American Mineralogist, Volume 108, pages 667–674, 2023

Volumes and spin states of FeH_x: Implication for the density and temperature of the Earth's core

Hua Yang[1,2], Joshua M.R. Muir[1], and Feiwu Zhang[1,*,†]

[1]State Key Laboratory of Ore Deposit Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, 550081, China
[2]University of Chinese Academy of Sciences, Beijing, 100049, China

Abstract

Hydrogen is the most abundant element in the solar system and has been considered one of the main light elements in the Earth's core. The hydrogen content in the Earth's core is determined normally by matching the volume expansion caused by the incorporation of hydrogen into FeH_x to the Earth's core density deficit. The magnitude of this volume expansion at the pressure (P) and temperature (T) conditions of the Earth's core is still unknown, and the effect of spin transition in FeH_x at high pressure is usually ignored. In this study, we simulate the Fe spin transition, equation of state, and hydrogen-induced volume expansion in Fe-H binaries at high P-T conditions using density functional theory (DFT) calculations. Our results indicate that hydrogen could stabilize the magnetic properties of fcc Fe from ~10 to ~40 GPa. A volume expansion induced by hydrogen is linear with pressure except at the Fe spin transition pressure, where it collapses significantly (~30%). The fcc FeH lattice is predicted to expand at an average rate of ~1.38 and 1.07 Å^3 per hydrogen atom under the Earth's outer and inner core P-T conditions, where the hydrogen content is estimated to be ~0.54–1.10 wt% and ~0.10–0.22 wt%, respectively. These results suggest that the Earth's core may be a potentially large reservoir of water, with up to ~98 times as much as oceans of water being brought to the Earth's interior during its formation. Based on our predicted hydrogen content in the Earth's core, we propose that the presence of hydrogen would induce a relatively lower core temperature, ~300–500 K colder than it has been previously speculated.

Keywords: Hydrogen, iron hydride, spin transition, volume expansion, Earth's core; Physics and Chemistry of Earth's Deep Mantle and Core