Crystal Chemistry of Iron Phosphides at Pressures to 71 GPa and 2000K

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Introduction

The Earth's crust is depleted in phosphorous relative to chondritic meteorites, lunar crust, and theoretical calculations of bulk earth composition. It is believed that this depletion is due to the incorporation of phosphorous into iron-nickel alloys, which differentiated into the Earth's core. Iron-nickel phosphides occur in meteorites as berringerite and schreibersite chondrules and as finegrained matrix material. The purpose of this study is to observe the behavior of stoichiometric iron-nickel phosphides with increased pressure and temperature.

Methods and Materials

Materials were synthesized in evacuated Si glass tubes at ambient pressure and temperatures ranging from 700° to 1200° C at the Geophysical Laboratory. Samples were examined by using x-ray diffraction and ion microprobe to ensure correct stoichiometry. Powdered samples were ground in agate under acetone to minimize the effects of preferred orientation. They were then loaded into a Mao-Bell type diamond anvil cell with a ~250- μ m culet, a rhenium gasket with a hole size of ~100 μ m, ruby chips as pressure calibrant, and NaCl as the pressure medium.

Experiments were carried out by using angle-dispersive diffraction and *in situ* laser heating at the GeoSoilEnviro Consortium for Radiation Studies (GSECARS) 13-ID-C beamline. The methodology included increasing the pressure in small increments (3 to 5 GPa per increase) and collecting diffraction data at ambient temperature and while the sample was being heated. This process was repeated until the diamond cell reached its maximum pressure. At this point, quenching experiments were conducted.

Results

Diffraction patterns collected (Figs. 1 and 2) indicate that a phase transformation may occur in Fe₂P from the hexagonal *P*-62*m* structure to a new, possibly monoclinic, structure between 30 and 50 GPa. At least one phase transformation is noted in FeP, from the orthorhombic *Pna*21 structure to a new, possibly monoclinic structure between 32 and 40 GPa. The overlapping of NaCl diffraction peaks with those of the sample has made solution of the new structures difficult to achieve.

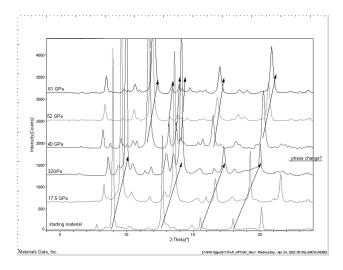


FIG. 1. Diffraction patterns of Fe_2P to 55GPa under laser heating. A structural change is apparent.

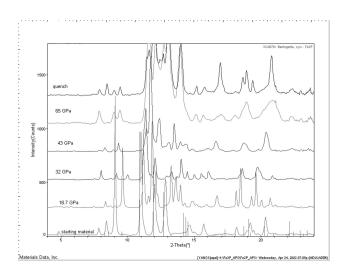


FIG. 2. Diffraction patterns of FeP between 17.5 and 61 GPa with laser heating. Sample peaks shift as the cell volume decreases. The sample exhibits a marked phase change after 32 GPa.

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