High-temperature in situ structural investigation on lead feldspar

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ABSTRACT

Single-crystal X-ray diffraction was performed in situ at T = 20, 230, 465, and 700 °C on a partially ordered lead feldspar (PbAl₂Si₂O₈, *I2/c*, a = 8.402, b = 13.043, c = 14.308 Å, $\beta = 115.30^\circ$, V = 1417.6 Å³; $Q_{od} = 0.71$). The unit-cell expansion (1.26×10^{-5} °C⁻¹) is close to that observed for other feldspars, sanidine in particular, and occurs predominantly along a^* . The electron-density at the Pb site evolves with temperature toward a bean-like configuration close to that observed in disordered lead feldspar. The average Pb position approaches the *c*-glide plane with increasing temperature. Consequently the intensity of the *b*-type reflections reduces dramatically without evidence of an increase of Al-Si disorder. The evolution of atomic displacement parameters of the Pb atom with temperature supports the view that at room temperature Pb shows considerable positional disorder. Dark-field in situ TEM observations show that *b* antiphase domains (APD) persist unchanged in shape and size up to T = 690 °C. No diffuse component appears in *b*-type reflections in SAD patterns up to 935 °C, showing that the above changes in the Pb configuration do not affect the APD. The results suggest that, at T > 700 °C, Pb reaches the glide plane assuming a configuration that may favor the Al-Si disorder.