

In situ p-V-T Measurements of Magnetite

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Magnetite Fe_3O_4 has an inverse spinel structure with space group $\text{Fd}\bar{3}\text{m}$. The tetrahedral positions are occupied by Fe^{3+} and the octahedral sites contain equal amounts of Fe^{2+} and Fe^{3+} , Fleet (1981). It occurs in earth crust and the upper mantle and is also an important material in industrial applications such as data storage. This work is part of systematic investigations of different spinels under high-pressure and high-temperature conditions to evaluate the thermal dependence of the bulk moduli.

The experiments were conducted at the Beamline F2.1 at the HASYLAB in Hamburg using a MAX80 multi-anvil-press. Synthetic magnetite powder was used for the experiments and NaCl acted as pressure standard. Pressure was stepwise increased up to about 5 GPa. Four different runs with a maximum temperature of 1100 Kelvin were made. The data were evaluated with the Rietveld-method using the GSAS/EXPGUI software suite to obtain the unit cell volume. Decker's equation of state was utilized to determine the pressure, Decker (1971).

The measurements yield an isothermal bulk modulus $K_{T0} = 186(9)$ GPa with a fixed $K' = 4$ and for dK/dT a value of -0.0339 GPa/K. In literature the values for the isothermal bulk modulus show values between 155 GPa and 222 GPa for powder data and between 181 GPa and 189 GPa for single crystal data, Haavik et al. (2000). The calculated bulk modulus of this work fits well within the single crystal data. The pressure derivative could not be fitted because of the narrow pressure range. There are no values for dK/dT reported before.

References

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