Poster

BIG BOX modelling of Pair Distribution Function using RMCProfile7 program

W. A. Sławiński

University of Warsaw, Faculty of Chemistry, Pasteura 1 Street, 02-093 Warsaw, Poland

wslawinski@chem.uw.edu.pl)

Nowadays, scientists have to work on more and more complicated materials. Description of crystal structures in terms of average structure as obtained from Bragg diffraction data analysis is no longer enough to understand material properties. Pair Distraction Function (PDF) is its natural extension and allows us to look deeper into the real (= both local and average) structure of materials. Big box modelling of PDF is currently the best method to understand local arrangement and/or short-range correlations of atoms without assuming any symmetry related constrains.

Here, I present the most recent development in the field of RMCProfile7 program and also some successful examples where only by using those new developments in the code new insight into the local structure could have been obtained.

The beauty of RMCProfile7 program and large box modelling is that it combines average structure modelling and local structure disorder and enables to find global minimum which gives a good picture of both avenge and local view of the same structure.

The most recent development of RMCProfile7 includes:

- Multiple phase refinement – useful for complex or mixed phases
- Multiples of datasets (i.e. multiple of Bragg datasets, joint X-Ray and neutron refinements, different PDF representations)
- Real space PDF calculation as a back Fourier transform of reciprocal space data – very useful for X-Ray PDF and neutron lower instrumental Qmax datasets
- 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) which enables more physical atomic configurations or fasted convergence to global minimum
- Molecular type moves (rigid body or molecular)

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

More detailed description of the program can be found in just accepted paper [1] in Journal of Applied Crystallography.

[1] Sławiński, W.A., Keer, C.J., Zhang Y.,Playford H.Y., Dove M.T., Phillips A.E., Tucker M.G., (2024) *Journal of Applied Crystallogrphy, accepted.*

RMCProfile7 development has been partially supported by National Science Centre of the Republic of Poland: Opus Project 2018/31/B/ST4/00943.