Grain Boundary Diffusion in Synthetic YAG-bicrystal

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Despite the fact that only a small volume fraction of a rock is represented by grain and phase boundaries, they strongly influence physical and chemical properties, such as elasticity, strength, electrical conductivity, and the efficiency of diffusive mass transport. Grain boundary diffusion is estimated to be three to five orders of magnitude higher than volume diffusion (Gleiter et al., 1972). A major practical problem in investigating the grain boundary structure and grain boundary diffusion of natural materials is the difficulty in controlling their purity and stoichiometry. Therefore, we used synthetic aluminium-garnet crystals.

The wafer direct bonding method (Heinemann et al., 2005) was used to obtain Yttrium-Aluminium-Garnet (YAG) bicrystals. Highly polished and ultra clean crystal surfaces are saturated with pure adsorbed water and are brought into contact. Hydrogen bonds of the opposing crystal surfaces are expected to form. The adsorbed water evaporates at elevated annealing temperatures and leaves a synthetic grain boundary behind. Analytical and High-Resolution Transmission Electron Microscopy (HREM) combined with Focussed Ion Beam (FIB) sample preparation were used to investigate the grain boundary structure and its width. Non-crystalline material is not observed in the straight grain boundaries of the bicrystals.

Diffusion experiments are carried out in thin-film geometry, such that the grain boundary is perpendicular to the surface covered with the thin-film. Pulsed Laser Deposition (PLD) (Dohmen et al., 2002) was used to deposit Nd doped YAG on the bicrystal. The initially amorphous thin-films crystallized during annealing and copied the structure of the bicrystal. Therefore, the grain boundary continues within the epitaxially grown thin-film.

After diffusion annealing of the bicrystals, diffusion profiles were measured with analytical TEM and/or Rutherford Backscattering (RBS). Volume diffusion profiles are compared to those measured by Cherniak (1998). Even though we choose the same T-t-parameters and analytical techniques, considerable differences in diffusion length are observed. Differences in defect structures, water activities, or the contact between substrate and source are possible explanations. More experiments at different temperatures, diffusion times, and thin-film compositions are planned.

References

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