Z-Contrast Imaging and Grain Boundaries in Semiconductors

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Interest in grain boundaries in semiconductors is linked to the application of polycrystalline semiconductors as photovoltaic and interconnect materials. In real devices such as solar cells and MOS structures as well as future devices such as flat-panel displays, the intergranular regions of the polycrystalline solid have a significant effect on the flow of electronic current. These grain boundary barriers exist because the chemical potential of the boundary atoms are shifted from the bulk value by the change in local symmetry. The chemical potential is also changed by impurities, other structural defects, and other phases in the boundary. The lack of knowledge on the atomic structure of grain boundaries is, at present, the greatest barrier to advancements in the understanding of the electrical properties of these defects.

The advances of the last few years have provided the tools with which to probe these interfaces at the true atomic scale. One such tool is the high-resolution scanning transmission electron microscope installed at Oak Ridge National Laboratory (VG Microscopes HB603) that can form a 1.27Å electron probe. Images are formed by scanning the probe across a thin sample and using an annular detector to collect electrons scattered to high angles. Because the annular detector collects electrons scattered over a wide range of angles, phase correlation and dynamical diffraction effects are averaged by this annular integration. Thus, an image with incoherent characteristics is produced and retained to relatively large specimen thickness. The key advantage of incoherent imaging is that when the microscope is focused to produce maximum image contrast, the bright image features directly correspond to the positions of the atomic columns. As long as the probe is smaller than the projected atomic column spacing and the inner detector angle is larger than the beam convergence, the observed atomic columns can be treated as independent incoherent scatterers. This column-by-column imaging is crucial when investigating interfaces and other unknown structures. Additionally, as the inner detector angle is increased beyond this minimum setting for incoherent imaging, the contribution of nuclear scattering increases, leading to increased compositional sensitivity of the images.

Atomic resolution of the grain boundary cores in silicon represents a severe test and remarkable demonstration of the technique. Figure 1 is a Z-contrast image of a section of a 39° <110> symmetric tilt boundary in silicon (Σ=9 {221}<110>) as viewed along the [110] direction. The boundary is seen to consist of a periodic array of perfect edge dislocation with their line direction parallel to the <110> tilt axis. While this grain boundary core structure had been previously identified to be the stable atomic configuration by both experiment and theory, the unprecedented resolution of the image clearly reveals the 5- and 7-atom rings of the distinct boundary dislocations.

The capabilities and advantages of the technique are more fully displayed in images from a 23° <001> symmetric tilt boundary in silicon (Σ=13 {310}<001>). As revealed in Figure 2, this boundary contains a more complex arrangement of boundary dislocations. Six distinct dislocation cores are present in each 13.84Å periodic repeat of the boundary. This structure had not been proposed previously as the preferred atomic configuration for this tilt boundary. The directly interpretable incoherent image removes the need for preconceived model structures.

The compositional sensitivity of the technique should allow the nature and distribution of impurities segregated to these structures to be obtained column-by-column. It is believed that the
combination of the detailed atomic structure data from the microscope along with theoretical modeling will improve our understanding of the physical processes that occur at grain boundaries.5

References

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4. M. F. Chisholm et al., Phil Mag. in press.
5. This research was sponsored by the Division of Materials Science, U.S. Department of Energy under contract number DE-AC05-96OR22464 with Lockheed Martin Energy Research Corp.

Fig. 1 [110] Z-contrast image of a 39° <110> symmetric tilt boundary in silicon.
Fig. 2 [001] Z-contrast image of a 23° <001> symmetric tilt boundary in silicon.