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Leucite at high pressure: Elastic behavior, phase stability, and petrological implications

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Abstract

Elastic and structural behavior of a natural tetragonal leucite from the volcanic Lazium district (Italy) were investigated at high pressure by in situ single-crystal X-ray diffraction with a diamond anvil cell under hydrostatic conditions. A first-order phase transition, never reported in the literature, was observed at $P = 2.4 \pm 0.2$ GPa from tetragonal ($I4_1/a$) to triclinic symmetry (analysis of diffraction intensities suggests the space group $P\bar{1}$), accompanied by a drastic increase in density of about 4.7%. The transition pressure was bracketed by several measurements in compression and decompression. No further phase-transition has been observed up to 7 GPa. Fitting a second-order Birch-Murnaghan equation of state (BM-EoS) to the pressure-volume data of the tetragonal polymorph, we obtain $K_0 =$ 41.9(6) GPa and $K' = 4$ (fixed). In the case of the triclinic polymorph, a second-order BM-EoS gives $K_0 = 33.2(5)$ GPa. The eulerian finite strain (f_e) vs. normalized stress (F_e) curves were calculated for the low- and high-P polymorphs, providing $F_e(0) = 42(1)$ and $F_e(0) = 33.2(4)$ GPa, respectively. The axial bulk modulus values of the tetragonal polymorph, calculated with a linearized BM-EoS, are $K_0(a) =$ 34.5(5) and $K_0(c) = 78(1)$ GPa. For the triclinic polymorph, we obtain $K_0(a) = 35.9(5)$, $K_0(b) = 34.9(7)$, and $K_0(c) = 35.5(7)$ GPa. The elastic behavior of the low-P polymorph appears to be more anisotropic than that of the high-P polymorph. The HP-crystal structure evolution of the tetragonal polymorph of leucite was studied on the basis of six structural refinements at different pressures between 0.0001 and 1.8 GPa. The main deformation mechanisms at high-pressure are due to tetrahedral tilting, giving rise to an increase of the ellipticity of the four- and six-membered rings of the tetrahedral framework. The T-O bond distances are practically invariant within the stability field of the tetragonal polymorph. The complex P-induced twinning, due to the tetragonal → triclinic phase-transition, and the low quality of the diffraction data at pressure above the phase-transition, did not allow the refinement of the crystal structure of the triclinic polymorph.

Keywords: Leucite, single-crystal X-ray diffraction, high pressure, compressibility, phase transition