SAND2008-7300C

Formation of Hexagonal Close Packing at a Grain Boundary in Gold by the Dissociation of a Dense Array of Crystal Lattice Dislocations

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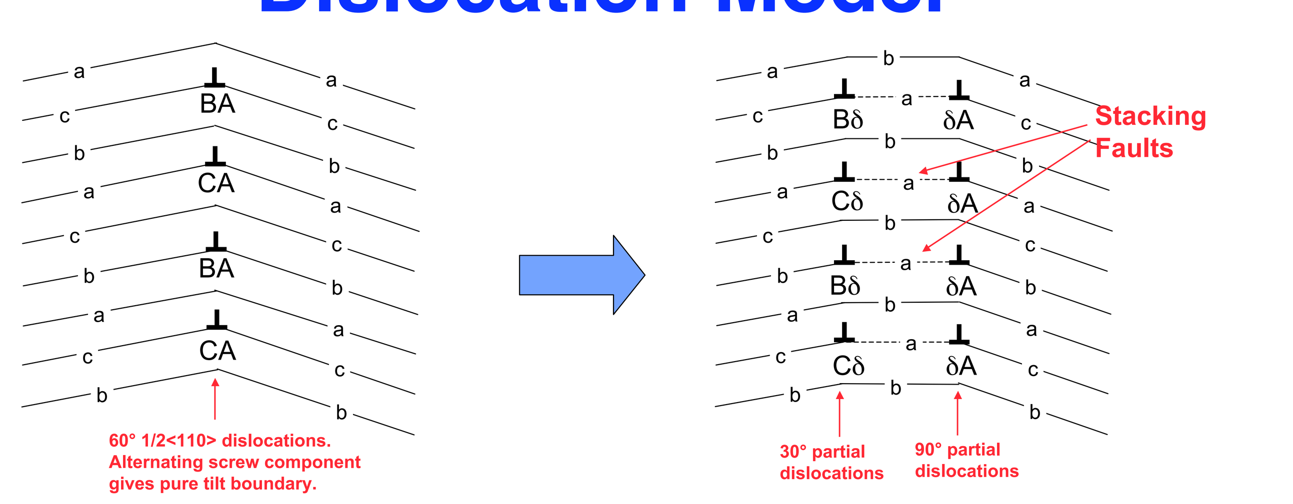
Introduction

Grain boundaries in face-centered-cubic (FCC) metals with low stacking-fault energies often form broad, three-dimensional structures that are composed of arrays of stacking faults [1-5]. A general question concerns how the pattern of such faults, and hence the structure of the boundary, is related to the orientational parameters that describe the macroscopic geometry of the interface. Here, we analyze the formation of a layer of hexagonal-close-packed (HCP) material at a grain boundary in gold. We present high-resolution transmission electron microscopy (HRTEM) observations and atomistic calculations of this interface. HCP has been predicted and observed previously at FCC grain boundaries [3,5], but at a higher misorientation than that of the boundary we analyze here. Thus, the specific questions we address here are: why does HCP form at this particular boundary and how is it related to the HCP that has been found at higher misorientations?

[1]K.L.Merkle Colloque de Physique 51: C1-251 (1990).
[2]F. Ernst et al., Physical Review Letters 66: 991 (1992).
[3]J.D. Rittner and D.N. Seidman, Physical Review B 54: 6999 (1996).
[4]T. Radetic T, F. Lançon F, and U. Dahmen, Physical Review Letters 89: 85502 (2002).
[5]G. Lucadamo and D.L. Medlin, Science 300: 1272 (2003).

Dislocation Model



Schematic of dislocation arrangement at the observed grain boundary. Here, an array of 60° 1/2<110> type dislocations, distributed at a spacing of one dislocation to every two {111} planes, has dissociated into Shockley partial dislocations. The arrangement of stacking faults in this dissociated layer gives an …abab… stacking sequence.

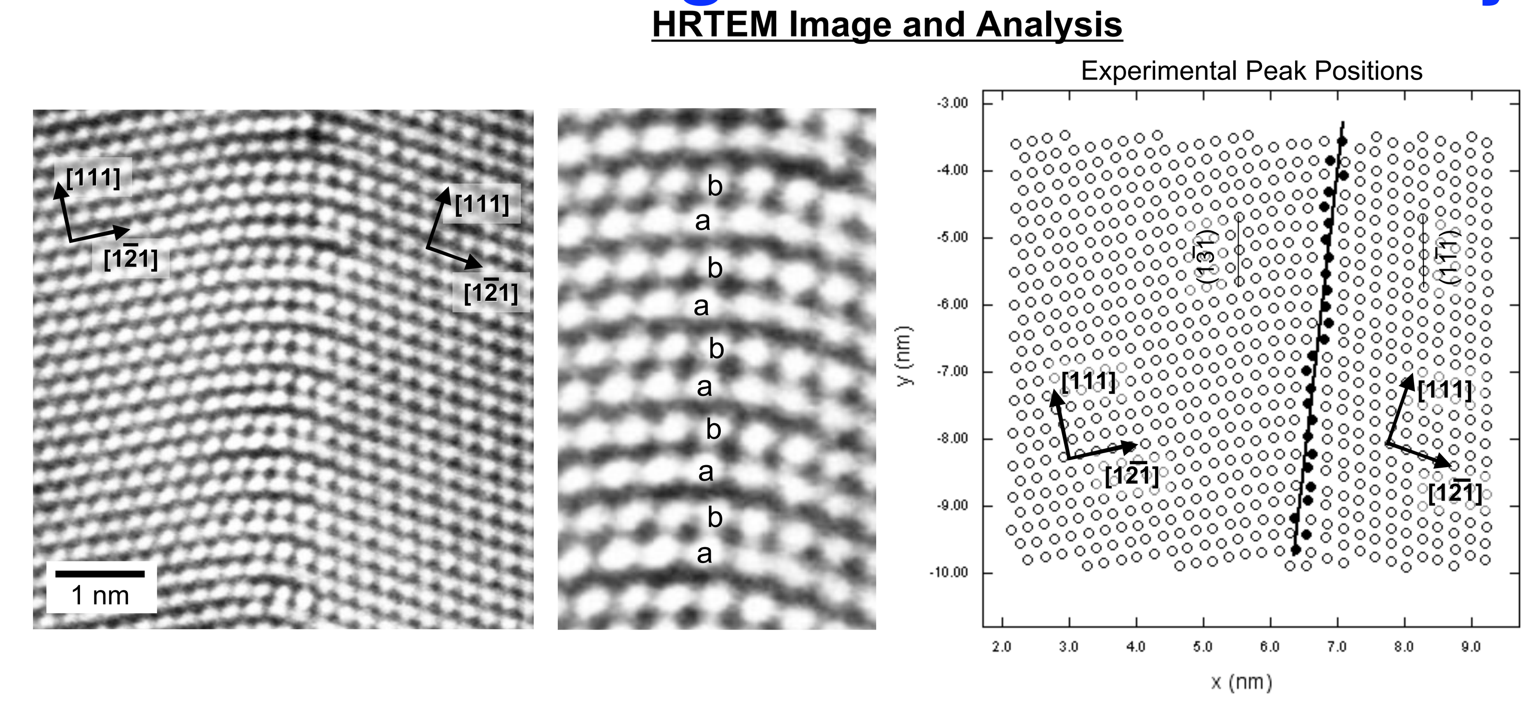
Solution of the Frank-Bilby equation for this dislocation content gives a misorientation of 29.7° and a boundary inclination with interface vectors: $1/2[19,10,19]_{left}$ and $1/2[13,22,13]_{right}$. The resulting boundary planes are vicinal to (1,-3,1) and (1,-1,1).

Frank-Bilby Equation

$$\mathbf{B}=(\mathbf{I}-\mathbf{P}^{-1})\mathbf{v}$$

HCP Stacking at a Grain Boundary in Au

HRTEM Image and Analysis

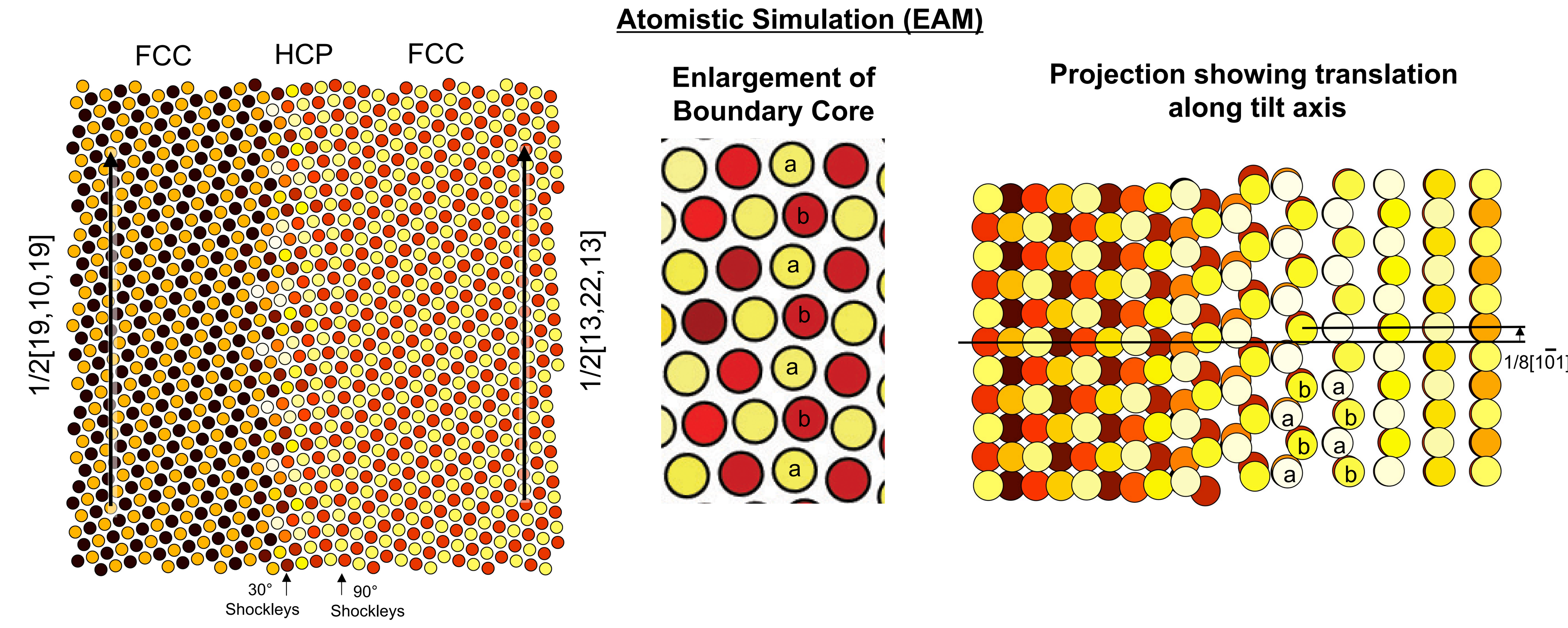


The boundary misorientation (28.8°) and inclination (16.1°) were measured from the HRTEM lattice fringe intensity peak positions.

To determine the boundary inclination we measured the local angle at each peak position based on its adjacent neighbors and defined the boundary position based on the peak positions with local angles closest to the midpoint of the far-field angle.

This analysis highlights the terraces along the (1,-3,1)/(1,-1,1) planes.

Atomistic Simulation (EAM)

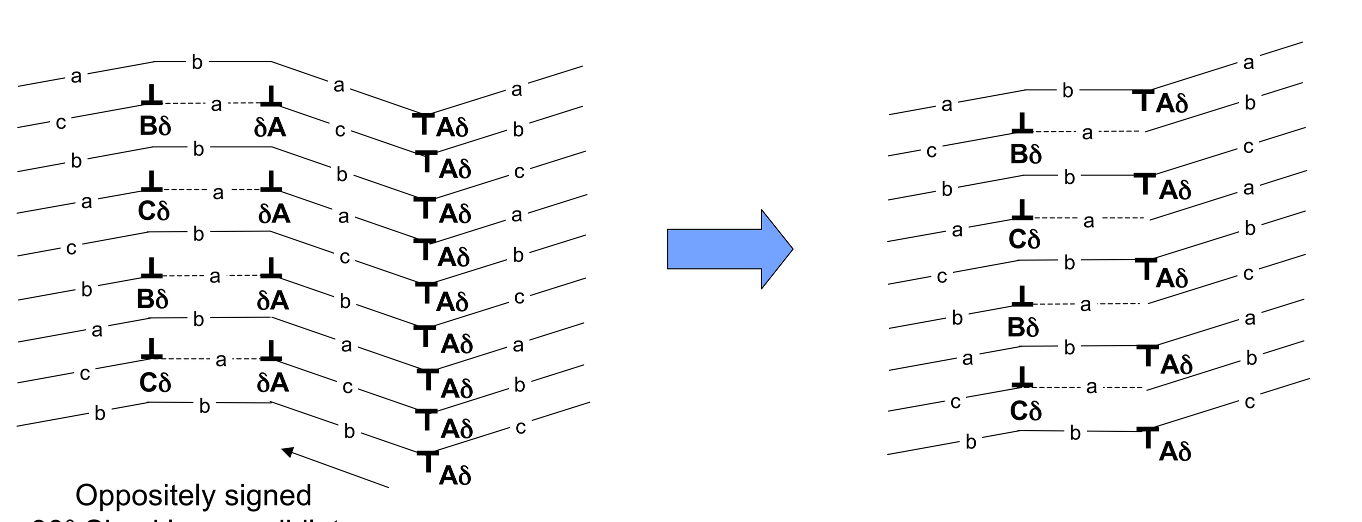


The HRTEM image shows a dissociated <110> tilt boundary in gold. The boundary is composed of dissociated lattice dislocations that are spaced on alternate {111} planes. The formation of stacking faults every two planes produces a local region of hexagonal-close-packed material. The boundary is vicinal to $(1,-3,1)_{left}$ and $(1,-1,1)_{right}$ and has a measured misorientation of 28.8°. We simulated this interface using an Embedded Atom Method potential. We chose a misorientation and periodic boundary conditions along the interface plane to be consistent with a Burgers vector density of one 60° 1/2<110> dislocation per 2 {111} planes intersected by the boundary. In addition to reproducing the broad, dissociated core region of HCP stacked material, the simulation also predicts a translation along the tilt axis of 1/8[-1,0,1]. This translation arises due to the alternating screw components of the array of 30° Shockley partial dislocations at the left side of the interface.

D.L. Medlin and J.C. Hamilton, Submitted to J. Mat. Sci. (2008)

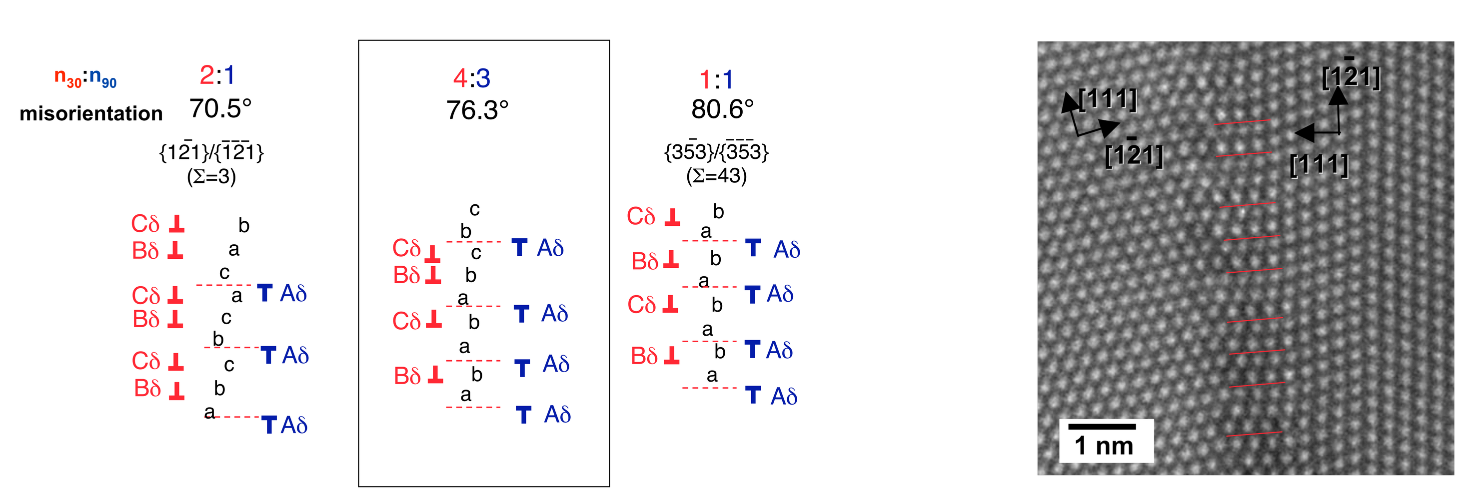
Relationship to Higher Angle Dissociated Boundaries

Because hexagonal close packing is the highest possible density of stacking faults in an FCC structure, the 29.7° boundary likely represents an upper misorientation limit for which such grain boundary structures can be meaningfully described in terms of the dissociation of individual 1/2<110> crystal lattice dislocations. However, dense arrays of stacking faults are also found at many boundaries at yet higher misorientation angles, and so it is important to consider how the present boundary is related to these other boundaries. Of specific relevance is the 80.63° <110> (Σ=43) symmetric tilt boundary, since this boundary also dissociates to form an interlayer of HCP material [1-3].



Previously, we have shown how the stacking fault patterns at a range of high angle<110> tilt boundaries can be understood by modeling the boundaries as a dense array of Shockley partial dislocations, distributed on adjacent close-packed planes[2]. The Σ=43 80.63° boundary is a special case in this description for which the ratio of 90° to 30° Shockley partial dislocations is 1:1[3]. The 29.7° boundary can be converted to the 80.63° boundary by reacting it with a wall of oppositely signed 90° Shockley partials dislocations (**Aδ**) and allowing the wall to reorient its inclination to eliminate coherency strains[4].

Local HCP stacking at 75° Boundary



Orientation given by:

$$\mathbf{v}_B=\mathbf{R}(\mathbf{v}_A-\Delta\mathbf{b}_A)$$

Net Burgers vector of partial dislocation array

Rotation due to twinning

[1] J.D. Rittner and D.N. Seidman, Physical Review B 54: 6999 (1996).
[2] D.L. Medlin DL, S.M. Foiles SM, and D. Cohen D Acta Materialia 49: 3689 (2001).
[3] G. Lucadamo and D.L. Medlin DL Science 300: 1272 (2003).
[4] D.L. Medlin, J.C. Hamilton, Submitted to J. Mat. Sci. (2008).

Steps at the {111}/{131} interface

Because the dissociated boundary is vicinal to {111}/{131}, it is instructive to analyze the steps in the boundary relative to a reference frame in which these planes are aligned. For this analysis, we adopt a *coherent* reference frame following an approach we have used previously for boundaries vicinal to {111}/{121} [1,2]. In this frame, {131} and {111} are rotated into alignment (θ=27.5°) and periodic lengths parallel to the interface in the upper (λ) and lower (μ) crystals ($1/2[323]_\lambda$ and $[121]_\mu$) are strained into coherency. By constructing circuits around defects at the interface and mapping these circuits into the reference frame, we characterize the topological properties of the defects and establish how they control the interfacial strain accommodation and inclination.

$$\mathbf{b}=-(C_\lambda+\mathbf{P}_{coh}C_\mu)$$

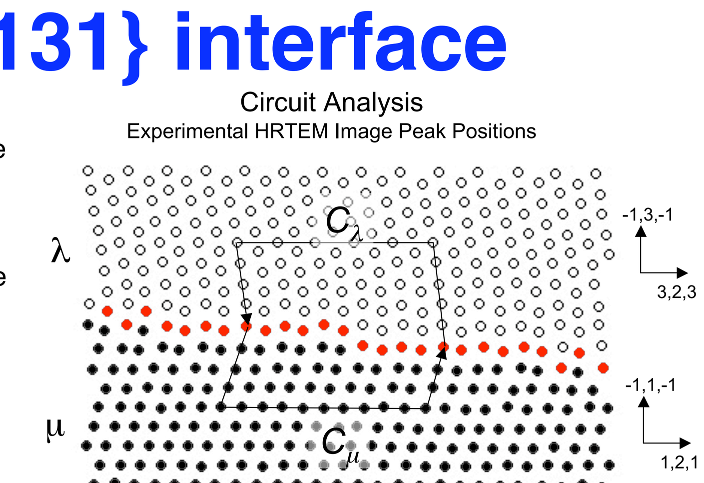
upper crystal circuit; lower crystal circuit

$$\mathbf{P}_{coh}=\mathbf{P}_{rel}\mathbf{U}\mathbf{A}\mathbf{U}^{-1}$$

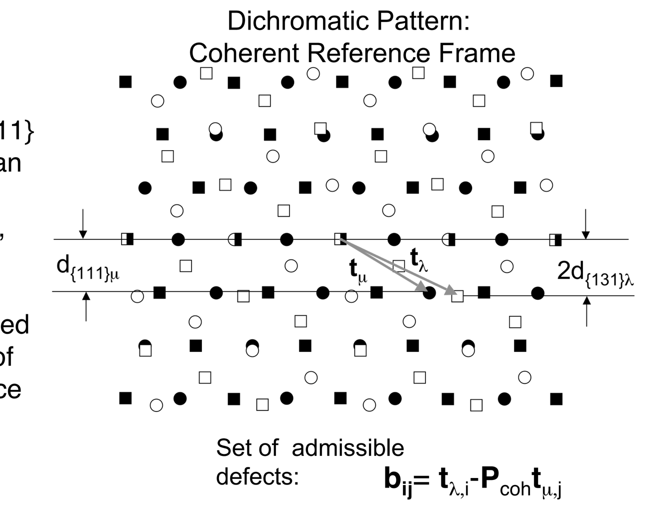
Relates coordinate frames of the two crystals in reference orientation; Describes strain to bring crystals into coherency

Circuit Analysis

Experimental HRTEM Image Peak Positions



Dichromatic Pattern:
Coherent Reference Frame



Set of admissible defects: $\mathbf{b}_{ij}=\mathbf{t}_{\lambda,i}-\mathbf{P}_{coh}\mathbf{t}_{\mu,j}$

The defect analyzed here joins two {131} planes in the upper crystal to one {111} plane in the lower crystal. In the plane of the interface, the defect possesses an edge component, $b_{||}$=0.302a, and a screw component, b_{screw}=±0.3535a. Additionally, the defect possesses an edge component normal to the interface, b_{norm}=-0.0256a, due to the mismatch in step-heights. When these steps are placed at the spacing required to fully accommodate the coherency strain, the resulting boundary inclination and misorientation is consistent with that predicted by the Frank-Bilby equation. This analysis, then, gives a microscopic picture of the relationship between the macroscopic geometric parameters of the interface and the specific atomic-scale defects that form at the interface.

[1] D.L. Medlin, D. Cohen, and R.C. Pond, *Phil. Mag. Letts* **83** (4) 223-232 (2003).
[2] R.C. Pond, D.L. Medlin, A. Serra, *Phil. Mag.* **86**(29-30) 4667 (2006).

Summary

The analysis here helps to link our understanding of low- and high-angle grain boundary structure. In this particular case, we have shown how the dissociation of a dense array of perfect crystal lattice dislocations into partial dislocations produces an interfacial layer of hexagonal close packed material and how this dislocation array is related the partial dislocations that produce HCP at the high angle Σ=43 boundary. The success in connecting these two boundaries of quite different misorientation suggests that similar analyses in terms of individual partial dislocations may have general utility in unifying our understanding of FCC boundary structure as a function of misorientation.

This work is supported at Sandia National Laboratories by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences, under contract DE-AC04-94AL85000.

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