American Mineralogist, Volume 108, pages 2043–2050, 2023

Magnetism and equation of states of fcc FeH_x at high pressure

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Abstract

Hydrogen is a strong candidate for light alloying elements in terrestrial cores. Previous first-principles studies on non-stoichiometric hexagonal close-packed (hcp) and double hexagonal close-packed (dhcp) FeH_x predicted a discontinuous volume expansion across the magnetic phase transition from non-magnetic (NM) or antiferromagnetic (AFM) to ferromagnetic (FM) state with increasing the hydrogen content, x at 0 K. However, previous high-pressure and -temperature neutron diffraction experiments on face-centered cubic (fcc) FeH_x did not reveal such nonlinearity. The discrepancy between theory and experiment may be due to differences in the crystal structure, magnetism, or temperature. In this study, we computed the equation of states for fcc FeH_x using the Korringa-Kohn-Rostoker method combined with the coherent potential approximation (KKR-CPA). In addition to the four types of ground-state magnetism (FM, AFM-I, AFM-II, and NM), we calculated the local magnetic disorder (LMD) state, which approximates the paramagnetic (PM) state with local spin moment above the Curie temperature. Our results show that even though FM, AFM-I, AFM-II, and NM calculations predict a discontinuity in the volume at 0 K, the volume becomes continuous above the Curie temperature, consistent with the previous neutron experiment. From the enthalpy comparison at 0 K, FM fcc FeH ($x = 1$) becomes the NM state above ~48 GPa. The magnetic transition pressure decreases with decreasing hydrogen content. Therefore, below the magnetic transition pressure, local spin moments affect the density and elastic wave velocity of fcc FeH_x, which may be important for small terrestrial bodies such as Mercury and Ganymede. By contrast, at the Earth's core pressure above 135 GPa, fcc FeH_x becomes NM. Thus, we calculated the density and bulk sound velocity as a function of pressure at 0 K for NM fcc FeH_x. The density at 360 GPa decreases with increasing hydrogen content, with $FeH_{0.5}$ best matching the preliminary reference Earth model (PREM) of the inner core. Since the density decreases with increasing temperature, this value constrains the upper limit of hydrogen content, assuming that the inner core is fcc FeH_x. On the other hand, the bulk sound velocity at 360 GPa increases with increasing hydrogen content, with $FeH_{0.3}$ best matching the PREM, which may give a lower bound. Assuming that Poisson's ratio of the FeH_x alloy is equal to that of the inner core, we examined the effects of temperature on density and bulk sound velocity. The results suggest that the fcc FeH_x alloy alone cannot explain the inner core density and bulk sound velocity simultaneously unless the temperature is extremely low ($T < 4000$ K).

Keywords: FeH_x, magnetism, equation of states, KKR-CPA, inner core