The 508th Geodynamics Seminar

First-principles study of iron diffusion properties with implications to inner core plasticity

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The mechanical properties of the Earth's inner core are key for understanding the evolution and dynamics of the core. However, little is known about the mechanical properties of iron (alloys) at conditions of the inner core. Therefore, long-standing questions remain open about the viscous strength of the inner core (Yoshida et al., 1996; Karato, 1999), about the origin of its seismic anisotropy (Deuss, 2014) and about its rotational dynamics (Buffett, 1997). Some, if not all, of these issues rely on plastic deformation of the inner core, which is barely constrained.

Under the extreme conditions of the Earth's deep interior, plasticity is expected to be rate limited by atomic diffusion. Experimental work on diffusion properties of iron-nickel alloys rely on extrapolation to inner core pressures (Yunker and Van Orman, 2007; Reaman et al., 2012). We use a density functional approach to study vacancy diffusion in iron at the appropriate inner core pressures. We quantify the associated defect energetics in order to constrain the self-diffusion coefficient of the hcp phase.

Vacancy diffusion controls many deformation mechanisms including dislocation creep, an effective strain producing mechanism in metals. Based on the pioneering works of Weertman (Weertman, 1955) and Nabarro (Nabarro, 1967), we derived a creep model to quantify the rate limiting bounds of climb-controlled dislocation creep in hcp iron to provide the first theoretical estimates of the inner core viscosity. Our results suggest an inner core viscosity that is significantly lower than that of Earth's mantle.

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