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High-pressure phase transitions in dalyite, a Zr-silicate

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Abstract

Dalyite, ideally $K_2ZrSi_6O_{15}$, space group $P\bar{1}$, is a rare potassium zirconium silicate in agpaitic alkaline rocks, i.e., rocks with $(Na + K)/Al \geq 1.2$ in which complex zirconosilicate minerals can form. The structural evolution and compressibility of dalyite have been studied by in situ single-crystal synchrotron X-ray diffraction up to 20.52(5) GPa. In the pressure (P) range investigated, we observed: (1) a second-order (distortive) phase transition, from dalyite to dalyite-II ($P\bar{1}$), between 9.90(5) and 10.68(5) GPa, and (2) a first-order phase transition, from dalyite-II to dalyite-III ($P\bar{1}$), between 11.06(5) and 12.03(5) GPa. Fitting the P–unit-cell volume (V) data with a second-order Birch-Murnaghan equation of state (EoS) yielded a value of $K_{V0} = 51.4(4)$ GPa for dalyite [$V_0 = 332.5(2)$ Å^3] and $K_{V0} = 39(1)$ GPa for dalyite-III [$V_0 = 670(4)$ Å^3]; due to the narrow stability field of dalyite-II (~1.3 GPa), its elastic parameters could not be determined. The structure accommodates the deformation induced by pressure by increasing anisotropy, from dalyite having a strain ellipsoid axial value of $\varepsilon_1:\varepsilon_2:\varepsilon_3 \sim 1.69:1.28:1$ [calculated between 0.22(5) and 9.90(5) GPa] to dalyite-III with $\varepsilon_1:\varepsilon_2:\varepsilon_3 \sim 6.4:2.0:1$ [calculated between 12.03(5) and 20.52(5) GPa]. Both phase transitions have been found to be fully reversible, and the high-pressure polymorph structures have been solved. From dalyite to dalyite-II and dalyite-III, the unit-cell is doubled, and the coordination of K polyhedra increases from eight- to ninefold. Interestingly, before the first phase transition, the SiO_4 tetrahedra have a significant role in accommodating the bulk compression and show different bulk moduli [47(4), 74(14), and 108(20) GPa], but after the transition the compressibility is accommodated mainly by deforming the ZrO_6 octahedra, the β-wollastonite chains and the 4- and 6-membered tetrahedra rings. The deformation of the SiO_4 tetrahedra and Zr polyhedra constitutes an unusual behavior, rarely observed in previous high-pressure studies.

Keywords: Dalyite, X-ray single-crystal diffraction, crystal structure, high-pressure, phase-transition, Zr-phases, accessory minerals