Diffuse scattering in protein crystals is dominated by rigid body motions.

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There is an ongoing debate on the origin of diffuse scattering arising from protein crystals in X-ray diffraction experiments. Although, many types of diffuse scattering from crystals can be observed, it is the cloudy diffuse scattering that is the subject of interest for protein crystals. While already in the 1980s different views were brought forward as to its cause, this discussion has revived in recent years, not the least because of advancements in equipment and computer resources. Two opposing views are prominent: either the diffuse scattering is caused by internal molecular motions on different size and time scales, or by overall whole molecule motions.

We modelled diffuse scattering for cyclophilin A (CypA) and HEW lysozyme by well-defined ensembles of molecules representing translational, rotational and internal motions. Amplitudes of the various motions were based on B-factors from structural refinement against Bragg reflections.
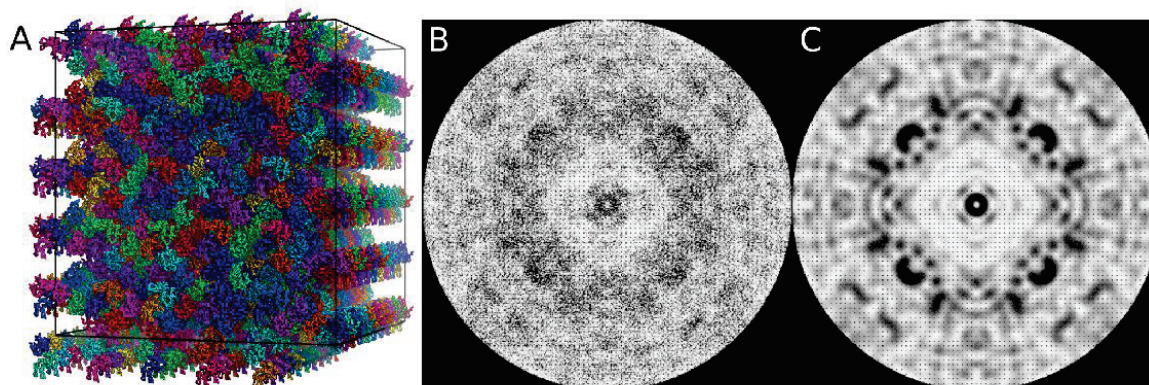
We developed a supercell approach [1], by which we can calculate diffuse scattering in between Miller indices of the lattice. The pixel resolution of experimental data for CypA [2] and lysozyme allows such oversampling of reciprocal space and was used to generate 3D diffuse maps. Global 3D features of these maps and speckle size agree largely with the maps from rigid body motion models. Although we included internal motions in our models, rigid body motions and especially translation, dominates the diffuse scattering as the movements of all atoms are fully correlated.

[1] T. de Klijn, A.M.M. Schreurs and L.M.J. Kroon-Batenburg (2019), IUCrJ, 6, 277-289. https://doi.org/10.1107/S2052252519000927

[2] Fraser, J. S. (2015), SBGrid Data Bank, http://dx.doi.org/10.15785/SBGRID/68