Atomic diffusion in solid iron at Earth’ s inner core conditions

*Sebastian Arthur Willem Ritterbex[1], Taku Tsuchiya[1]

1. Geodynamics Research Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama 790-8577 Ehime Japan

Crystalline iron is the main constituent of the Earth’ s inner core[1]. The thermomechanical properties of solid iron at high pressure and temperature therefore mainly control the dynamics and evolution of the inner core. One of those properties is atomic diffusion which plays a key role in many processes, such as plastic deformation (viscosity) and crystal growth. Ongoing debate about the seismologically observed elastic anisotropy of the Earth’ s inner core[2,3] has led to several suggestions whether to find its origin in non-uniform core growth[4], dendritic crystal growth[4,5] (core solidification) or in solid-state flow[4,6,7] (formation of LPO), all which depend on atomic diffusion processes. In addition, the diffusion anisotropy of iron at inner core conditions provides a link between seismic anisotropy and plastic deformation of the inner core. Therefore, a thorough understanding of atomic diffusion mechanisms in iron polymorphs is essential to gain better insight into the evolution of the Earth’ s inner core.
Since experiments are extremely difficult to perform at inner core pressure and temperature conditions, computational mineral physics provides an alternative to study atomic diffusion in iron under those conditions. In this work, the effect of pressure on vacancy diffusion is investigated by means of defect energetics as it largely determines the rate of vacancy diffusion. First principles simulations have been performed to calculate activation enthalpies for self-diffusion in FCC- and BCC- and HCP-Fe at a pressure range up to the conditions of the Earth’ s inner core. Our results show that pressure significantly increases defect energetics and in particular is responsible for suppressing defect concentration substantially in iron at inner core conditions. Consequently the rate of vacancy diffusion will be strongly inhibited. Intrinsic vacancy concentration plays an important role in metals in contrast to ionocovalent minerals where extrinsic vacancy concentration may determine effective vacancy diffusion. The question then arises whether other mechanisms allow to enhance vacancy concentration in iron under inner core conditions. If not, the latter will have direct consequences for the interpretation of the seismologically observed inner core anisotropy in terms of intracrystalline plasticity.

[1] Birch, F., Journal of Geophysical Research, 57(2), 227-286 (1952). [2] Tanaka, S., Hamaguchi, H., Journal of Geophysical Research, 102, 2925-2938 (1997). [3] Creager, K.C., Journal of Geophysical Research, 104, 23127-23139 (1999) . [4] Wookey, J., Helffrich, G., Nature, 454, 873-876 (2008). [5] Bergman, M., Nature 389, 60-63 (1997). [6] Karato, S.-I., Nature, 402, 871-873 (1999) . [7] Buffett, B.A., Wenk, H.-R., Nature, 413, 60-63 (2001) .

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