ESRF	**Experiment title:** High-pressure breakdown of Fe_3O_4	**Experiment number**: HS-1525
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Report:

Lazor P., Shebanova O., Annersten H., High-pressure study of stability of magnetite by thermodynamic analysis and synchrotron X-ray diffraction, Journal of Geophysical Research, 109, B05201: 1-16, 2004.

Abstract: Thermodynamic analysis and synchrotron x-ray diffraction experiments aiming at the investigation of stability of magnetite were carried out in the pressure temperature range 0 - 36 GPa and 300 - 800 K, respectively. The thermodynamically predicted breakdown of magnetite to hematite and wüstite was not observed, but the trace amounts of hematite detected in the sample assemblage may signify a presence of nucleation centers of breakdown products, the growth of which is kinetically hindered due to the energetic requirements for the reaction. A number of phase equillibria were considered and evaluated in the Fe-O system. The pressure - temperature stability field for the mixture of oxides Fe_2O_3 + FeO is defined by a triangle with maximum temperature 850 K at 14.6 GPa. At 298 K, the equilibrium pressure for the breakdown of magnetite is 13.3 GPa, while the pressure for the synthesis FeO + Fe_2O_3 $\Leftrightarrow$ h-Fe_3O_4 is located between 35 and 47 GPa, depending on the choice of input parameters. The calculations also predict that the h-Fe_3O_4 becomes unstable with respect to h-Fe_2O_3 + FeO at pressures higher than 50 GPa. The 298 K isotherm derived from the compression experiment is in good agreement with results of earlier studies. The 1 - confidence ellipsoid shows large negative correlations for the fit parameters K_T, K_0`, and V_0. The transformation of magnetite to the dense polymorph was observed already at 19 GPa. The Rietveld refinement of the diffraction pattern of h-Fe3O4 is consistent with the $CaTi_2O_4$-type structure. The values of Gibbs formation energies for the high-pressure polymorphs h-Fe_3O_4 and h-Fe_2O_3 were estimated to be -962 kJ/mol and -610 kJ/mol, respectively. The standard-state entropy of h-Fe_3O_4 is 172.4 J/K/mol.