Characterization of Grain Boundary Geometry in the TEM, exemplified in Si thin films

János Lábár[1], Ákos Koppány Kiss[1], Zsolt Fogarassy[1], Silke Christiansen[2], Fritz Falk[2]

[1] Research Institute for Technical Physics and Materials Science, Hungarian Academy of Sciences H-1121 Budapest, Konkoly-Thege ut 29-33 Hungary

[2] Institute for Photonic Technologies, Jena, Germany

2012

Keywords: Si, Grain boundary, TEM, GB-plane, method

Abstract.

It has been long observed that phenomena associated with grain boundaries (GB) in metals (e.g. corrosion, energy, segregation, etc) are influenced by the grain boundary geometry. For many years the coincidence site lattice (CSL) model, which describes the grain boundary in terms of the misorientation between neighbouring grains, has been a cornerstone of grain boundary research and formation of special boundaries with low-Σ (assumed to result in better material properties) was pursued. Further work subsequently indicated that a low-Σ CSL was a necessary but not sufficient criterion for specialness, but the interpretation of similar results is complicated by the effect of impurities on boundary energies. The structure of the GB is more related to the orientation of the GB plane (planar density of coincidence sites), which is difficult to determine experimentally. Bicrystals with known misorientation and BG plane indices were artificially fabricated and studied both by HRTEM and other characterization methods from the 80's. Structural characterization (including indexing the GB plane) in real-life polycrystalline materials proved to be more challenging. One approach involves following the change in the location of GB traces in a scanning electron microscope (SEM) while thin layers of material are removed mechanically (either by polishing or by focused ion beam, FIB). The other approach reported here, records the projections of the GB at two different tilt values in a transmission electron microscope (TEM) and deduces the orientation of the GB plane from them.

The method relies on calibrating rotation of the image as compared to the diffraction and determining orientations of both neighbouring grains from the Kikuchi-bands (or Kikuchi-lines) seen in convergent beam electron diffraction (CBED) patterns, recorded with low camera length (to include the maximum available angular range in the TEM). The direction of the trace is determined from is direction as related to the diffraction axes and the elevation (tilt) of the GB plane from the beam-direction is determined from the width of its trace as compared to local sample thickness (determined from 2-beam CBED). The resulting plane normal, together with the misorientaion (determined from CBED Kikuchi-bands) gives a complete geometrical characterization of the GB.

GB-plane distribution in a thin film is not necessarily identical to the distribution of similar planes in bulk materials. It was observed in low dimensional fcc metals (wires or thin films) that energy minimization of GBs can follow two (mainly alternative) routes. Either low energy planes (like {111}) are formed in Σ3 boundaries, or alternatively, it is observed in Σ3 boundaries that the GB plane has a general index (and high energy) but it ends at both free surfaces of the sample, resulting in a GB, almost normal to the sample surface, minimizing the total area of the GB. We observed similar distribution in thin Si films, crystallized from melt on glass substrates (separated by a thin SiN barrier layer). This observation is important for the expected recombination properties of the multicrystalline Si (m-Si) in planned solar cell (SC) applications.