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Ab-initio investigation of diffusion properties of Earth's inner core and the role 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 be the result of the collective alignment of iron crystals. This provides evidence that the inner core may be subject to plastic deformation. The plastic properties of iron are therefore believed to be a key issue 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 of the deep Earth, it is likely that plastic deformation becomes more influenced by the local chemistry via extrinsic mechanisms (Ita and Cohen, 1998). Especially the interaction between point defects and light elements may thus be quintessential to inner core plasticity. Diffusion of these point defects, such as vacancies, may control many mechanisms of plastic deformation including dislocation creep via climb. A deep insight into the mechanisms of (anisotropic) atomic diffusion is therefore important to understand creep mechanisms which control the plasticity of 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 strongly suppresses defect concentration rather than to affect the mobility of the defects. We found that some light elements, and particularly hydrogen, influence metallic bonding and enhance atomic diffusion. The latter 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. Here we discuss how light elements may influence the rheological properties of the inner core iron alloy.