Mean field theory calculations to model single crystal diffuse scattering

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Correlated disorder in crystalline materials gives rise to single crystal diffuse scattering. While the average structure determination via Bragg data analysis is considered a standard procedure, disorder analysis is thought of as a lengthy and complicated process. We present a mean field approximation to model single crystal diffuse scattering in molecular materials from a simple pair-interaction Hamiltonian.

Mean filed theory is a self-consistent field theory, which is widely used in statistical physics to model high-dimensional random systems. It has proven a valuable tool in the analysis of magnetic diffuse scattering data [1]. Here, the formalism is applied to describe orientationally disordered molecular crystals,.

We present a computational study based on the mean field model suggested by Naya [2] and proof its applicability to strongly correlated disorder, where the local building block geometry dictates allowed and prohibited local configurations. The system that will be analysed in detail is a two-dimensional analogue of $Hg(NH_3)_2Cl_2$ as depicted in Figure 1 (a) [3]. The Hg atoms are disordered over the cubic face centres to form $[H_3N - Hg - NH_3]^{2+}$ molecules. The local arrangement is strictly dictated by these building rules.

We compare the results of the diffuse scattering analysis using the mean field model as introduced by Naya [2] to the results of RMC modelling and ΔPDF models based on a Warren-Cowley short range order parameter refinement (see Figure 1 (b)). Finally, the stability of the mean field analysis on limited data availability is demonstrated: Diffraction experiments under pressure or electric field yield a limited reciprocal space coverage. Here, we demonstrate the robustness of the proposed method against incomplete data sets.

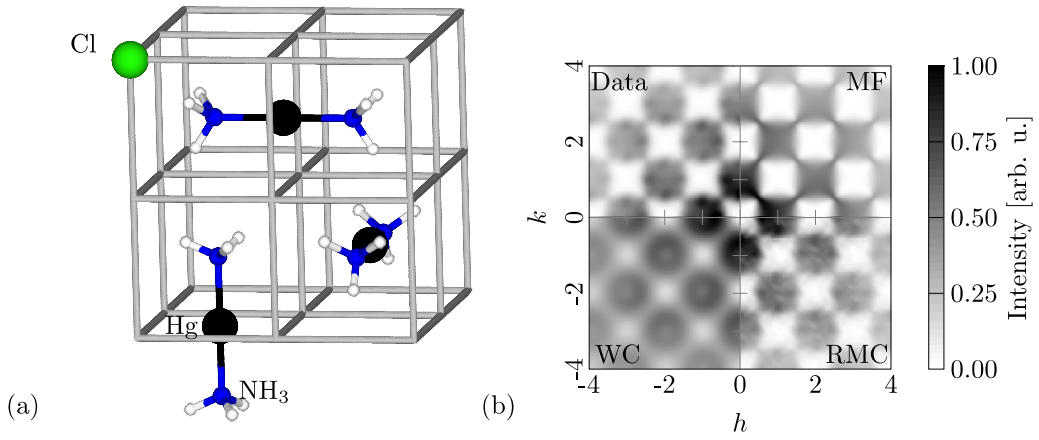

Figure 1. (a) $Hg(NH_3)_2Cl_2$ [3], where the Hg is disordered over the cubic face centres. (b) Simulated data for a two dimensional analogue compared to refinements using mean field theory (MF), ΔPDF analysis for the Warren-Cowley short-range order parameters (WC) and reverse Monte Carlo modelling (RMC).

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