Hydrogen occupation and hydrogen-induced volume expansion in Fe$_{0.9}$Ni$_{0.1}$D$_x$ at high P-T conditions

Chikara Shito$^1$, Hiroyuki Kagi$^{1, *}$§, Sho Kakizawa$^2$‡, Katsutoshi Aoki$^1$, Kazuki Komatsu$^1$, Riko Iizuka-Oku$^1$, Jun Abe$^3$, Hiroyuki Saitoh$^4$, Asami Sano-Furukawa$^{5, 6, *}$, and Takanori Hattori$^5$

$^1$Geochemical Research Center, Graduate School of Science, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
$^2$Earth and Planetary Systems Science Program, Graduate School of Advanced Science and Engineering, Hiroshima University, 1-3-1, Kagamiyama, Higashi-Hiroshima-Shi, Hiroshima, 739-8526, Japan
$^3$Neutron Science and Technology Center, Comprehensive Research Organization for Science and Society, 162-1, Shirakata, Tokai-mura, Naka-gun, Ibaraki 319-1106, Japan
$^4$Quantum Beam Science Research Directorate, National Institutes for Quantum and Radiological Science and Technology, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5198, Japan
$^5$J-PARC Center, Japan Atomic Energy Agency, 2-4, Shirakata, Tokai-mura, Naka-gun, Ibaraki 319-1195, Japan
$^6$Institute of Materials Structure Science, KEK, 203-1 Shirakata, Tokai-mura, Naka-gun, Ibaraki, 319-1195, Japan

ABSTRACT

The density of the Earth’s core is several percent lower than that of iron-nickel alloy under conditions of pressure and temperature equivalent to the Earth’s core. Hydrogen is one of the most promising constituents accounting for the density deficit, but hydrogen occupation sites and density decrease of iron-nickel alloy caused by hydrogenation have never been investigated. In this study, the phase relation and crystal structure of Fe$_{0.9}$Ni$_{0.1}$H$_x$(D$_x$) at high pressures and temperatures up to 12 GPa and 1000 K were clarified by in situ X-ray diffraction and neutron diffraction measurements. Under the P-T conditions of the present study, no deuterium atoms occupied tetragonal (T) sites of face-centered cubic (fcc) Fe$_{0.9}$Ni$_{0.1}$D$_x$, although the T-site occupation was previously reported for fcc FeH$_x$(D$_x$). The deuterium-induced volume expansion per deuterium v$_D$ was determined to be 2.45(4) and 3.31(6) Å$^3$ for fcc and hcp Fe$_{0.9}$Ni$_{0.1}$D$_x$, respectively. These v$_D$ values are significantly larger than the corresponding values for Fe$_2$. The v$_D$ value for fcc Fe$_{0.9}$Ni$_{0.1}$D$_x$ slightly increases with increasing temperature. This study suggests that only 10% of nickel in iron drastically changes the behaviors of hydrogen in metal. Assuming that v$_D$ is constant regardless of pressure, the maximum hydrogen content in the Earth’s inner core is estimated to be one to two times the amount of hydrogen in the oceans.

Keywords: Neutron diffraction, high pressure, metal hydride, Earth’s core; Physics and Chemistry of Earth’s Deep Mantle and Core

INTRODUCTION

Cosmochemical studies suggested that the iron in the Earth’s core contains 5–15 wt% of nickel (e.g., Anderson 1989). It has been a long-standing subject that the core would contain light elements (H, C, N, O, Si, and S) because the density of the Earth’s core is about 10% lower in the outer core and about 5% lower in the inner core than that of pure iron (e.g., Birch 1952). Hydrogen, the most abundant element in the solar system, is thought to be the most plausible candidate among the light elements. According to Fricker and Reynolds (1968), a deep magma ocean, which once existed on the primordial Earth’s surface, would have dissolved about 1 wt% of water. Okuchi (1997) suggested that most of the dissolved water was incorporated into metallic iron by metal–silicate partitioning in the lowermost of the magma ocean. Iizuka-Oku et al. (2017) directly observed the formation process of iron hydride through the reaction between iron and water using high-pressure and -temperature (high P-T) neutron diffraction. The H-bearing iron at the base of the magma ocean formed through such processes would sink to form the current core because of the gravitational instability. Tagawa et al. (2021) found that the partition coefficient of hydrogen between molten iron and silicate melt is greater than 29, and hydrogen is strongly siderophile at the conditions of core formation. Kato et al. (2020) determined the stability of stoichiometric fcc FeH up to 137 GPa and showed that fcc FeH is stable at the P-T conditions of the Earth’s core. Ohta et al. (2019) indicated that the resistivity of stoichiometric fcc FeH is smaller than that of fcc Fe by measuring resistivity of iron hydrides at high pressures up to 65 GPa and high temperatures up to 2100 K. The chemical composition of the Earth’s core has been estimated by comparing density (e.g., Anderson and Isaak 2002) and sound velocity measurements (e.g., Sakamaki et al. 2016) of prospective constituent phases to the 1-D averaged seismic models such as PREM (Dziewonski and Anderson 1981). However, the definitive chemical composition has not been determined because the behavior of light elements in the core is unknown.

* E-mail: kagi@eqchem.s.u-tokyo.ac.jp. Orcid 0000-0002-8587-1213
† Orcid 0000-0002-1652-1623
‡ Present address: Research and Utilization Division, Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo-cho, Hyogo 679-5198, Japan.
§ Special collection papers can be found online at http://www.minsocam.org/MSA/AmMin/special-collections.html.

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