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Diffusion in yttrium aluminium garnet at the nanometer-scale: Insight into the effective grain boundary width

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ABSTRACT

Atomic diffusion along grain boundaries in solids is a key process in many geological environments and in ceramics research. It is closely related to the grain boundary width, which is an important parameter in numerous equations describing diffusional or rheological processes, including plastic deformation of polycrystals, intergranular failure, and recrystallization. Here, we studied diffusion along a single well-characterized, near Σ5 grain boundary in yttrium aluminum garnet (YAG) using different transmission electron microscopy methods at atomic resolution. For the diffusion experiment, YAG thin-films containing Yb as diffusant were deposited perpendicular to the grain boundary on the bicrystal. We investigated the grain boundary using a focal series in combination with multislice calculations that yield the electron exit wave. This, coupled with chemically sensitive *Z*-contrast images, as well as the Yb distribution over the grain boundary measured using electron energy loss spectroscopy, show the zone of enhanced Yb diffusion parallel to the grain boundary. This zone of enhanced diffusion is often considered as the effective grain boundary width.

Profiles from the boundary into the crystal volume suggest a highly permeable zone of about 18 nm, which we assume to be the effective grain boundary width for diffusional processes. The effective width strongly differs from the structural grain boundary width of about 2 nm in the present study. Furthermore, it is much shorter compared to the calculated volume diffusion profile. We conclude that the combination of small samples and transmission electron microscopy at atomic resolution are excellent tools to study varying processes, such as diffusion, deformation, or reactions at the atomic scale.

Keywords: Grain boundary, diffusion, width, grain boundary width, deformation, rheology, recrystallization