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Ab initio investigation of the intercrystalline mechanical behavior of ferropericlase at extreme pressures of planetary mantles

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Ferropericlase is the second most abundant phase of Earth's lower mantle and is also considered to be one of the main constituents of the mantles of super-Earth exoplanets. Since ferropericlase is more ductile compared to silicates (Girard *et al*. 2016), it is expected to control the rheological behavior of mantle aggregates which governs solid-state convection of planetary mantles. The mechanical behavior of polycrystalline aggregates is strongly affected by the presence of grain boundaries. Despite previous work on MgO grain boundaries (*e.g*. Verma & Karki 2010; Hirel *et al*. 2019), little is yet known about the properties and mobility of ferropericlase grain boundaries at pressure conditions of deep planetary interiors.

In this study, we carried out atomistic simulations based on the density functional theory to model the structures, energies and spin states of iron of a series of [001] symmetrical tilt grain boundaries in ferropericlase as a function of pressure. Based on these results, we investigated the mechanical behavior of the Σ5 tilt grain boundary by applying simple shear increments to the simulation cell to trigger grain boundary migration. Here, we will present the different mechanisms of grain boundary migration and the evolution of the ideal shear strengths up to a pressure of 400 GPa. Our results show that the mechanical strength of the grain boundaries and the directionality of their motion strongly varies with increasing pressure. Especially at pressure conditions of super-Earth exoplanets, significant grain boundary weakening is observed with increasing depth. Implications for the deformation of ferropericlase at conditions of Earth's and super-Earth's mantles will be finally discussed.