MS38 Computations with/for Pair Distribution Functions

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Most recent development big box modelling in RMCProfile7

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Abstract

Big box modelling of Pair Distribution Function (PDF) is becoming more and more popular and powerful tool to describe local structure of materials. To a large extent this id because it allows move freely and create a structure having non-symmetry restrained distortions. Therefore, this enable the solution which complies both the average structure (as obtained from Bragg diffraction data) and local order/disorder as obtained from Pair Distribution Function. In order to follow the increasing need in the PDF analysis tools, we are currently implementing new capabilities in new RMCProfile7 program. This piece of software grown out from very well-known RMCProfile6, gives multiple of new capabilities implemented very recently.

Here, we present new functionalities which are now available in RMCProfile7:

1. Multiple phase refinement
2. Variety of experimental dataset types (real space, reciprocal space, Bragg)
3. Multiples of datasets of the same type (i.e. multiple of Bragg datasets, joint X-Ray and neutron refinements)
4. Real space data calculation also possible as back Fourier transform of reciprocal space data
5. Variety of constraints (minimum distance, moveout) and restraints (bond valence sum; broad variety of potentials – bond, angles, torsion angles, inversion angle, planarity, planar rings; tails)
6. Multiple atom type swaps, fully compatible with all constraints/restraints
7. Implementation of molecule type move (collective move, rotation and/or swap for a rigid molecule or rigid group of atoms)
8. Implementation of Bragg profile calculation based on GSAS-II program for both X-ray and neutron time of flight data
9. Scale and offset refinement, also background for Bragg datasets

RMCProfile7 is freely available in beta form on https://rmcprofile.pages.ornl.gov/