MS27- Quasicrystals: theory and experiment

Chairs: Prof. Marc de Boissieu, Prof. Janusz Wolny

MS27-P01

AlCuRh decagonal quasicrystal – new techniques for the refinement

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Quasicrystals are still challenging when it comes to the structure refinement. The complexity of the structure requires the use of sophisticated mathematical models to properly describe the structure. In addition, the range of diffraction peaks' intensities is wide with small peaks especially being affected by multiple disorder effects which are still not included in the refinement. What is important those small peaks carry essential structural information and without them the structure model cannot be considered correct. Recently we invented and applied a variety of new models [1, 2] to describe the structure of decagonal AlCuRh quasicrystal. The quality data allows us to test which approach could be beneficial for the refinement. We testes new phononic correction assuming local statistical deviation obeying sinusoidal oscillations resulting in the Bessel function in the Foureir space. We also included phason flips in the quasilattice of the Penrose Tiling, providing long-range order, to correct for the deviation of the structure units locations. Last but not least, we phenomenologically included the effect of the multiple scattering which appears to be a significant effect in terms of weak reflections. All those corrections have proven to improve the quality of agreement between theoretical model and the experimental data. In the best fit we could obtain an R-factor equal to 5.84%, which is the best result yet for the quasicrystal. In the presentation we explain the reasons for the application of each corrective term and the effect on the final structure model.

References:

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MS27-P02

Statistical method of structural description of complex systems

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The statistical method is a commonly approved and confirmed by many results approach to structural and diffractional studies of crystals. It is particularly successful in terms of complex systems, like modulated crystals or quasicrystals. In our presentation we will show the fundamentals of the method, including the basic concept behind – called the average unit cell concept [1], and discuss its application to modulated crystals and quasicrystals [2,3].

The average unit cell is the probability distribution function P(u) of atomic positions calculated against some periodic reference lattices. A Fourier transform of P(u) gives the diffraction pattern. Structural modeling within the statistical approach involves a modeling of the P(u) distribution, which is an object in physical space, and enables including all kinds of structural disorder in a derivation of the structure factor. We will show how this methodology applies for the harmonically modulated crystal (with harmonic modulation and incommensurate scattering vector), including its correspondence to a quasicrystal, and selected decagonal quasicrystals.

The method has no limit in applying it also to such complex systems, like proteins of macromolecules, where the structural disorder appears to play a crucial role, and attempts to use crystallographic methods known for periodic crystals are rather doubtful. We will shortly introduce a possible benefits from applying the statistical method to complex organic systems.

References:

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