Ab-initio study of Earth’s inner core diffusion properties and the effect of light elements

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Seismic observations provide evidence that the Earth’s inner core exhibits global anisotropy (Tanaka and Hamaguchi, 1997; Creager, 1999). This anisotropy is thought to result from the collective alignment of crystals and suggests that the inner core may be subject to plastic deformation. The plastic properties of the inner core are therefore believed to be of paramount importance for understanding inner core dynamics and core evolution.

The inner core is expected to be composed of a solid iron-nickel alloy with some unknown light elements (Mao *et al*., 1998). Under high pressure conditions in the deep Earth, plastic deformation is likely to be influenced by local chemistry via extrinsic mechanisms (Ita and Cohen, 1998). Especially the interaction between light elements and point defects may thus contribute to inner core plasticity. Diffusion of these point defects, such as vacancies, may control many mechanisms of plastic deformation including dislocation creep via climb. Therefore, understanding the mechanisms of (anisotropic) atomic diffusion is important to gain insight into the creep processes in Earth’s inner core.

Using *ab-initio* calculations, we study vacancy diffusion in hcp, bcc and fcc iron at pressure conditions up to the Earth’s inner core. Our results demonstrate that pressure suppresses defect concentration but does not strongly affect defect mobilities. We found that some light elements, particularly hydrogen, influence metallic bonding and enhance atomic diffusion. This allows for extrinsic deformation mechanisms in iron at inner core conditions. This extrinsic mechanism is totally different from those expected in the silicates and oxides of the Earth’s mantle. We will discuss how light elements, and especially hydrogen, may influence the rheological properties of the inner core iron alloy.

Keywords: Earth's inner core, self-diffusion, extrinsic mechanisms