American Mineralogist, Volume 104, pages 1781–1787, 2019

Static compression of Fe_4N to 77 GPa and its implications for nitrogen storage in the deep Earth

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Abstract

Compression and decompression experiments on face-centered cubic (fcc) γ′-Fe_4N to 77 GPa at room temperature were conducted in a diamond-anvil cell with in situ X-ray diffraction (XRD) to examine its stability under high pressure. In the investigated pressure range, γ′-Fe_4N did not show any structural transitions. However, a peak broadening was observed in the XRD patterns above 60 GPa. The obtained pressure-volume data to 60 GPa were fitted to the third-order Birch-Murnaghan equation of state (EoS), which yielded the following elastic parameters: K_0 = 169 (6) GPa, K' = 4.1 (4), with a fixed V_0 = 54.95 Å at 1 bar. A quantitative Schreinemakers' web was obtained at 15–60 GPa and 300–1600 K by combining the EoS for γ′-Fe_4N with reported phase stability data at low pressures. The web indicates the existence of an invariant point at 41 GPa and 1000 K where γ′-Fe_4N, hexagonal closed-packed (hcp) ε-Fe_7N_3, double hexagonal closed-packed β-Fe_7N_3, and hcp Fe phases are stable. From the invariant point, a reaction γ′-Fe_4N = β-Fe_7N_3 + hcp Fe originates toward the high-pressure side, which determines the high-pressure stability of γ′-Fe_4N at 56 GPa and 300 K. Therefore, the γ′-Fe_4N phase observed in the experiments beyond this pressure must be metastable. The obtained results support the existing idea that β-Fe_7N_3 would be the most nitrogen-rich iron compound under core conditions. An iron carbonitride $Fe_7(C,N)_3$ found as a mantle-derived diamond inclusion implies that β-Fe_7N_3 and Fe_7C_3 may form a continuous solid solution in the mantle deeper than 1000 km depth. Diamond formation may be related to the presence of fluids in the mantle, and dehydration reactions of high-pressure hydrous phase D might have supplied free fluids in the mantle at depths greater than 1000 km. As such, the existence of $Fe_7(C,N)_3$ in diamond can be an indicator of water transportation to the deep mantle.

Keywords: Iron nitrides, Earth's core, equation of state, diamond-anvil cell, in situ X-ray diffraction, high pressure; Physics and Chemistry of Earth's Deep Mantle and Core