Simulation of a Polytypic Family from an Incommensurately Modulated Member

Alla Arakcheeva, Gervais Chapuis, *Laboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne. BSP, CH-1015 Lausanne, Switzerland.* E-mail: Alla.Arakcheeva@epfl.ch

The superspace formalism is applied in order to simulate a polytypic family from the structure of an incommensurately modulated member.

The complete set of structure characteristics (symmetry, unit cell parameters and atomic coordinates) of both periodic and aperiodic members can be generated from the incommensurate structure by changing the value of the modulation vector $\boldsymbol{q}$.

One of the interesting properties of the aperiodic structure is to present the full spectrum of the crystal chemical information (*e.g.* interatomic distances, tilts and displacements of rigid building units and rules defining the sequence of layers) for the most probable members of the polytypic family, respectively for the most probable values of the modulation vector $\boldsymbol{q}$.

These conclusions are illustrated on the basis of the incommensurately modulated phase β-$K_5Yb(MoO_4)_4$. The simulated structures of the highest-temperature phase α ($\boldsymbol{q}$ = 1) and the lowest-temperature phase γ ($\boldsymbol{q}$ = 1/2) show a good agreement with the corresponding experimental data [1].

[1] Morozov V.A., Lazoryak B.I. et al., *J. of Solid State Chemistry*, 2003, **176**, 76-87.

Keywords: polytypes, incommensurate modulated structures, crystal structure prediction