Poster

Quarter century of the statistical method in crystallography

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Higher-dimensional crystallography first introduced to modulated crystals by de Wolff, Janner, and Janssen is about to celebrate 50 years. The discovery of quasicrystals by Dan Shechtman recently celebrated 40 years. Also, just above 25 years ago the first paper on the statistical method with a concept of the average unit cell was published [1,2], the date since a real-space analysis of quasicrystals and other aperiodic systems was introduced. The basic idea behind the AUC approach is to describe the aperiodic system in real space (3D), rather than going to high dimensions. Atoms (replaced by atomic surfaces in multidimensional crystallography) are represented here by statistical distributions of positions calculated with respect to some reference grids. The structure factor is obtained by a Fourier transform of the distributions [3].

Since its development, the AUC approach has found its application to structure and diffraction description of modulated crystals, aperiodic sequences (like Thue-Morse sequence without Bragg-like diffraction spectrum), cluster aperiodic coverings, decagonal and icosahedral quasicrystals. About 10 quasicrystalline structures were refined in real space. The AUC method due to its functioning in the real space found also a very good application in modeling disorder (phonons and phasons) in quasiperiodic systems. Recently, the concept of avoiding high dimensions was transferred to special relativity, where it was shown that all relativistic phenomena can be obtained by Newtonian dynamics (in 3D) of variable-mass systems with no need of going to 4-dimensional Minkowski spacetime.

In this poster presentation, the 25 years of crystallography of aperiodic systems in real space will be briefly summarized with the most prominent examples of its successful application presented [4].

[4] Wolny, J. (1998*) Phil. Mag. A***77**, 395.

[5] Wolny, J. (1998) *Acta Cryst. A***54**, 1014.

[7] Strzalka, R., Buganski, I., Wolny, J. (2016) *Crystals* **6**, 104.

[6] Wolny, J., Buganski, I., Strzałka, R., Smietanska-Nowak, J., Wnek, A. (2024) *Isr. J. Chem.* (published online)