Oral presentation

One dimensional diffuse scattering and homometry

B. Stöger[1]

[1]*X-ray center TU Wien, Getreidemarkt 9, 1060 Wien, Austria*

bstoeger@mail.tuwien.ac.at

Homometric structures are distinct structures that possess the same weighted vector-distance set [1]. Pairs of homometric structures therefore cannot be distinguished by classical diffraction experiments. Actual examples of homometric structures have been described for polytypes, *i.e.* structures built of the same layers arranged in different ways [2]. However, these are exceedingly rare in periodic polytypes, because typically homometry only appears for long stacking sequences. For example, for the dense packings of spheres, only polytypes of period 15 or more feature homometry [3]. In contrast, for disordered polytypes, which feature one-dimensional diffuse scattering, very simple and realistic growth models may result in homometry.

Recently, we modelled the diffuse scattering of a (POCOP-^{t}Bu)CrBr crystal (Fig. 1) using a two-neighbor growth model (Fig. 2).

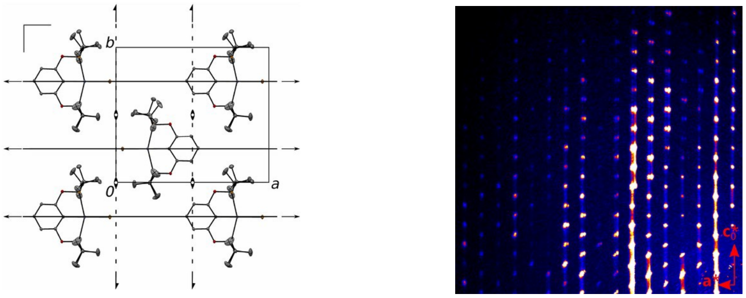

Figure 1. Left: layer in the structure of (POCOP-^{t}Bu)CrBr with *pbmm* (pseudo-)symmetry. Right: One-dimensional diffuse scattering in the $k = 5$ plane of reciprocal space.

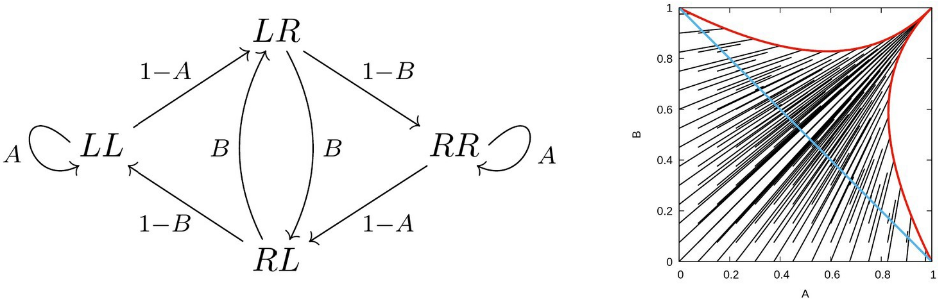

Figure 2. Left: Two-neighbor growth model with transition probabilities A and B (L and R are translations with $+\mathbf{a}/4$ and $-\mathbf{a}/4$ components, respectively). Right: Homometric pairs (A, B) connected by black line segments. The blue line represents parameters degenerating to a single-neighbor model.

It is shown mathematically that distinct (A, B) pairs of the parameters produce distinct structures with the same diffraction pattern and thus can be considered as homometric. A definition of structural equivalence and homometry in the case of disordered layer structures is proposed. Moreover, it is shown how desymmetrization (small deviations from the ideal model) can break homometry. Even in that case it has to be stressed that the parameter landscape possesses practically identical local minima, making the analysis of such structures treacherous. It is therefore suggested to use global searches such as the MCS algorithm [4] to locate all the minima.

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