High pressure behavior of the Ni end-member schreibersite, (Ni_3P), up to 50 GPa

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Abstract

Earth's core is believed to be primarily composed of iron-nickel (Fe-Ni) alloy, however, observed seismic velocities suggest the presence of an appreciable amount of one or more light elements. Among several other alloys and compounds, Fe-Ni phosphides are considered as candidates for minor core phases and would have the effect of lowering the core density. While Fe-phosphides have been the subject of earlier experimental and computational studies, the effects of Ni, the second major element in the core, have not been systematically investigated. This project focuses on the investigation of the crystal structure and behavior of the most metal-rich of Ni-P binary compounds, the Ni end-member schreibersite (Ni_3P), using synchrotron X-ray diffraction (XRD) experiments. Ni_3P is isostructural with Fe_3P and has a tetragonal symmetry with $I\bar{4}$ space group. In our experiments both powder and two single crystal samples of synthetic Ni_3P in different orientations, with respect to the axis of the diamond anvil cell, were compressed up to approximately 50 GPa at ambient temperature. The compressional data were fitted by 3rd order Birch–Murnaghan equation of state, and yielded V_0 = 351.44(8) Å^3, K_{T0} = 190(4) GPa, K' = 4.9(4) for powder data below 35 GPa, K_{T0} = 199(5) GPa, K'= 4.7(4) for single-crystal 1 data below 30 GPa, and K_{T0} = 194(5) GPa, K' = 4.7(8) for single crystal 2 below 25 GPa. All data suggest that at low pressure (~< 30 GPa), the *c*/*a* ratio of unit cell parameters remains approximately constant but starts to increase steadily above that pressure and experience a second slight discontinuity at approximately 40 GPa. The change in unit cell parameters at ~30 GPa and ~40 GPa suggests discontinuous changes in magnetic ordering. Moreover, the threshold of these subtle discontinuities is sensitive to the stress state and orientation of the crystal in the diamond anvil cell. This study is the first report of compressional behavior of both powder and single crystal Ni_3P up to 50 GPa and offers insights into the effects of Ni_3P components on the compressional behavior of schreibersite in the Earth's core.

Keywords: Schreibersite, High pressure, Diamond Anvil Cell, Synchrotron X-ray diffraction, Single-crystal X-ray diffraction, Crystallography