MS23-P01 | CORRECTION FOR PHONONS, PHASONS AND MULTIPLE SCATTERING IN QUASICRYSTALS

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In modern crystallography of quasicrystals and aperiodic systems a proper diffraction data treatment and structure refinement are still a challenge. In this presentation new approach to corrective terms to diffraction data for phonons and phasons will be discussed within a statistical method (or average unit cell method) of diffraction and structure investigation of aperiodic systems. Both phenomena, i.e. thermal vibrations and phasonic flips of atoms, are well reflected in the shape of the statistical distribution of atomic positions in the aperiodic tiling, which makes it possible to model phonons and phasons at the stage of constructing a structure factor. In this sense, corrective terms (Debye-Waller factors) for phonons and phasons become additive terms to the structure factor with a small number of parameters to fit (for phasons it will be a probability of flips of a given kind) [1]. Also a new approach to multiple scattering effect treatment will be discussed. It is based on the Rossmanith theory and considers a redistribution of peak intensities among all reflections with a given probability (the probability parameter is to be fitted). New corrections are tested against model quasiperiodic systems and real quasicrystals [2].

[1] J. Wolny, I. Buganski, P. Kuczera, R. Strzalka, J. Appl. Cryst. **49**, 2106 (2016).
[2] I. Bugański, R. Strzalka, J. Wolny, Acta Cryst. A **75**, 352 (2019).