



## HREM STUDY OF 45° [100] QUASIPERIODIC GRAIN BOUNDARY IN ALUMINUM

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### Introduction

The structural study of grain boundaries is central to a better understanding of many physical properties of polycrystalline materials. In recent years, there has been remarkable progress in research on the atomic structure of grain boundaries, with the publication of theoretical and experimental structures of many grain boundaries [1-5] and comprehensive reviews [6,7]. The availability of intermediate voltage electron microscopes (300-400 keV) now provides easy access to atomic resolution images of grain boundaries in many metals and semiconductors in low-index zone axis projections [8]. These studies are complemented by geometrical models of grain boundaries based on the coincident site lattice (CSL) [9], displacement-shift-complete (DSC) lattice [10-12] and the O-lattice theories [10]. These models provide an adequate framework for structural characterization of the atomic-resolution images of grain boundaries. However, this approach to studying grain boundary structures has limitations in the sense that it only provides structural information on periodic boundaries. The current body of knowledge on interface structures is almost entirely accumulated from grain boundaries and interfaces with periodic structure.

The vast majority of grain boundaries in polycrystalline materials are more general and possess complex atomic structure. Structural information on these grain boundaries remains sketchy because of the lack of theoretical and experimental tools for their structural characterization. It is thus recognized [6] that efforts should be directed to gaining knowledge about the structure. Owing to the complex structure of these boundaries, it seems desirable initially to perform structural investigations on boundaries intermediate to periodic and complex general boundaries. Quasiperiodic grain boundaries do not possess translational periodicity, but have some degree of structural order. Thus, they can be considered as a bridge between periodic and general boundaries, and they offer an opportunity to study structures that may be prototypes of more complex boundaries. The structure of quasiperiodic boundaries can be characterized within the framework of the crystallography of quasicrystals [13]. So far, only a few structural studies of quasiperiodic boundaries have been reported [14-16]. This paper focuses on quasiperiodic boundaries and presents for the first time an HREM study of a 45° [100] twist quasiperiodic grain boundary.

### Experimental Procedure

The aluminum grain boundary used in this study was prepared by cross-rolling and annealing using a method described elsewhere [17]. In order to obtain a thin foil suitable for transmission electron microscopy, a cylindrical specimen of 3mm diameter containing the boundary was prepared by spark cutting. The cylindrical disc thus obtained was polished gently on 600 grade SiC paper to reduce its thickness to 0.16mm. Finally, the disc was electropolished at a voltage of 14V at  $-25^{\circ}\text{C}$  in a solution of 30% nitric acid and 70% methanol. Polishing was halted just after perforation. The thin foil was first examined with a 200keV Hitachi H-8000 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 400keV. All high-resolution images were recorded near optimum defocus at a typical magnification of 500,000 times. Under these experimental conditions, atomic columns appeared black so that images could be interpreted intuitively in terms of atomic column positions to within about 0.03nm [18].

### Results and Discussion

Figure 1 shows an HREM image of the investigated grain boundary and associated bicrystal. The image exhibits atomic columns projected along [011] and [001] of crystals 1 and 2, respectively, and therefore, defines a  $45^{\circ}$  [100] twist misorientation for the bicrystal. The boundary is thus expected to assume a crystal symmetry and structure consistent with this misorientation. Representative dichromatic patterns (DCP) of a  $45^{\circ}$  [100] twist misoriented Al bicrystal, projected along  $[100]_{1,2}$  twist axis and  $[011]_1$  or  $[001]_2$  axes are shown in Figures 2a and 2b, respectively. These patterns exhibit an  $8'/mmm'$  point group symmetry, where operations indicated with a prime are colored operations relating atoms of two interpenetrating crystals, and unprimed symmetry operators relate atoms within their respective crystals. The eight-fold colored axis is parallel to the rotation axis and perpendicular to a mirror plane that runs parallel to (100) of both crystals. The  $8'/mm'n$  symmetry of the DCP is not compatible with any periodicity, but it is consistent with the presence of quasiperiodicity in the bicrystal [19]. Thus, the structure present at any interface of an identically oriented experimental bicrystal such as the present boundary should exhibit quasiperiodicity.

The HREM micrograph of Figure 1 indicates that the experimental bicrystal locally exhibits close contact between (100) of both crystals at its interface, but fails to maintain a well-defined boundary plane

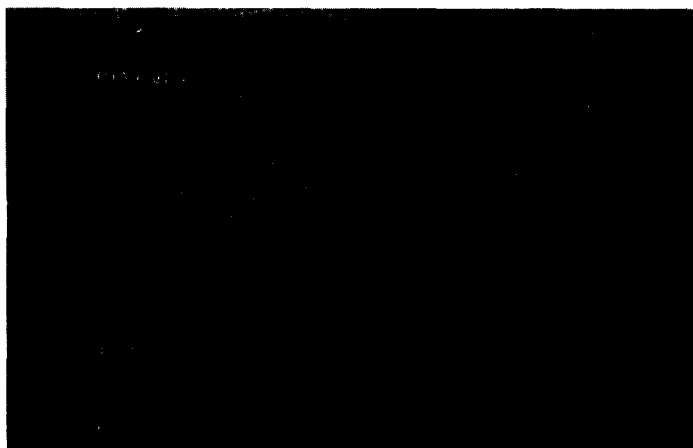


Figure 1. HREM micrograph of  $45^{\circ}$  [100] twist bicrystal as viewed along [011] and [001] of crystal 1 and 2. The boundary is not strictly parallel to (100) of either crystal.

over an extended length. This suggests that the orientation of the boundary plane varies regularly along the boundary. Closer inspection immediately reveals that regular occurrence of grain-boundary stepping causes these variations in the orientation of the boundary plane. In a magnified view of a boundary segment (Figure 3), such steps are visible at the positions marked by arrows.

In the event of stepping, periodic grain boundaries conserve their lowest energy boundary structure by rigid-body translation. This translation generally produces a secondary grain boundary dislocation (SGBD) to accompany such stepping. The SGBD usually assumes a DSC-lattice Burgers vector. For quasiperiodic grain boundaries, the  $\Sigma$  value of the related CSL assumes infinity and the corresponding DSC lattices become infinitely small [20]. As a consequence, no SGBD is expected to be associated with stepping in quasiperiodic grain boundaries. Thus, any step in a quasiperiodic grain boundary neither brings about any rigid-body translation nor produces any change in the structure and energy of the boundary. The boundary segments produced by such steppings are commonly referred to as locally isomorphic [13], i.e., they all possess the same type of local atomic environment. An important question that remains is how quasiperiodic grain boundaries, in the event of stepping, minimize their energy. A structural study of the atomic arrangement existing at the experimental boundary is likely to provide answers to this question. However, consideration of the fact that the  $(100)_{1,2}$  boundary plane of the DCP shown in Figure 2b depicts a close geometrical description of the experimental boundary plane, seems to suggest that prior structural study of the boundary of the DCP is desirable. It not only provides knowledge on the structure of the experimental boundary, but also helps to identify locations in the experimental boundary at which the structural study should be directed.

Inspection of the  $(100)_{1,2}$  grain boundary plane present in the DCP of Figure 2b reveals that apart from the coincident point O, which lies on the eight-fold colored axis, the lattices belonging to crystal 1 and 2 do not exhibit one-to-one lattice correspondence across the boundary. However, owing to a ratio of periods along the boundary plane equal to  $2^{1/2}$  one may be able to interpret the lattice matching at the boundary in terms of "pseudo-coincidence." For instance, the lattice points labeled A and B can be considered as being almost coincident, and that they exhibit 17  $(02\bar{2})$  planes of crystal 1 and 12  $(020)$  planes of crystal 2 between them. The points A and B are also separated from the coincident point O by 7 and 10  $(02\bar{2})$  planes of crystal 1 and 5 and 7  $(020)$  planes of crystal 2, respectively. Boundary segments existing between OA, OB and AB exhibit respective stacking ratio of 1.400, 1.428 and 1.417 for the  $(02\bar{2})_1$  and  $(020)_2$  planes. It appears that atomic environment surrounding these "pseudo-coincident" points of the

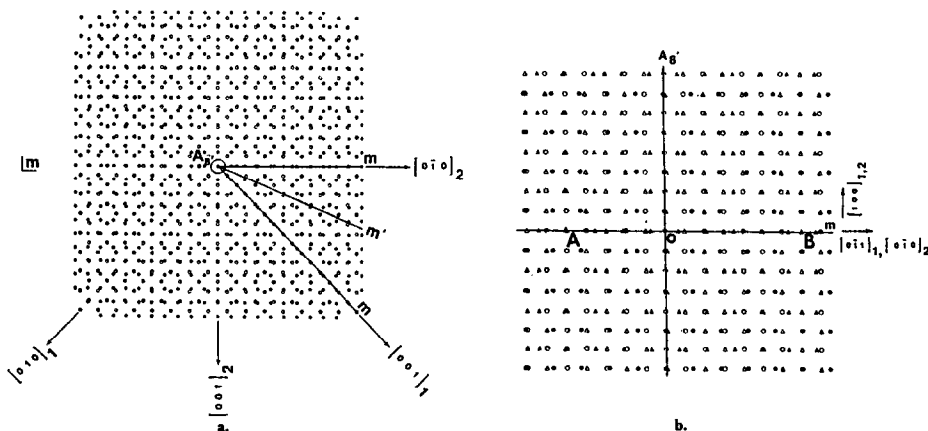


Figure 2. (a)  $45^\circ$   $[100]$  dichromatic pattern as viewed along  $[100]$  of crystals 1 and 2. Circles and triangles represent lattices of crystals 1 and 2, respectively. (b) Dichromatic patterns of (a) as viewed along  $[011]_1$  and  $[001]_2$ . Filled and unfilled circles and triangles represent successive  $(011)_1$  and  $(001)_2$  planes, respectively.

boundary is expected to be favored for strong atomic interactions. Therefore, these boundary locations are likely to play critical roles in the overall stability of the boundary. Analyses of the experimental image (Figure 3) revealed that the grain boundary steps at "pseudo-coincident" points which are separated by distances identical to that mentioned for AO and AB of the DCP of Figure 3b. It appears that atomic interactions at the special locations of "pseudo-coincidence" allow the experimental boundary to destabilize to such an extent that steps occur to minimize energy, and then it assumes some stable structure. Boundary segments, thus formed by successive stepping, possess structures in which terminal planes of constituent crystals, i.e.  $(02\bar{2})_1$  and  $(020)_2$ , maintain a stacking ratio close to  $2^{1/2}$ .

### Conclusion

The present HREM study on a  $45^\circ$  [100] twist grain boundary in an Al bi-crystal provides experimental evidence that the structure of quasiperiodic grain boundaries is regulated by the local atomic environment existing at the boundaries. The boundary investigated reveals certain special locations at which the local atomic environment favors stepping. These special locations owe their origin to the existence of dissimilar planar stacking between  $(02\bar{2})_1$  and  $(020)_2$  across the boundary. This dissimilarity in stacking allows the boundary to exhibit close correspondence for  $(02\bar{2})_1$  and  $(020)_2$  when the stacking ratio of the two planes approaches the irrational number,  $2^{1/2}$ . The boundary appears to destabilize at such locations and undergoes stepping in order to relax its structure.

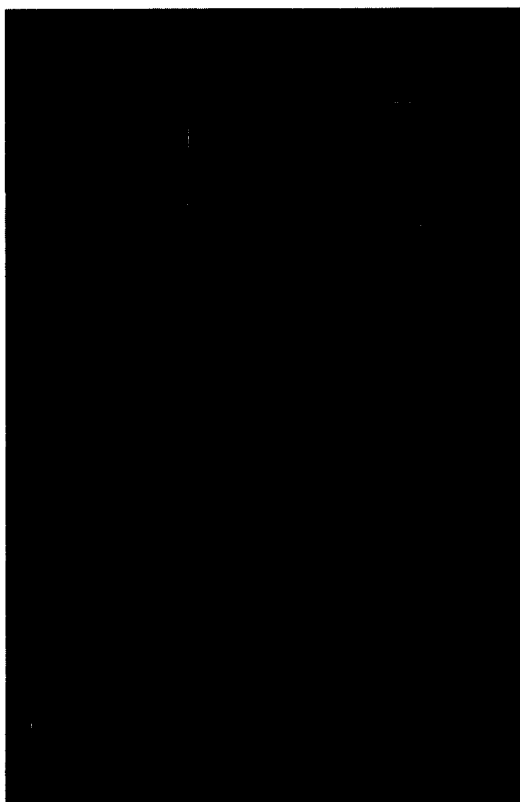


Figure 3. Magnified image of grain boundary steps taken from segment of  $45^\circ$  [100] twist boundary shown in Figure 1.

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