

High pressure X-ray studies of iron-nickel alloy and iron-nickel hydride

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The Earth's core is composed of iron-nickel alloy with a small amount of light element(s). Hydrogen has long been suggested as the possible major light element. In last decade, physical and chemical properties of iron hydride were studied by X-ray and Neutron diffraction experiments, Mossbauer spectroscopy, and nuclear resonance X-ray inelastic scattering measurements, and theoretical calculations. There are much fewer studies on iron-nickel alloys and its hydrides, while pure iron and iron hydride has been studied by many authors.

The behavior of hydrogen in metals has long been great interest to scientists in physics and chemistry as well as geophysics. Most of transition d-band metals form metal hydride under high pressure. The hydrogen molecule is dissociated and incorporated in the octahedral and/or tetrahedral interstices of the host metals. The partial hydrogen volume (PHV) in metal-hydrogen systems can be estimated by the difference in unit cell volume between pure metal and its hydride. However, compression behavior of hydrogen atom in metal hydrides remains unclear. Here, we report in situ X-ray observation of iron-nickel alloy and iron-nickel hydride at high pressures up to 53 GPa.

Powder X-ray diffraction spectra were collected by the angle-dispersive method at BL04B2 beamline (~37.8 keV) of SPring-8 and BL18C (~20 keV) of Photon Factory, High Energy Accelerator Research Organization (KEK), Japan. High pressure was generated by a diamond-anvil cell. The sample of iron-nickel alloy, Fe-10.50 wt.% Ni, was used as a starting material. Helium was the pressure transmitting medium in the experiment of iron-nickel alloy, while, in the study of iron-nickel hydride, fluid hydrogen was loaded into a sample hole with iron-nickel alloy. Pressure was determined using the ruby fluorescence method. The samples and ruby chips were not bridged between diamonds to highest pressure in the present study.

X-ray diffraction patterns of iron-nickel hydride showed that the double hexagonal close packed (dhcp) phase was stable from 6 GPa up to at least 53 GPa and no further structural phase transformation of iron-nickel hydride was observed, similar to iron hydride. The diffraction peaks of iron-nickel hydride except for (004), (110), and (114) were not sharp in spite of the pressure medium of hydrogen. This is likely to be due to random stacking faults. On the other hand, we observed the transformation from the body-centered cubic (bcc) phase of iron-nickel alloy to the bcc + hcp phases at 15 GPa upon compression, and the phase transformation to the hcp phase was completed around 19 GPa, compared to the bcc to hcp phase transition of pure iron in experiments using a pressure medium of helium.

We found anomalous behavior of the axial ratio, $(c/a)/2$, for the dhcp phase of iron-nickel hydride. The axial ratio decreases monotonically to 1.630 with increasing pressure around 22 GPa, and then increases to 1.635 at 45 GPa. Whereas in iron-nickel alloy no significant dependence of axial ratio on pressure was observed and the axial ratio decreases smoothly to 53 GPa. The difference in the compression behavior of the axial ratio results from incorporating hydrogen into iron-nickel alloy, compared to that of pure iron and its hydride. A loss of magnetism on the dhcp iron hydride phase at 22 GPa was reported with synchrotron Mossbauer spectroscopy (W. Mao et al. 2005). Recently, the effect of magnetic spin transition on compression behavior was studied on magnesiowustite (Mg,Fe)O with X-ray diffraction measurements and Mossbauer and/or X-ray emission spectroscopy. Thus, compression behavior of iron-nickel hydride are likely to be associated with a change of the magnetic properties. In the presentation, we will discuss the compression behavior of hydrogen in iron-nickel alloy.