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Collective Atomic Motion at a 90° <110> Tilt Grain Boundary in Gold

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Grain boundaries in crystalline materials affect many macroscopic properties such as strength, electrical resistivity, and corrosion resistance. Processing techniques to enhance these properties are therefore often aimed at modifying the existing grain boundary content via processes such as recrystallization and grain growth. While much is known about the structural character of grain boundaries and the variables that affect their mobility, the atomic-scale mechanisms of migration are still poorly understood. Recent experimental work suggests that step nucleation and cooperative, string-like motion of many atoms near a boundary may contribute to its advancement [1,2]. Molecular dynamics simulations indicate that these atomic cascade events can be triggered by volume fluctuations at the grain boundary and may occur in the absence of an external driving force [3].

In this contribution, we investigate step propagation and collective atomic motion at an incommensurate 90° <110> tilt grain boundary in gold. The samples used in this study were prepared by physical vapor deposition of high purity Au onto <100> Ge substrates. This results in a {110} mazed bicrystal thin film where all grains are rotated 90° about a common <110> axis. Characteristic segments of these boundaries were imaged using the aberration-corrected TEAM microscopes at the National Center for Electron Microscopy in both HAADF-STEM and HRTEM modes at 300kV. Imaging parameters such as beam current and dwell time were systematically varied to optimize the detection of transient events, as well as to investigate the effect of the electron beam on event frequency. Large time series were acquired to allow for cumulative averaging of frames between events and enable precise atomic displacement measurements for comparison to simulations [4]. Custom MATLAB routines were employed to track and analyze structural fluctuations near the interface.

Figure 1(a) shows an intensity-averaged image of an incommensurate {110}/{001} boundary segment that contains two steps in the boundary plane. The five-fold structural units that are characteristic of this boundary are outlined in yellow. Over the course of imaging, many structural fluctuations are observed at ambient temperature under the influence of the electron beam. Figure 1(b) shows a red/green/blue (RGB) overlay of frames before, during, and after one such event. The white atoms indicate sites that have not moved over the course of the experiment, while red and blue illustrate the trajectory of atoms during the cooperative motion. This clearly shows a string-like motion of atoms in the lower grain that serves to advance the boundary upward. This structural fluctuation persisted for several seconds and changed the local structure of the boundary segment as shown in Figure 2. The boundary steps have been defined in terms of the number of planes involved on each side of the step, n:m, where n is the number of {001} planes and m {110} planes. This structural analysis suggests that the observed collective motion of atoms consolidates a 1:1 and a 2:3 step into a single 3:4 step.

The implications of the observed structural transitions for grain boundary migration will be presented. Molecular dynamics simulations are used to further clarify the experimental observations and to explore the z-component of the transition. The defect character of the atomic shuffles as well as consideration of intrinsic factors, such as stacking fault energy, are utilized in the description of this migration mechanism.

References

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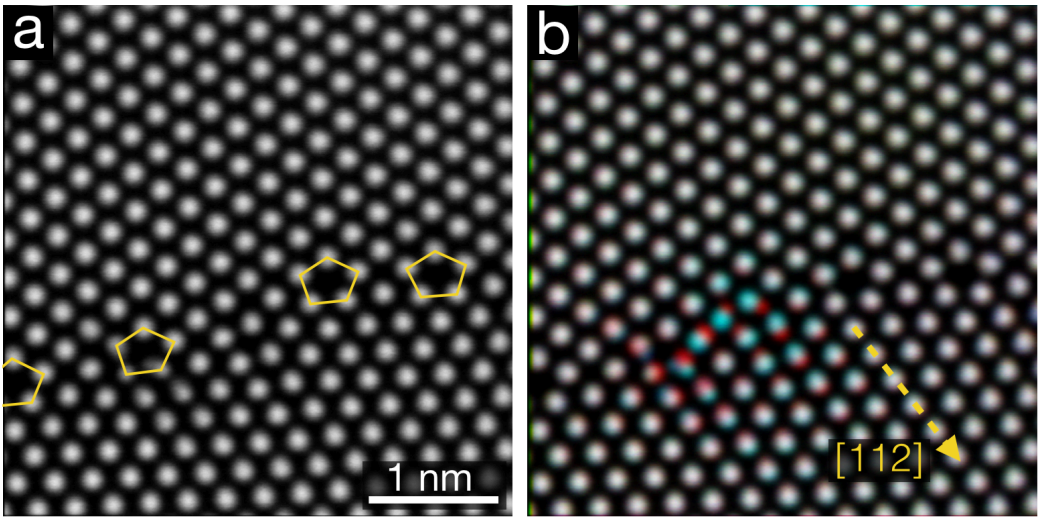

Figure 1: (a) Intensity average of 40 HAADF-STEM fast scan (0.5μs dwell time) images showing an incommensurate boundary segment containing two steps. Five-fold structural units are outlined in yellow. (b) RGB overlay of averaged intensities before, during, and after a structural event to highlight the atomic displacements.

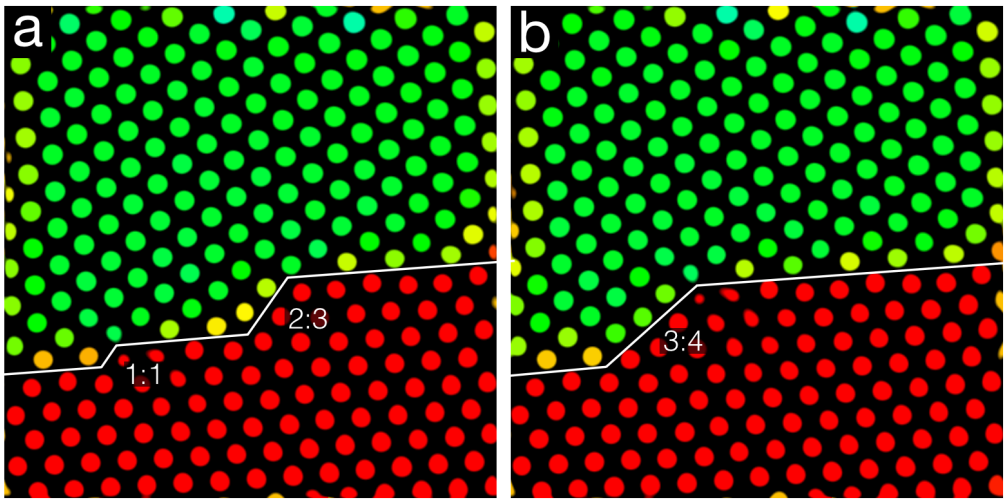

Figure 2: Grain boundary structure before (a) and after (b) collective rearrangement, colored by local coordination. Green and red correspond to the unique grain orientations, while yellow and orange show local distortions near the boundary. The boundary is highlighted for clarity.