

### **Refinement of Partially Disordered OD Structures**

Jiří Hybler<sup>a</sup>, Slavomil Ďurovič<sup>b</sup>, <sup>a</sup>*Institute of Physics, Academy of Sciences of the Czech Republic, Prague.* <sup>b</sup>*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava.* E-mail: hybler@fzu.cz

In the diffraction pattern of OD structures two kinds of reflections can be distinguished: (i) Family reflections represent the Fourier transform of the so called family structure: a fictitious structure comprising all possible positions of OD layers superimposed with equal probability. They are always sharp, even for totally disordered crystals, and common for all polytypes of the family. (ii) Non-family, or polytype reflections, characteristic for a given polytype. These are sharp only for ordered (3D periodic) polytypes, otherwise they are more or less smeared out into diffuse streaks [1]. For partially disordered crystals, the intensities of the non-family reflections are underestimated due to their diffusivity and the moduli of their structure factors are reduced by a common factor.

If both kinds of reflections are constrained on the same scale in the refinement process, spurious "ghost" peaks can appear on the Fourier map [2]. These peaks are in fact residuals of the family structure. The structure can be in most cases successfully refined if separate scale factors are assigned to either of the two kinds of reflections [3]. Several artificial and real examples are presented in order to demonstrate how various degree of disorder affects diffraction pattern, Fourier maps, and structure refinements.

[1] Ďurovič S., *International Tables for Crystallography*, 1999, C, 752-765. [2] Nespolo M., Ferraris G., *Eur. J. Miner.*, 2001, **13**, 1035-1045. [3] Ďurovič S., Hybler J., Kogure T., *Clays Clay Min.*, 2004, **50**, 613-621.

**Keywords: OD structures, polytypism, fourier methods**