

Nuclear Resonant Inelastic X-ray Scattering of Iron Hydride at High Pressure

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Introduction

As major constituents of the Earth's core, iron and its alloys have long been of great interest to geophysicists. Information on their high-pressure dynamic behavior, such as phonon dispersion, is essential for interpreting seismic and geomagnetic observations and for numerical modeling of the Earth's deep interior. Seismic observations coupled with laboratory research indicate that the density of the outer core and perhaps the inner core is lower than that of pure iron, which has led to extensive research on possible lower-atomic-weight components in the Earth's core [1]. Hydrogen has been suggested as a possible candidate for one of the light elements. If it is, it would have profound implications on the hydrogen budget within the Earth and our understanding of the physics and chemistry of the core. X-ray diffraction experiments show that stoichiometric FeH is formed at 3 GPa from the reaction of iron and fluid hydrogen [2], and this compound is stable to at least 62 GPa [3]. Experiments conducted at a limited pressure and temperature (P-T) range also demonstrate that FeH can be formed by the reaction of iron and silicates [4] and that FeH has increased stability relative to iron, silicate, and water over increasing P-T conditions [5]. The partitioning of hydrogen into the molten iron core has important implications with regard to core-mantle interactions [6]. Because of the limitations of x-ray diffraction alone, however, important geophysical and crystal chemical information about FeH is still lacking. The phonon dynamics of FeH at high pressure certainly warrant in-depth investigation and could prove crucial for comparison with seismic observations.

Methods and Materials

Samples of isotope-enriched ⁵⁷Fe were loaded into a Be gasket in a diamond anvil cell with fluid hydrogen. Fe and H reacted to form FeH above 3 GPa. The remaining hydrogen acted as a pressure medium that provided hydrostatic conditions. We carried out a series nuclear resonant inelastic x-ray scattering (NRIXS) experiments on iron hydride at ambient temperature at XOR undulator beamline

3-ID at the APS. The high-resolution (1-meV) monochromator was scanned over a range of ± 80 meV in 0.25-meV steps about the ⁵⁷Fe Mossbauer line. NRIXS spectra at 4, 7, 10, 12, 22, 30, 42, 47, and 52 GPa were collected *in situ* and converted to phonon density of state (DOS) for final analysis. Nuclear resonant forward scattering (NRFS) was used to monitor magnetic transition. Pressure was calibrated by using the ruby scale at sector 13 at the APS [7]. The phase was confirmed by x-ray diffraction at beamline station 16-ID-B.

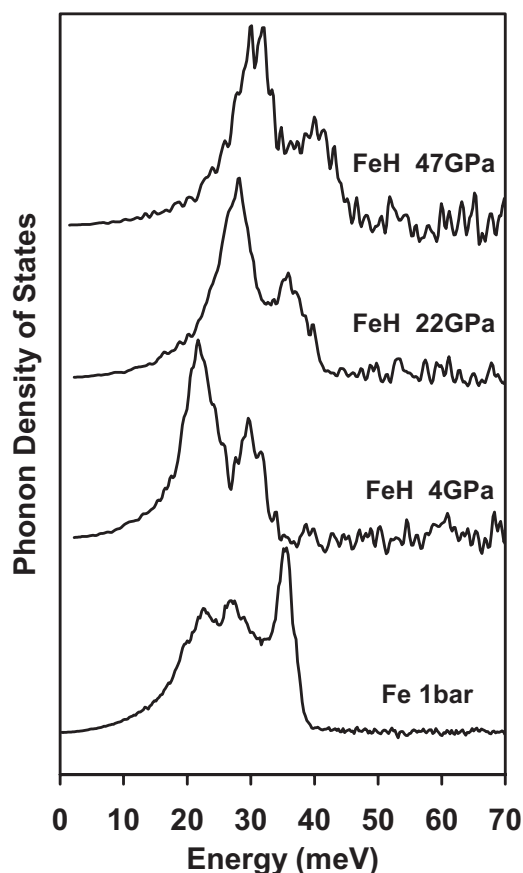


FIG. 1. NRIXS for three of the pressures showing the partial phonon DOSs for FeH at 4, 22, and 47 GPa. For comparison, the DOSs of pure Fe at ambient pressure are shown.

Results

FeH was in double hexagonal closed-packed (dhcp) structure over the range of pressure studied. Loss of magnetism was observed at 22.2 GPa. The partial (Fe-related) phonon DOSs for iron hydride were determined (Fig. 1). The spectra shape are quite different from those of pure Fe and FeO [8, 9]. The initial slope, coupled with hydrostatic equation of state data, yields V_p and V_s for comparison to seismic observations, thereby providing insight into core chemistry and physics.

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