

First-principles study of the mechanical behavior of (Mg,Fe)O tilt grain boundaries in planetary mantles

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Ferropericlase is the second most abundant phase of the Earth's lower mantle and other terrestrial planets. Ferropericlase is polycrystalline, making grain boundary properties critical to describe its mechanical behavior, important to understand dynamic processes as grain growth, plastic deformation and seismic attenuation. Since ferropericlase is relatively ductile compared to lower mantle silicates (Girard *et al.* 2016), its rheological behavior is thus expected to play a key role in the dynamics of the Earth and planetary interiors. Despite previous theoretical work (e.g. Verma & Karki 2010; Hirel *et al.* 2019), little is known about the spin state of iron and the mechanical behavior of grain boundaries in ferropericlase as a function of pressure.

In this study, we carried out atomistic simulations based on the density functional theory combined with the Hubbard type correction to the on-site Coulomb interaction between the Fe *d* orbitals to model the structures, energies and spin state of iron in a series of [001] high-angle tilt grain boundaries as a function of pressure. Segregation energies of iron are quantified showing the ability of iron to host at specific grain boundary sites which affects the local spin transition of iron in the grain boundary with respect to bulk ferropericlase.

Based on those results, we investigated the ideal shear strength of the Σ 5 tilt grain boundary by applying simple shear strain increments to the simulation cell in order to induce a gradual increase in the shear stress to the atoms directly above and below the interface until a critical value is reached that it required to migrate the grain boundary through the crystal lattice. Our results show that the grain boundary strength strongly varies both non-monotonously and monotonously with increasing pressure resulting in grain boundary hardening and weakening, respectively across a broad pressure range. The latter is expected to influence the mechanical behavior of polycrystalline ferropericlase across a broad depth range in planetary mantles.

Keywords: Ferropericlase, Grain boundaries, Mechanical behavior