American Mineralogist, Volume 94, pages 1596–1602, 2009

The high-pressure–high-temperature behavior of bassanite

Paola Comodi,[1,*] Sabrina Nazzareni,[1] Leonid Dubrovinsky,[2] and Marco Merlini[3,4]

[1]Dipartimento di Scienze della Terra, Università di Perugia, Piazza dell'Università, 06100 Perugia, Italy
[2]Bayerisches Geoinstitut, Universität Bayreuth, Universität Strasse 30, 95440 Bayreuth, Germany
[3]European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP220, F-38043 Grenoble, France
[4]Dipartimento di Scienze della Terra, Università di Milano, Via Botticelli 23, 20133 Milano, Italy

Abstract

The pressure evolution of bassanite ($CaSO_4 \cdot \frac{1}{2}H_2O$) was investigated by synchrotron X-ray powder diffraction along three isotherms: at room temperature up to 33 GPa, at 109 °C up to 22 GPa, and at 200 °C up to 12 GPa.

The room-temperature cell-volume data, from 0.001 to 33 GPa, were fitted to a third-order Birch-Murnaghan equation-of-state, and a bulk modulus K_0 = 86(7) GPa with K' = 2.5(3) was obtained. The axial compressibility values are β_a = 3.7(2), β_b = 3.6(1), and β_c = 2.8(1) GPa^{-1} (×10^{-3}) showing a slightly anisotropic behavior, with the least compressible direction along *c* axis. The strain tensor analysis shows that the main deformation occurs in the (010) plane in a direction 18° from the *a* axis.

The bulk moduli for isotherms 109 and 200 °C, were obtained by fitting cell-volume data with a second-order Birch-Murnaghan equation-of-state, with K' fixed at 4, and were found to be K_{109} = 79(4) GPa and K_{200} = 63(7) GPa, respectively. The axial compressibility values for isotherm 109 °C are β_a = 2.4(1), β_b = 3.0(1), β_c = 2.5(1) (×10^{-3}) GPa^{-1}, and for isotherm 200 °C they are β_a = 3.5(3), β_b = 3.4(3), β_c= 2.6(4) (×10^{-3}) GPa^{-1}. These two bulk moduli and the 20 °C bulk modulus, $K_{0,20}$ = 69(8) recalculated to a second-order Birch-Murnaghan EoS to be consistent, as well as the axial compressibilities, are similar for the three isotherms indicating that the thermal effect on the bulk moduli is not significant up to 200 °C. The size variation of the pseudo-hexagonal channel with pressure and temperature indicates that the sulfate "host" lattice and the H_2O "guest" molecule in bassanite do not undergo strong change up to 33 GPa and 200 °C.

Keywords: Bassanite, Ca-sulfate, compressibility, high temperature, high pressure, X-ray diffraction