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The effects of ferromagnetism and interstitial hydrogen on the equation of states of hcp and dhcp FeH_x: Implications for the Earth's inner core age

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Abstract

Hydrogen has been considered as an important candidate of light elements in the Earth's core. Because iron hydrides are unquenchable, hydrogen content is usually estimated from in situ X-ray diffraction measurements that assume the following linear relation: $x = (V_{FeHx} - V_{Fe})/\Delta V_H$, where x is the hydrogen content, ΔV_H is the volume expansion caused by unit concentration of hydrogen, and V_{FeH_x} and V_{Fe} are volumes of FeH_x and pure iron, respectively. To verify the linear relationship, we computed the equation of states of hexagonal iron with interstitial hydrogen by using the Korringa-Kohn-Rostoker method with the coherent potential approximation (KKR-CPA). The results indicate a discontinuous volume change at the magnetic transition and almost no compositional (x) dependence in the ferromagnetic phase at 20 GPa, whereas the linearity is confirmed in the non-magnetic phase. In addition to their effect on the density-composition relationship in the Fe-FeH_x system, which is important for estimating the hydrogen incorporation in planetary cores, the magnetism and interstitial hydrogen also affect the electrical resistivity of FeH_x. The thermal conductivity can be calculated from the electrical resistivity by using the Wiedemann-Franz law, which is a critical parameter for modeling the thermal evolution of the Earth. Assuming an $Fe_{1-y}Si_yH_x$ ternary outer core model ($0.0 \leq x \leq 0.7$), we calculated the thermal conductivity and the age of the inner core. The resultant thermal conductivity is ~100 W/m/K and the maximum inner core age ranges from 0.49 to 0.86 Gyr.

Keywords: FeH_x, ferromagnetism, chemical disorder, equation of states, KKR-CPA