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Constraining Grain Boundary Diffusion within the Earth's Lower Mantle

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Diffusion creep is widely acknowledged as a fundamental process defining lower mantle viscosity. It is comprised of both lattice and grain boundary diffusive events. And, while significant progress has been made in constraining the self-diffusion rates through crystalline structures, far less is known about the nature of grain boundary diffusion at lower mantle conditions. Representing the largest interconnected defect structure, grain boundaries are of intrinsic mechanical significance, allowing for both fast diffusion pathways and impurity accumulation.

Before the kinetics of a diffusion event can be calculated, the most stable atomic arrangements of an interface at a given P-T condition must first be established. Here a fully ab-initio random structure search has been applied to construct a library of low energy interfacial structures, enabling variation in both the atomistic configuration and local chemistry alike. The construction of such a library provides a means of understanding trends in interfacial energies and volumes as a function of pressure and chemistry.

Grain boundaries, much like crystalline lattices, are thought to facilitate self-diffusion via the propagation of vacancies. The self-diffusion coefficients of a given low interface is calculated by applying harmonic transition state theory to the vast range of migration pathways for each of the six tilt grain boundaries that comprise this study, ((011)/[100], (012)/[100], (013)/[100], (014)/[100], (021)/[100], (032)/[100]). Harmonic transition state theory requires knowledge of both the ion-specific vacancy concentration and the energy barrier of a migration event. A value for the interfacial vacancy concentration is calculated by considering the formation enthalpy of Mg, Si and O within the grain boundary region. Whilst, the climbing image nudged elastic band method is used to minimise the energy barrier for a given diffusion pathway.

By following this approach and referring to known lattice diffusivities, an expression for a grain size dependance viscosity between pressures 20-140GPa and grain-sizes between 10-1000 microns has been estimated.