

more than one (direct) lattice element exists which is quasi-perpendicular to the twin element, where "quasi" mean within the accepted limit on the obliquity. In a hybrid twin, each sublattice is responsible for a partial restoration of the lattice nodes; the degree of approximation of this restoration differs for each sublattice and is directly related to the obliquity of each sublattice. The overall restoration is measured by the *effective twin index*, which is the ratio of the multiplicity of the cell of the sublattice with higher index and the number of lattice nodes quasi-restored by all the concurrent sublattices [3]. In the case of the Saint Andrews twin, there are two lattice planes quasi-perpendicular to the [313] twin axis.

- (231), corresponding to an index of 12 and an obliquity of  $0.90^\circ$ ;
- (352), corresponding to an index of 10 and an obliquity of  $6.21^\circ$ .

When these sublattices, which are both monoclinic, are taken into account, two nodes out of the 12 in the cell defined by [313] and (231) are quasi-restored, although with different obliquity, and the effective twin index is 6. The degree of lattice restoration is therefore comparable to that of the Greek cross twin.

[1] Donnay, J.D.H., Donnay, G. (1983). *Tschermaks Min. Petr. Mitt.*, 31, 1-15.

[2] Nespolo, Ferraris, G (2007). *Acta Cryst.* A63, in press.

[3] Nespolo, Ferraris, G (2006). *Acta Cryst.* A62, 336-349.

#### MS41 P09

**MXL – a program for analysis of mix-layered structures** Max Nickolsky<sup>a</sup>, Victoriya Krupskaya,<sup>a</sup>  
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**Keywords: mixed-layer structures, X-ray diffraction, modular crystallography**

A method of identification and evaluation of the main probability parameters characteristic of mixed-layer structures, with no need for more than a good tracing of the basal reflections were suggested by Djakonov [1].

The method is based on the analysis of so-called Z-function. Physically Z-function is the self-convolution of electron density. Thus Z-function is proportional to 1-dimensional Patterson function such that its value at each point  $z$  is proportional to the product of the electron densities in planes separated by the distance  $z$ . Z-function presents principle and secondary maxima. For mixed-layer structures Z-function contain principle peaks if  $z$  is equal to the distance between identical layers. Positions and the heights of the secondary peaks depend to the internal structure of the layers. Analysis of the Z-function for mixed-layer structures is complicated by the secondary peaks which can overlap with principal peaks.

Accurate interpretation of Z-function provides information about type of layers, their relative concentration and way of alteration in the mixed-layer mineral.

MXL software package which calculate and interpret Z-function has been developed. The only required data is the set of integral intensities and positions of the reflections on the X-ray profile. Experimental data is corrected by Lorentz factor. Output data contain Z-function values for given thickness, positions of the principle and secondary maxima, probability parameters characteristic of mixed-layer structure.

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[1] Djakonov J.S., *Crystallography (in Russian)*, 1961, 6, 4.

#### MS41 P10

**Crystal chemistry of disordered layer-like oxonitridosilicates** Oliver Oeckler, Juliane A. Kechele, Florian Stadler, Tobias Rosenthal, Hans Koss, Wolfgang Schnick, *Department of Chemistry and Biochemistry, LMU Munich, Germany.* E-mail: [oliver.oeckler@gmx.de](mailto:oliver.oeckler@gmx.de)

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Oxonitridosilicates have received remarkable attention owing to their suitability as host lattices for rare-earth doped phosphors in light-emitting diodes [1]. The luminescence properties of the compounds  $\text{MSi}_2\text{O}_2\text{N}_2$  ( $M = \text{Ca, Sr, Ba}$ ) are particularly promising [2-4]. For the profound understanding of these properties, detailed knowledge of the associated crystal chemistry is essential; however, numerous real structure effects complicate its investigation.

Unlike oxosilicates, layered structures such as those of  $\text{MSi}_2\text{O}_2\text{N}_2$  [5, 6] exhibit highly condensed  $\text{SiO}_3$  tetrahedra interconnected by  $\text{N}^{3-}$  atoms. These layers are interconnected via cations coordinating terminal O atoms of the tetrahedra. Both the cation arrangement and the silicate layers are highly pseudosymmetric. This fact gives rise to numerous real structure effects, which have been investigated in detail by means of high-resolution electron microscopy (HRTEM) complemented by the analysis of X-ray data including diffuse scattering and powder methods.

Comparable to the role of  $\text{SiO}_2$  in silicate chemistry, the defect wurtzite structure of sinoite ( $\text{Si}_2\text{N}_2\text{O}$ ) provides a basis for many oxonitridosilicates structures, and parts of it are frequently retained in complex structures. In addition, silicate layers may be interconnected by  $\text{AlN}_4$  tetrahedra, for example in the compound  $\text{SrAlSi}_4\text{N}_7$  [7]. Only a few basic structural motifs build up a number of compounds with compositions in the range  $\text{SrAl}_{\leq 1}\text{Si}_{4.5}\text{N}_{6.8}\text{O}_{0.1}$  where silicate layers are partially interconnected by additional tetrahedra as well as larger cations. Owing to pronounced pseudosymmetry and versatile modes of interconnection, all of these compounds are highly disordered. However, they possess long-range ordered average structures that are evident from sharp Bragg reflections. The disorder involves the interchange of structure parts that accept different, but similar surroundings, ultimately leading to phasoids in some cases. As evidenced by HRTEM, complex diffraction patterns can be understood assuming domain structures, polytypism, and low-dimensional defects.

[1] Mueller-Mach, R., Mueller, G., Krames, M. R., Höpfe, H. A., Stadler, F., Schnick, W., Juestel, T., Schmidt, P., *Phys. Status Solidi A* 2005, 202, 1727.

[2] Li, Y. Q., de With, G., Hintzen, H. T., *Chem. Mater.* 2005, 15, 4492.

[3] Li, Y. Q., Delsing, A. C. A., de With, G., Hintzen, H. T., *Chem. Mater.* 2005, 17, 3242.

[4] Bachmann, V., Jüstel, T., Meijerink, A., Ronda, C., Schmidt, P. J., *Journal of Luminescence* 2006, 121, 441.

[5] Höpfe, H. A., Stadler, F., Oeckler, O., Schnick, W., *Angew. Chem. Int. Ed.* 2004, 43, 5540.

[6] Oeckler, O., Stadler, F., Rosenthal, T., Schnick, W., *Solid State Sci.* 2007, 9, 205.

[7] Stadler, F., *Ph. D. thesis*, LMU Munich, 2006.