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A high-pressure polytypic transformation in type-I chlorite

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ABSTRACT

The compressional behavior of a natural chromian-clinochlore-I*a* polytype has been studied by synchrotron powder X-ray diffraction to 8 GPa at 298 K under hydrostatic conditions. A reversible polytypic transformation occurs at 6 GPa from the I*a*-4 to a I*b* polytype in which all *a*-type interlayers are converted to *b*-type by sheet translation across the interlayer, thus removing the high degree of cation superposition between the brucite-like sheet and the adjacent 2:1 layer that is associated with *a*-type interlayers. The isothermal bulk modulus for the I*a* polytype to 5.9 GPa was determined by fitting pressure-volume data to a second-order Birch-Murnaghan equation of state: K_0 = 78.7 ± 1.4 GPa. This value is close to that of clinochlore-II*b* (K_0 = 81 GPa). Elastic moduli for *a*, *b*, and d_{001} obtained from second-order fits to a Birch-Murnaghan equation of state are: K_{a0} = 113(5) GPa, K_{b0} = 91(2) GPa, and $K_{001,0}$ = 54(1) GPa. A possible relationship is discussed between the 6 GPa polytypic transformation observed in chromian-clinochlore and the non-polytypic transformation at 9 GPa in clinochlore-II*b* reported recently. Both transformations are dominated by contraction of the interlayer, with negligible in-plane compression of the polyhedral sheets. Both may also involve an increase in oxygen close-packing across the interlayer. However, in chromian-clinochlore, the destabilization of *a*-type interlayers is a further significant structural factor that may cause the transformation to occur at a lower pressure. Both transformations also involve an increase in the compressibility of chlorite. Although the transformation in chromian-clinochlore is influenced by the vertical superpositions of cations across the *a*-type interlayer, the hydrogen bonding is robust and does not reorganize until a considerable pressure (6 GPa) is reached.