American Mineralogist, Volume 89, pages 647–653, 2004

A single-crystal study on the pressure behavior of phlogopite and petrological implications

P. COMODI,[1] P. FUMAGALLI,[2] M. MONTAGNOLI,[1] AND P.F. ZANAZZI[1,*]

[1]Dipartimento di Scienze della Terra, Università di Perugia, Piazza Università, I-06100 Perugia, Italy
[2]Dipartimento di Scienze della Terra, Università di Milano, Via Botticelli 23, I-20133 I-Milano, Italy

ABSTRACT

The structural behavior of phlogopite was studied by in situ single-crystal X-ray diffraction (XRD) in a diamond-anvil cell, using crystals of composition $[(K_{0.91}Na_{0.02}Ba_{0.03})\ (Fe^{2+}_{0.65}Fe^{3+}_{0.163}Al_{0.123}Mg_{1.81}Ti_{0.149})Si_{2.708}Al_{1.292}O_{10}OH_{1.725}F_{0.175}]$. Lattice parameters were measured from 0.0001 to 6.5 GPa and fitted with a third-order Birch-Murnaghan equation of state (EoS). The resulting EoS parameters are: V_0 = 497.1(1) Å^3, K_0 = 54(2) GPa^{-1}, and K' = 7(1); a_0 = 5.336(1) Å, K_0 = 123(9) GPa, and K' = 3(2); b_0 = 9.240(3) Å, K_0 = 128(15) GPa, and K' = 3(2); c_0 = 10.237(6) Å, K_0 = 25(2) GPa, and K' = 5(1); the β angle increases linearly with pressure from 100.02(5) to 100.4(1)°.

The structural evolution of phlogopite was studied by comparing five structural refinements performed with intensity data collected at 0.0001, 1.2, 3.2, 5.0, and 6.0 GPa. The interlayer site, where K is located, is about 4.5 times more compressible than the T-O-T unit. At the same time, the greater compression of the octahedral layer with respect to the tetrahedral one induces an increase in tetrahedral rotation angle α from 9.29 to 11.9°.

Structural evolution with pressure yields a crystallographic rationale for the larger baric stability of K-deficient and Si-rich phlogopites, as observed from natural and experimental data.

Combined high-pressure and thermal expansion data yield the approximate EoS: $V = V_0(1 + 4.6 \times 10^{-5}\Delta T - 0.0167\ \Delta P)$, where P is in GPa and T in °C. This equation was used to calculate phase equilibria in lherzolite compositions modeled in the simplified K_2O-CaO-MgO-Al_2O_3-SiO_2-H_2O (KCMASH) system. The results show that the effect of phlogopite on bulk density is particularly significant at high pressure and temperature since, above the chlorite stability field, phlogopite is the only hydrous phase able to lower bulk density properties by about 0.5% with respect to the K-free bearing system.