Abstract:

Structure and Equation of State of Fe_3P up to 1 Mbar: Implications for Phosphorus in Earth's Core

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The Earth's core is predominantly iron and nickel alloyed with one or more light elements. In addition to the major light elements such as hydrogen (H), carbon (C), oxygen (O), sulfur (S) and silicon (Si), phosphorus (P) is considered to be present in the Earth's core partly due to its high metal/silicate partitioning coefficients and its abundance of iron phosphide minerals, such as schreibersite, $(Fe, Ni)_3P$, in iron nickel meteorites. In addition, the concentration of phosphorus in the Earth's silicate mantle prominently deviates from the volatility trend, unambiguously indicating the presence of phosphorus in the core. In this study, we performed synchrotron powder X-ray diffraction (XRD) measurements using laser heating diamond anvil cells up to 102 GPa to determine the densities of Fe_3P at high pressure. We observed a spin transition accompanied by a volume collapse at about 18 GPa at 300 K and the spin transition completed at 47 GPa according to the *c*/*a* ratio as a function of pressure. The *P*-*V* relationship of Fe_3P could be well represented by Birch-Murnaghan equation of states. No further transformation was observed up to 76 GPa, 1700K or up to 102 GPa. As Fe_3P can form solid solution with its isostructural compound Fe_3S, the crystal structure of Fe_3P will provide insights into the crystal chemistry of the binary Fe-P system and the ternary Fe-S-P system. The determined elastic properties of Fe_3P will examine the Fe-P or Fe-P-S core composition model and contribute to the mineral physics database for iron alloys.