Structure and behavior of the Ni end-member schreibersite, (Ni_3P), under deep Earth conditions

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Abstract

Natural schreibersite consists of iron-nickel phosphide [$(Fe, Ni)_3P$], is common in iron meteorites and is believed to have a similar composition as that of Earth's core. Although, there are a few environments to find schreibersite, the implication of schreibersite might be important for the Earth's life. It is believed that meteoritic phosphides minerals including schreibersite is a source of phosphorus in the early Earth. Seismic velocity measurements of Earth's core indicate that the density of the outer core and inner core is about 10% and 3% lower than pure iron at the relevant pressure and pressure conditions. The density deficit of the core with respect to pure iron can be explained by assuming the presence of Fe-Ni- light element alloys. Although, there have been numerous previous studies investigating solid solutions between Fe and light elements, including the schreibersite Fe end-member (Fe_3P), the effect of Ni, the second major element in the core, on the high-pressure and temperature behavior and physical properties of Fe_3P has not been systematically investigated. The crystal structure and behavior of the Ni end-member schreibersite at high pressure and temperature conditions were studied by using single-crystal synchrotron-based X-ray diffraction in combination with the laser-heated diamond anvil cell and using Vienna ab-initio simulation package (VASP) in MedeA program to study atomic scale materials phenomena at different conditions as the First-principle calculations. The volume data of Ni_3P at high pressures and ambient temperature below 35 GPa were fitted by 3rd order Birch–Murnaghan equation of state, yielded the values V0 = 352.63(7) Å^3, K0 = 163(18) GPa, K'=17(2). The volume decreases by approximately 1.5 % between pressure at 30 and 35 GPa. At approximately 35 GPa, the trend of c/a ratio changes from negative to positive, which might be a sign for a magnetic transition of $I\bar{4}$ of the structure. Moreover, around 30 GPa, the trend of a lattice parameter changes the slope while the trend of c lattice parameter follows the lower pressure curve, which leads to a discontinuous behavior of c/a ratio and volume at high pressure. A better understanding of the effects of the potential presence of light element alloys of Fe and Ni, such as schreibersite, will provide new constraints on the evolution and formation of the Earth, and will improve our ability to interpret seismic observations of the Earth's core.

Keywords: schreibersite, diamond anvil cell, the Earth's core