New techniques for the refinement of quasicrystals

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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 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. It cooperates with well-known generalized Debye-Waller formula. 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 yes 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.

1. Wolny J., Buganski I., Kuczera P., Strzalka R., J. App. Cryst., **49**, (2016), pp. 2106-2115.
2. Wolny J., Buganski I., Strzalka R., Cryst. Rev., **24**, (2017), pp. 22-64.