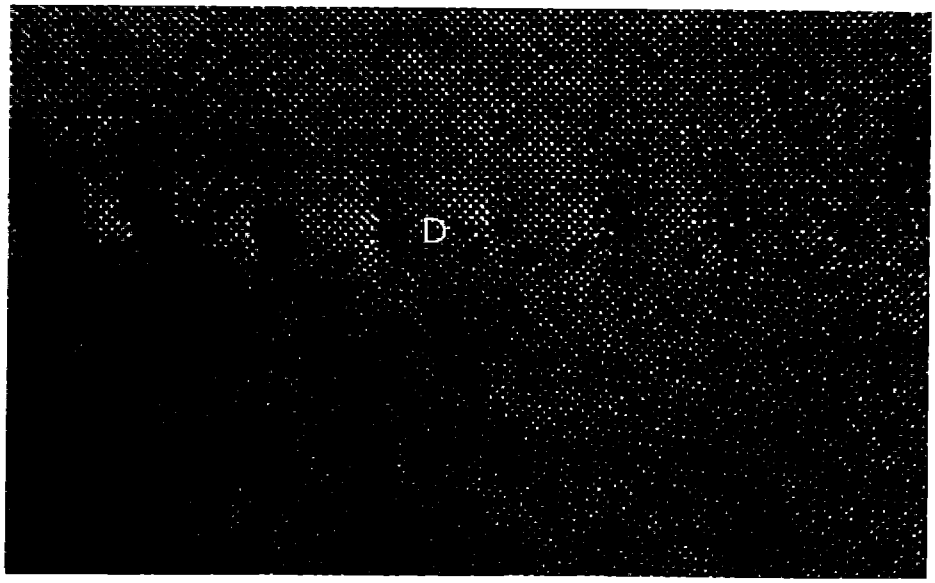

FIG. 1. HREM micrograph recorded at 400 kV showing a 6°[001] symmetric tilt grain boundary in Al with dislocation spacing shown as D.

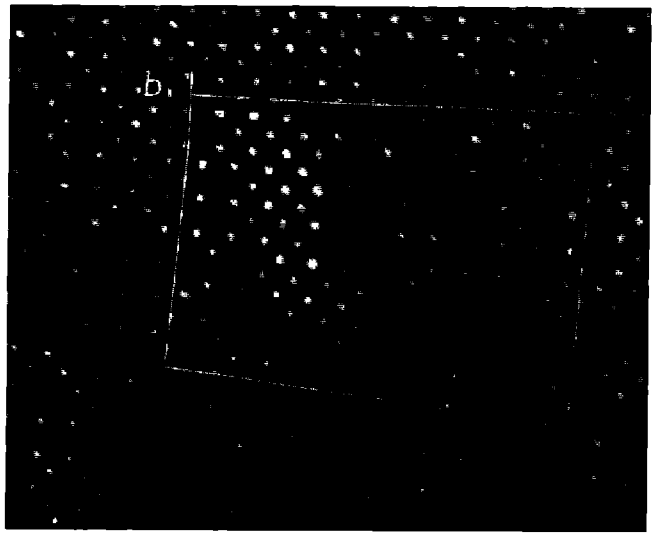

FIG. 2. Magnified image of a single dislocation taken from Fig. 1. A Burgers circuit drawn around the dislocation indicates a Burgers vector $\bar{b} = \frac{1}{2}[\bar{1}10]$.

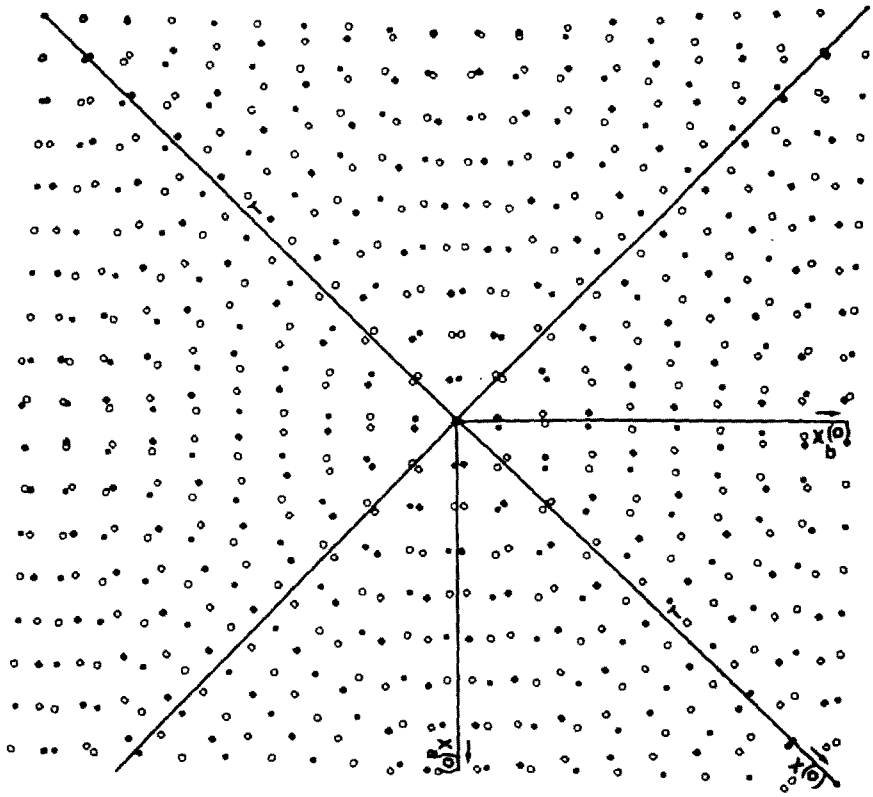

FIG. 3. Dichromatic pattern and the 0-lattice for a 6° [001] misorientation between two F.C.C. lattices. ("∘" and "•" stand for atoms in two successive (001) planes of crystal 1. "□" and "■" similarly represent two successive (001) planes in crystal 2.) The edge dislocation symbols appear at the position of maximum misfit between the two lattices.