MS23-1-1 Quasicrystalline structure modelling with the statistical method
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Abstract
Since the discovery of quasicrystals, the higher-dimensional method was extensively used to model the atomic structure of quasicrystals and refinement. The basic idea behind this method is a considering of a quasicrystal as a multidimensional object with periodicity. Only by projecting it on the 3D real space, a quasiperiodic arrangement of atoms is obtained. Higher-dimensional method combined with a cluster approach was used to model a vast majority of quasicrystalline systems [1]. An alternative method, named a statistical method, working in real space only and making use of the concept of the average unit cell, was proposed [2]. Results of using both methods are equivalent to some extent, but some differences, e.g., in modelling structural defects, may appear [4].
Over the last years, the statistical method has found its application in the structure refinement of numerous decagonal and icosahedral quasicrystals (e.g., [1, 2] or very recently [3]). For the very last result of icosahedral CdYb phase, no assumptions on the cluster type were not made, but only 3D Penrose quasilattice was used to refine the structure. In addition, the influence of phasonic flips on the atomic structure at high temperatures was recently discussed. Finally, the macromolecular system with modulation of the atomic positions was investigated [ASIA].
In this presentation, a short introduction to the statistical method will be followed by some exemplar applications of the approach to real systems, including modelling of phonons and phasons.

References
[1] W. Steurer, Acta Cryst. A 74 (2018) 1.
[2] J. Wolny, B. Kozakowski, P. Kuczera, R. Strzalka, J. Wnek, Isr. J. Chem. 51 (2011) 1275.
[3] R. Strzalka, I. Buganski, J. Wolny, Crystals 6 (2016) 104.
[4] J. Wolny, I. Buganski, P. Kuczera, R. Strzalka, J. Appl. Cryst. 49 (2016) 2106.
[5] P. Kuczera, J. Wolny, W. Steurer, Acta Cryst. B 68 (2012) 578.
[6] I. Buganski, J. Wolny, H. Takakura, Acta Cryst. A 76 (2020) 180.
[7] I. Buganski, R. Strzalka, J. Wolny, et al., in preparation.
[8] J. Smietanska, J. Sliwiak, M. Gilski, Z. Dauter, R. Strzalka, J. Wolny, M. Jaskolski, acta Cryst. D 76 (2020) 653.