LAYERED STRUCTURES: EXAMPLE OF DISORDER

by

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Three examples of layered structures from the authors recent work will be presented. All structures show disorder due to stacking fault mechanisms.
The first example, is the *layered brownmillerite* $Ca_4Fe_2Mn_{0.5}Ti_{0.5}O_9$. This material shows strong one-dimensional diffuse scattering (Fig. 1). A simulation study revealed the stacking fault mechanism and using high-resolution transmission electron microscopy the faults could be imaged (KRÜGER et al., 2011).

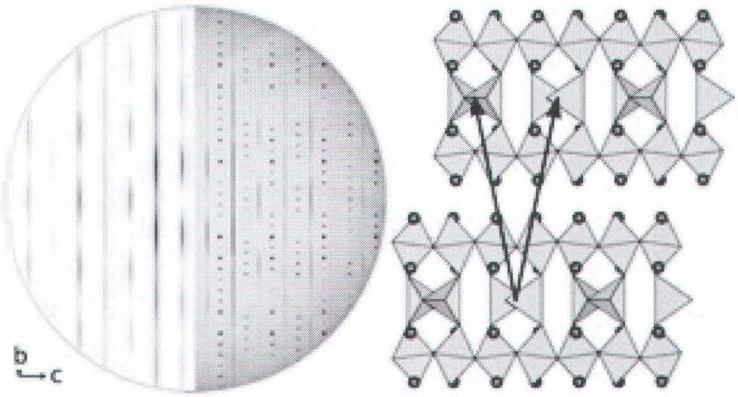

Figure 1:
Left side: a combination of calculated (left, Bragg scattering neglected) and observed (right) diffraction patterns (3kl) is shown. The right side shows two brownmillerite layers with alternative stacking vectors.

Potassium aluminate KAl_9O_{14} exhibits a mullite-type structure. In single crystals grown from a vapour phase, we found a monoclinic superstructure which causes a complex nano- and micro-structure due to multiple twinning and stacking faults (Fig. 2, LAZIĆ et al., 2013).

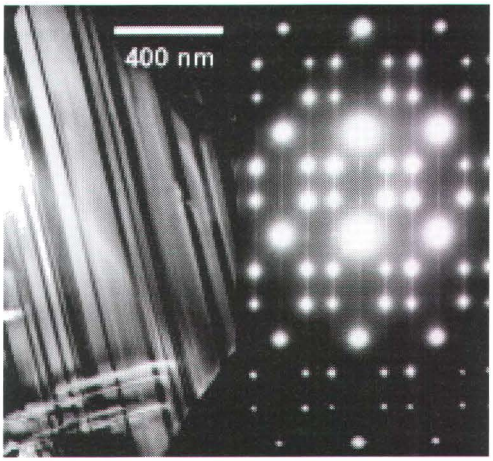

Figure 2:
TEM of monoclinic KAl_9O_{14}: electron micrograph (left) showing the nano-sized twin domains, and electron diffraction pattern [010] (right) with super-structure reflections and diffuse scattering.

The third example highlights an interesting case of stacking faults in an ordered aluminosilicate framework structure: the monoclinic kalsilite phase $KAlSiO_4$-O1 (KREMENOVIĆ et al., 2013). Our recent results revealed that the stacking faults are related to non-stoichiometry with silicon excess and potassium vacancies according to $K_{1-x}\square_xAl_{1-x}Si_{1+x}$. The proposed stacking faults do not break the framework, however, its topology is modified at the fault planes. Pseudo-hexagonal twinning causes a complex diffuse scattering pattern (Fig. 3).

Figure 3:
Reciprocal space section hk0 of non-stoichiometric $KAlSiO_4$-O1. Strong one-dimensional diffuse scattering with twin-related additional directions.

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