Phase Relations in the Fe-C-H Ternary System: Implications to Deep Carbon and Hydrogen Cycles

Xiaojing Lai[1,2], Feng Zhu[2], Eran Greenberg[3], Vitali B. Prakapenka[3], Bin Chen[2]

[1] Department of Earth Sciences, University of Hawai‘i at Mānoa, Honolulu, Hawai‘i, USA.

[2] Hawai‘i Institute of Geophysics and Planetology, University of Hawai‘i at Mānoa, Honolulu, Hawai‘i, USA.

[3] Advanced Photon Source, Argonne National Laboratory, Chicago, Illinois, USA.

Carbon (C) and hydrogen (H) are essential elements for life on our habitable planet. The deep carbon and hydrogen cycles are crucial for our understanding of the physiochemical processes and evolution of Earth’s deep interior and its interaction with the surface. Native iron (Fe) has been proposed to exist as minor component in the deep mantle below the depth of ~250 km, and as major element in the Earth’s core. Phase relations in the Fe-C-H system at high pressure and high temperature are thus important to understand the deep C and H cycles. Recent studies on the reactions between Fe and excess hydrocarbon showed that Fe carbide and molecular hydrogen formed first at high pressures and relatively low temperatures. With increasing temperature, Fe hydride and diamond were formed instead due to the inversed stability between Fe carbide and Fe hydride at the experimentally investigated pressure-temperature conditions (Hirose et al., 2019; Narygina et al., 2011; Thompson et al., 2018); In addition, a recent study demonstrating the failure of hydrogenation of Fe_3C also led to the conclusion that C and H cannot coexist in Fe (Litasov et al., 2016). However, this may only occur when the content of C and H are in excess compared with Fe. In the present study using laser-heated diamond anvil cell combined with in situ synchrotron-based X-ray diffraction, we investigated the reactions of Fe with excess C-H content and demonstrated the inversed stability between Fe carbide and Fe hydride at high pressures with increasing temperatures. We also successfully synthesized a *hcp*-type Fe-C-H alloy (Fe-1.2wt.%C-H_x, x=0.5-0.6) at high pressures when Fe was in excess. In this case, both C and H can coexist in the structure and accommodate the interstitial sites of *hcp*-type Fe. We found that the density of *hcp*-type Fe can be significantly reduced by adding C and H in its crystal structure at high pressures. The equation of state of this Fe-C-H alloy was obtained and

compared with Fe to understand the effect of hydrogen on the elastic properties of Fe alloys. The discovery of Fe-C-H alloy indicates that C and H can coexist in Fe and the Fe-C-H can serve as a potential reservoir for both C and H cycled into the mantle by subduction process and a potential iron alloy in the Earth's core.

References

Hirose, K., Tagawa, S., Kuwayama, Y., Sinmyo, R., Morard, G., Ohishi, Y., Genda, H., 2019. Hydrogen Limits Carbon in Liquid Iron. Geophysical Research Letters.

Litasov, K., Shatskiy, A., Ohtani, E., 2016. Interaction of Fe and Fe 3 C with hydrogen and nitrogen at 6–20 GPa: a study by in situ X-ray diffraction. Geochemistry International 54, 914-921.

Narygina, O., Dubrovinsky, L.S., McCammon, C.A., Kurnosov, A., Kantor, I.Y., Prakapenka, V.B., Dubrovinskaia, N.A., 2011. X-ray diffraction and Mössbauer spectroscopy study of fcc iron hydride FeH at high pressures and implications for the composition of the Earth's core. Earth and Planetary Science Letters 307, 409-414.

Thompson, E., Davis, A., Bi, W., Zhao, J., Alp, E., Zhang, D., Greenberg, E., Prakapenka, V., Campbell, A., 2018. High-Pressure Geophysical Properties of Fcc Phase FeHX. Geochemistry, Geophysics, Geosystems 19, 305-314.