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The high-pressure behavior of an Al- and Fe-rich natural orthopyroxene

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Abstract

A single crystal of a natural orthopyroxene with composition $^{M2}[Fe^{2+}_{0.818}Mg_{0.156}Ca_{0.010}Mn_{0.016}]^{M1}[Fe^{2+}_{0.081}Mg_{0.767}Al_{0.084}Fe^{3+}_{0.068}]^{TA}[Si]^{TB}[Si_{0.848}Al_{0.152}]O_6$ and space group *Pbca* (sample S95) was investigated at high pressure by X-ray diffraction using a diamond-anvil cell up to 9.56 GPa. No phase transitions were detected in the pressure range investigated. The unit-cell parameters, *a*, *b*, and *c*, decrease non-linearly with pressure and show an axial compression anisotropy with a ratio $\beta_a:\beta_b:\beta_c = 1.00:1.64:1.16$. The unit-cell volume decreases non-linearly as well and with a negative variation, by about 6.3% up to 9.56 GPa. The equation of state calculated using high-accuracy volume-pressure data up to 5.5 GPa gave the following coefficients: $V_0 = 846.02(4)$ Å^3, $K_{T0} = 115.4(6)$ GPa, $K' = 7.7(3)$. Among the Mg-orthopyroxenes investigated at high pressure so far S95 shows the highest bulk modulus.

Six complete intensity data were collected at 0, 0.16, 1.72, 3.95, 8.03, and 9.56 GPa. The results confirm previous conclusions regarding the compressional mechanism in orthopyroxenes. At lower pressures, compression is mostly connected to a decrease in volume of the two M-coordination octahedra, accompanied by an increased kink in the B-tetrahedral chain. At higher pressures, compression of the M sites decreases, the kink of the tetrahedral chains stops to change, and reduction in unit-cell volume is accompanied mainly by compression of tetrahedra.

This change in compressional trends results in a relatively large *K*' parameter and a pronounced stiffening of the structure with pressure. The presence of Al in the TB tetrahedral site influences the kink of the B tetrahedral chain, which depends on the ratio of sizes of the M2 and TB coordination polyhedra. The increased stiffness of the M polyhedra, caused by the presence of Fe, is the main reason for the high bulk modulus of S95 and its resistance to shortening of the **c** axis. This explains the limited shortening of the **c** axis in S95 and the different compressional axial anisotropy with respect to other orthopyroxenes investigated under high pressure.

Keywords: Orthopyroxene, high pressure, crystal structure, X-ray diffraction