Superspace description of brownmillerites and layered brownmillerites

H. Krüger
Institute of Mineralogy and Petrography, University of Innsbruck, Austria
E-mail: Hannes.Krueger@uibk.ac.at

Brownmillerite-type materials exhibit a wide range of structures, which vary in the arrangement of tetrahedral chains. In brownmillerites perovskite-like layers of octahedra alternate with layers of tetrahedral chains. The tetrahedral chains can adopt two mirror-related configurations, which allow different inter- and intra-layer ordering patterns to form. The simplest of which result in space groups \( \text{Pnma} \) and \( \text{I2mb} \).

High-temperature modifications of the brownmillerite solid solution series \( \text{Ca}_2(\text{Al},\text{Fe})_2\text{O}_5 \) show modulated intra-layer order, which exhibits commensurate or incommensurate sequences depending on composition and temperature [1-3]. All structures of this series can be described using the superspace group \( \text{Imma}(00\gamma s0) \).

D'Hondt et al. [4] found an alternating intra-layer sequence in \( \text{Sr}_2\text{Fe}_2\text{O}_5 \), which allows stacking faults and various stacking sequences, which are all covered by superspace group \( \text{I2/m}(0\beta\gamma\beta 0) \).

We observed diffuse scattering related to stacking faults in layered brownmillerites \( \text{Ca}_4(\text{Fe},\text{Al})(\text{Mn},\text{Ti})\text{O}_9 \), which exhibit separated blocks (OTO) of the brownmillerite structure. Similar to \( \text{Sr}_2\text{Fe}_2\text{O}_5 \) [4], the layered brownmillerites show a certain degree of order according to superstructures with different stacking sequences, as evident by electron diffraction experiments. All possible superstructures can be described using superspace group \( \text{A2}_1/m(0\beta\gamma\beta 0) \) with different modulation wave vectors.

As shown by these examples, the superspace approach is a powerful tool to unify the description of brownmillerites, layered brownmillerites and their superstructures.

References