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LETTER

High-pressure phase transition in clinochlore: II*a* polytype stabilization

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ABSTRACT

Structural variations of natural clinochlore with pressure have been studied by in situ single-crystal X-ray diffraction (XRD) in a diamond-anvil cell in the pressure range 0–20 GPa at room temperature. High-resolution XRD data allowed for the identification of a polytypic phase transition at about 9 GPa. Around 4.32(5) GPa, the unit-cell parameters exhibited a significant deviation from linear behavior, particularly the *c* and β values, abruptly interrupted when the phase transition occurs. XRD patterns showed a drastic reduction of diffuse scattering due to the stabilization of the high-pressure structure, suggesting that the atomic reorganization of the layers led to a disorder reduction. The phase transition showed complete reversibility during the experiment. Ab initio structural refinements identified the transition as polytypic, from the initial II*b*-4 triclinic polytype (space group $C\bar{1}$) to the II*a*-1 monoclinic structure (space group *C*2/*m*), with unit-cell parameters $a = 5.2058(6)$ Å, $b = 9.0208(4)$ Å, $c = 13.560(7)$ Å, $\beta = 97.34(3)°$. The latter was theoretically derived in the 1960s as the least stable chlorite polytype but has never been observed in natural chlorites. The phase transition also has a significative effect on the bulk modulus, with a reduction from $K_0 = 81.2(13)$t to $K_0 = 56.0(6)$ GPa for the high-pressure structure. An isothermal run at 600 K from ambient pressure to 14 GPa showed the same phase transition at 7.8(5) GPa. Its occurrence at lower pressures suggests a negative *P*/*T* slope for the transition. Therefore, at high-temperature and high-pressure conditions compatible with impact phenomena, the polytypic phase transition could prevent chlorite from early destabilization and dehydration.

Keywords: Chlorite, high pressure, single crystal, phase transition