Geophysical Research Abstracts,
Vol. 10, EGU2008-A-10220, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-10220
EGU General Assembly 2008

H*P*-phase transition of natural *P*2_1/*c* pigeonite: spontaneous strain and structure evolution

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The only available HP data on $P2_1/c$ pyroxene, concern so far synthetic samples of clinoenstatite, $Mg_2Si_2O_6$ clinoferrosilite, $Fe_2Si_2O_6$, and of a sample with composition $Ca_{0.15}Mg_{1.85}Si_2O_6$[1,2,3]. Although these studies have concluded that composition affects the pressure of transformation (P_c), the mechanism remains to be fully characterized. Moreover, there are as yet no high pressure data on natural pigeonite samples.

In this study a sample of natural pigeonite from the Paranà ryodacite with composition $^{M2}(Ca_{0.20}Mg_{0.15}Fe_{0.65})^{M1}(Mg_{0.80}Fe_{0.20})Si_2O_6$ and free of exsolved augite was studied by means of single-crystal X-ray diffraction using a diamond anvil cell at 13 different pressure values up to about 8 GPa and room temperature. In the $P2_1/c$ LP-phase the unit-cell parameters showed a non-linear decrease almost isotropic linear axial compressibility with a ratio of β_a:β_b:β_c = 1.0:1.3:1.0, while the unit-cell parameters of the $C2/c$ HP-phase decreased almost linearly and with an isotropic linear axial compressibility (β_a:β_b:β_c =1.02:1.26:1.00). Between 3.3 and 3.4 GPa the variation in the unit-cell volume showed a strong discontinuity (about 2%) typical of a first order behavior phase transformation. A small hysteresis (~0.2 GPa) was observed. Diffraction data clearly indicate that the transition occurs from $P2_1/c$ to $C2/c$ symmetry as expected for this composition.

By fitting the pressure-volume data for the $P2_1/c$ phase using a third-order Birch-Murnaghan equation of state (EoS) we could refine simultaneously its unit-cell volume V_0, the bulk modulus K_{T0} and its first pressure derivative, K', obtaining the following EoS coefficients: V_0 = 431.9(2)Å^3, K_{T0} = 96.8(8) GPa and K'= 8.5(6). For the $C2/c$ phase K_{T0}, calculated fixing the K' to 4, was significantly higher than that of the $P2_1/c$ phase, with values of V_0= 423.64(11) and K_{T0}= 111.9(8) GPa.

We used the fitted EoS parameters $(a_0$, b_0, c_0, V_0 and $c\sin\beta_0)$ of the HP-phase to calculate the spontaneous strain due to the phase transition to the LP-phase. The evolution of every single component of the strain tensor with pressure compares well with the observed evolution for the same phase transition in $ZnSiO_3$ [4]. Scalar spontaneous strain (ε_s) scales almost linearly with volume strain (V_s) as ε_s= 0.169(16) - 5.8(9) •V_s.

Crystal structure evolution with pressure in the low-symmetry phase $(P2_1/c)$ indicated that M1-O and M2-O mean bond lengths decreased as 0.006 Å•GPa^{-1} and 0.013 Å•GPa^{-1} respectively, with no significant change in tetrahedral T-O bond lengths. For the high-symmetry phase $(C2/c)$ the M1-O and M2-O mean bond lengths showed a decrease of 0.006 Å•GPa^{-1} and 0.008 Å•GPa^{-1} respectively. A shrinking of 2.2 and 5.1% were observed in the two non-equivalent A and B tetrahedra chains respectively. At the transition, the A-chain changed from S-rotated to O-rotated reaching a value of 142.4° for the single chain of the HP-phase.

References

[1] Hugh-Jones D. A. et al. (1994) Am. Mineral. 79, 405-410

[2] Hugh-Jones D. A. et al. (1994) Am. Mineral. 79, 1032-1041

[3] Nestola F. et al. (2004) Am. Mineral. 89, 189–196

[4] Arlt, T., and Angel, R.J. (2000) Phys. Chem. Minerals, 27(10), 719-731.