P-V and *T-V* Equations of State of natural biotite: An in-situ high-pressure and high-temperature powder diffraction study, combined with Mössbauer spectroscopy

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Abstract

The *P-V* and *T-V* equations of state of a natural biotite sample (Mg/Fe ratio $\approx$ 1) have been studied using in-situ high-pressure (0.0001–11 GPa) synchrotron radiation powder diffraction at the European Synchrotron Radiation Facilities (ESRF) in Grenoble, France, and in-situ high-temperature (298–610 K) laboratory X-ray powder diffraction. A third-order Birch-Murnaghan model [$V_0 = 498.7(1)$ Å^3, measured value] provides the following elastic parameters: $K_0 = 49(1)$ GPa, $K' = 8.1(5)$. The volume thermal expansion is satisfactorily described by a constant value resulting in $37(2) \cdot 10^{-6}$ K^{-1}. Mössbauer spectroscopy proves that REDOX reactions have occurred upon heating, presumably $2(OH^- + Fe^{2+}) \rightarrow 2O^{2-} + 2Fe^{3+} + H_2^\uparrow$ and/or $4Fe^{2+} + 2OH^- + O_2 \rightarrow 4Fe^{3+} + 3O^{2-} + H_2O$. On the basis of the elastic and thermal parameters measured we have modeled the deformation contribution (G_{deform}) to the Gibbs energy. The third-order Birch-Murnaghan model with V_0 fixed at its experimental value and the model with refined V_0 do not significantly differ from one another in terms of G_{deform}. A comparison based on G_{deform} between biotite and phlogopite shows a better compliance to *P* of the former, though balanced in mineral reactions by a difference of molar volume, i.e., V_0(biotite) > V_0(phlogopite).

Keywords: High-pressure studies, high-temperature studies, biotite, *P-T* stability