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Melting temperature of FeHx at high pressures determined by in situ X-ray observation

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Density of the Earth's outer core is 10% less than that of the pure iron under relevant pressure and temperature conditions, probably due to the existence of some light elements. After the discovery of stability of FeHx at high pressures, hydrogen is considered to be one of the candidate light elements in the Earth's outer core. Thus, melting temperature of FeHx is important for understanding of temperature in the Earth's outer core.

Because hydrogen escapes from the iron metal, FeHx can not be recovered to the room pressure. Thus, it is very difficult to the investigate behavior of FeHx by observation of quenched run products. For this difficulty, accurate determination of melting curve and phase diagram of FeHx have been carried out up to10 GPa.(Yagi and Hishinuma; 1993, Okuchi and Takahashi; 1997) Furthermore, in most previous experiments, hydrogen was supplied through the iron-water reaction, so that sample iron may not be saturated with hydrogen, Thus, melting temperature could be lower than previous estimate under the hydrogen saturated conditions. In this study, we have determined the melting temperature of FeHx up to 15 GPa by in situ X-ray observation at SPring-8 synchrotron.

Starting material was a mixture of pure iron and MgO with equivalent atomic ratio to prevent grain growth of iron. Sample was heated by a tube heater made of TiC and diamond powder (1:1 in weight ratio) and temperature was measured by W5%Re-W26%Re thermo couple. We have determined experimental pressure using MgO and NaCl pressure markers(Jamieson et al.; 1982, Decker; 1971). Sample was packed in NaCl capsule with hydrogen source of $LiAlH_4$. Since $LiAlH_4$ decompose into LiAl and H_2 above 673K at room pressure, sample iron is considered to be saturated with pure hydrogen gas during heating. Pressure was generated by Kawai-type multi anvil apparatus, SPEED Mk-2, installed in SPring-8. In this study, we have determined the melting temperature by disappearance of the diffraction peaks of FeHx. In order to avoid the effect of grain growth on the diffraction peaks, the SPEED Mk2 was oscillated during X-ray diffraction measurements.

In this study, onset of the iron hydrogen reaction was detected by the occurrence of the phase transition from hcp phase to d-hcp phase or rapid expansion of lattice parameter. At 10GPa, we observed phase transition from hcp FeHx to d-hcp FeHx at 973K. This phase transition was consistent with the previous phase diagram (Y. Fukai and K. Mori; 2003). At 15GPa, an abrupt and large expansion of fcc iron was observed at 1073K. The reason why phase transition from hcp to d-hcp was not detected at 15 GPa is probably due to the absence of the reaction between iron and hydrogen at that temperature where hcp iron is stable. (fig.) Diffraction peaks of FeHx disappeared at 1473K and 1553K, at 10GPa and 15GPa, respectively. This is judged to be due to the melting of FeHx because broad X-ray halo is observed in the high temperature diffraction patterns. The observed melting temperature at 10GPa is consistent with previous estimate of melting temperature of FeHx by Okuchi and Takahashi (1997). The temperature increases monotonously with pressure to 15GPa. The low Clapeyron slope of the melting curve for FeHx may significantly lowers the possible temperature range for the Earth's outer core (4173 - 4673 K when the mantle specific heat is 3 - 4.5, Boehler; 1996), which were estimated by melting curves of Fe, FeS and FeO, if substantial amount of hydrogen is there.