Average Patterson analysis of disordered structures

Dariusz Orzechowski and Janusz Wolny

Faculty of Physics and Nuclear Techniques,
AGH University of Science and Technology,
al.Mickiewicza 30, 30-059 Krakow, Poland

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The diffraction pattern of ideal crystals is discrete - consists of separated Bragg peaks. On the other hand it is known that diffraction of amorphous materials (as well as liquids) leads to continuous diffraction pattern due to structural disorder. In fact, diffraction always leads to this continuous component because of phonons, phasons and structural defects. Besides, there is a big class of materials that are not perfectly crystalline nor perfectly amorphous, e.g. polymers. Diffraction pattern of such materials consists of three components: background, crystalline and amorphous.

Classic crystallographic approach based on concept of unit cell and reciprocal lattice fails if unit cell doesn't exist. It has been shown that diffraction pattern of such structures may be described in average unit cell approach based on reference lattice concept. This approach has been used to calculate diffraction pattern of model one-dimensional disordered structures.

Inverse problem (i.e. determination of structure given its diffraction pattern) is still unsolved in general case. One can nevertheless obtain certain amount of information about structure calculating so-called average Patterson function. This approach has proven so far successful if used to describe perfect quasicrystals and modulated structures. Numerical calculations have been performed to check this approach when applied to disordered structures.

[1] Wolny, J., Philos.Mag. A **77**, 395-412, (1998)