Spin transition in (Mg,Fe)O tilt grain boundaries across the Earth's lower mantle

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Iron-bearing MgO periclase is the second most abundant phase of the Earth's lower mantle and is relatively ductile compared to the lower mantle silicates (Girard *et al.* 2016). Its rheological behavior is thus expected to play an important role in the dynamics of the Earth. Ferrous iron in ferropericlase undergoes an electronic spin transition across the pressure range of the lower mantle (*e.g.* Tsuchiya *et al.* 2006). Previous studies reported that changes in iron spin state induce an anomalous compressibility of ferropericlase across the spin transition, which is thought to affect its mechanical strength (*e.g* Wentzcovitch *et al.* 2009; Wenk *et al.* 2009). Lower mantle ferropericlase however is polycrystalline, making the properties of grain boundaries critical to describe its mechanical behavior, important to understand plastic deformation and seismic attenuation. Yet, little is known about the effect of the pressure-induced iron spin transition on the properties of grain boundaries in ferropericlase.

Prior to understanding the kinematics of iron-bearing grain boundaries in ferropericlase, their structural properties must be established at lower mantle conditions. Here, we apply a density functional based first-principles approach combined with the Hubbard type correction to the onsite Coulomb interaction between the iron 3*d*-orbitals to describe the correct electronic structures of ferropericlase. This method has been used to determine the pressure-induced spin transition of ferrous iron in the Σ5 {310}/[001] tilt grain boundaries, enabling variation in the iron grain boundary site configurations and local chemistry alike as a function of pressure.

We quantify the iron segregation energetics into the Σ5 tilt grain boundary and demonstrate their ability to host iron at specific boundary sites, affecting the grain boundary formation energies and volumes. We show that the resulting spin transition pressure is significantly higher than that of monocrystalline ferropericlase, suggesting a non-homogenous iron spin transition in polycrystalline ferropericlase throughout the pressure range of the lower mantle. The latter should be taken into account regarding the mechanical behavior of polycrystalline ferropericlase across the lower mantle.

Keywords: Spin transition, Grain boundaries, Ferropericlase

