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Bicrystals to study grain boundary diffusion: special vs. random grain boundaries

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Grain boundary (GB) diffusion affects many processes such as grain growth, recrystallization, grain boundary migration and related discontinuous reactions. GB diffusion is a fundamental process for understanding transport properties of polycrystalline materials. One of the parameters that control GB diffusion is the structure of the grain boundary itself, which is difficult to control during experiments. Previous experimental studies on grain boundary diffusion mainly addressed polycrystalline materials and consequently, only the bulk properties of the GBs are extracted. Other diffusion studies were carried out on special grain boundaries, for example twins of natural minerals, and the structure of the grain boundaries was only rarely characterized, let alone investigated at atomic resolution before and after the experiment.

Here, a new approach to quantify GB diffusion along structurally and chemically defined single grain boundaries is presented. The study profited from new experimental and analytical developments, and volume and grain boundary diffusion data from one explicitly defined experiment were extracted. The main benefits are: (i) simple experimental geometry by using bicrystals produced by wafer direct bonding to control the grain boundary parameters. The diffusant source is deposited by Pulsed Laser Deposition perpendicular to the straight grain boundary. (ii) Applying high-resolution analyses: focused ion beam (FIB) sample preparation is used to produce site specific and oriented lamellae for transmission electron microscopy (TEM). ATEM and HRTEM allow for the extraction of chemical and structural information at very high spatial resolution. Volume and grain boundary diffusion parameters can be determined on the same sample. (iii) data extraction: numerical simulations account for all specific experimental observations and the volume and GB diffusion coefficients are quantitatively extracted.

The feasibility of this approach is presented using the example of an yttrium aluminium garnet (YAG) bicrystal with an Yb-doped YAG-thin-film as diffusant source. Inter-diffusion of ytterbium with yttrium is investigated. The grain boundary diffusion coefficient of Yb, was determined to equal 3x10ˆ-15 m^2/s at 1723 K and was found to be 4.85 orders of magnitude faster than volume diffusion. This difference is discussed with respect to the investigated grain boundary structure. Finally, the nature of the grain boundary width for diffusional element transport and its determination are critically discussed with respect to the structural grain boundary width.