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The phase problem for quasicrystals in reciprocal space

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The phase problem is very well-known in crystallography and is particularly important for structure solution of quasicrystals. Structure solution (initial phasing of the diffraction pattern) is the first step of atomic structure determination against the diffraction data. Many tools for solving the phase problem in crystallography were developed over the years. Besides the pioneer Patherson function method or direct methods, also the low density elimination method and, more recently, maximum entropy method or charge flipping algorithm are widely used. We propose another way of phase recovery, directly from the diffraction pattern. It has been shown, that diffraction patterns of aperiodic structures (quasicrystals and modulated structures) consists of periodic series of peaks [1,2]. The peaks are, of course, aperiodically distributed in reciprocal space. However, the envelopes of such peaks are strictly periodic. For Fibonacci sequence the shape of envelopes is given by a sinx/x – type function. In the centrosymmetric case all peaks belonging to a given series have the same phase (0 or π). Moreover, once we rescale peak positions to obtain the reduced envelope of structure factor (intensity), we can easily find the shape of the average unit cell, by applying the inverse Fourier transform. The functionality of such approach has been shown in [3] for d-AlNiCo quasicrystal. In this paper we show a few examples of model structures with recovered phases. Decorated Fibonacci sequence, Penrose tiling and Ammann tiling are used as model structures for 1D, 2D, and 3D quasicrystals respectively. We compare the results with conventionally used charge flipping method.

[1] *J. Wolny, B. Kozakowski, P. Kuczera et al, Acta Cryst. A70, 2014, doi:10.1107/S2053273313034384.,* ***[2]*** *J. Wolny, B. Kozakowski, P. Kuczera et al, Acta Phys. Pol. A, 2014, (in press).,* ***[3]*** *B. Kozakowski, J. Wolny, Aperiodic Crystals, 2013, 125-132.*

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