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How high-pressure phase transitions can alter mantle rheology: on self-diffusion in B2-type MgO

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The mantle of the Earth as well as those of terrestrial exoplanets (super-Earths) is expected to be composed of a mixture of high-pressure silicates and the oxide ferropericlase, which is considered to be the weakest phase. Thus, knowlegde of the rheological properties of periclase is of major importance for understanding the dynamics and evolution of terrestrial planets. Although B1-type (Fm-$3m$) MgO is stable over the pressure range of the Earth's mantle, it changes into the B2 phase (Pm-$3m$) if pressure exceeds $\sim$500 GPa in the interior of super-Earths. So far no creep mechanisms in B2-type MgO has been studied. Generally, MgO becomes denser with increasing pressure and is likely to undergo a viscosity increase. On the contrary, based on results from analogue materials, Karato (2011) suggested that the B1-B2 transition of MgO may rather affect mantle rheology by a viscosity decrease with increasing depth in super-Earths.

Relying on first-principles calculations, we investigate the above paradox by studying the behavior of vacancy diffusion in B2-type MgO. We show that non-interacting vacancy pairs are the most important Schottky defects in the B2 phase in the intrinsic and extrinsic regimes which may govern ionic diffusion. Most important however is the reduction we found in defect energetics across the B1-B2 transition. We demonstrate that a reduction in the enthalpy of ionic vacancy migration alone accounts for an increase in the effective diffusion coefficient of $\sim 10^4$ across the B1-B2 transition of MgO with increasing pressure. Careful examination of atomic relaxations indicates that diffusion controlled viscosity may generally decrease across high-pressure phase transitions with increasing coordination number. Our study suggests that mantle convection in the deep interior of super-Earths may be less sluggish than previously thought.