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Diffuse single crystal scattering corrected for molecular formfactor effects

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The determination of the average structure of a crystalline material via analysis of Bragg scattering data has long since become a routine method, at least for materials with moderate complexity. No technique equivalent to direct methods has been established to date for the analysis of disordered crystalline materials. For full data analysis the weaker diffuse scattering in between the Bragg peaks has to be considered.
We show that chemical short range order (SRO) in two component molecular crystals can be solved directly by separating the influence of the molecular form factor from the diffraction pattern. This is demonstrated by analyzing the diffuse scattering of tris-tert-butyl-1,3,5-benzene tricarboxamide.
For our development [1] we used the theoretical model for SRO in two component systems:
$I(h_1,h_2,h_3) = Nm_1m_2|f_1-f_2|^2(1+\Sigma_{lmn}\alpha_{lmn}\cos(2\pi(h_1l + h_2m + h_3n)))$
Here I is the diffuse intensity due to SRO, which is a function of the reciprocal space coordinates h_1 h_2 and h_3. The crystal consists of N atoms/molecules of species 1 and 2. m_1, m_2 and f_1, f_2 are the respective concentrations and atomic/molecular form factors of the species. The summation over lmn is a summation over all interatomic vectors, and the α_{lmn} are the Warren-Cowley SRO parameters.
For simple materials with a primitive unit-cell where only one site is occupied, the diffuse scattering can simply be divided by the absolute molecular form factor difference squared $|f_1-f_2|^2$. A consecutive projection into one reciprocal unit cell allows a linear regression algorithm to obtain the α_{lmn}.
The suggested algorithm was tested on the diffuse scattering of tris-tert-butyl-1,3,5-benzene tricarboxamide. The data was taken from [2] with kind permission. The results obtained by the division and projection algorithm are in very well agreement with the results from the 3D-ΔPDF analysis performed with YELL [2].
The suggested algorithm requires prior knowledge of the exact molecular form factors, hence it is necessary to obtain excellent results form the average structural refinement. Often it is not possible to distinguish disordered side groups in the average structure refinement. Therefore it is possible, that the exact molecular form factors cannot be calculated given the average structure refinement. The division of the data by an average atomic form factor and the consecutive projection into one reciprocal unit cell allows the determination of the SRO parameters nevertheless. This was also tested with the diffuse scattering of tris-tert-butyl-1,3,5-benzene tricarboxamide and the resulting SRO parameters coincide for both techniques. This opens up new opportunities in the average structure refinement, similar to what is demonstrated by Chodkiewicz et al. in [3].
The projection algorithm suggested for data analysis is fast and does not require starting values for the fit of the SRO parameters. Furthermore the algorithm is robust against incomplete data sets, which makes the algorithm a powerful tool, that can be applied to a wide variety of disordered materials.
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