s3.m11.p3 The dependence of the structure amplitude on the amplitudes of the terms of a finite harmonic expansion of the modulation function. Tamara Sliwinska, Pawel Gusin, Jerzy Warczewski, University of Silesia, Institute of Physics, ul. Uniwersytecka 4, PL-40007 Katowice, Poland. E-mail: pgusin@us.edu.pl

Keywords: Modulation function; Structure amplitude; Displacive modulation

The structure amplitude is analysed in terms of the harmonics of a modulation function for the case of a one-dimensional displacive modulation. This modulation function is expressed by a finite series of N sine functions. It turns out that: 1. for the high values of the amplitudes of the terms of a finite harmonic expansion of the modulation function the structure amplitude tends to zero for the arbitrary value of the order of the satellite reflections, 2. for certain values of the amplitudes of the harmonic expansion mentioned above the module of the structure amplitude assumes its maximum value, whereas the intensity of a satellite reflection of a given order can be expressed as a function of both the intensity of a main reflection closest to this satellite reflection and the intensities of the finite set of the satellite reflections of the lower orders, the number of these reflections depending on N.

s3.m11.p4 Average Patterson analysis of disordered structures. <u>Dariusz Orzechowski</u> and Janusz Wolny, Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, al.Mickiewicza 30, 30-059 Krakow, Poland. E-mail: orzech@fatcat.ftj.agh.edu.pl

Keywords: Disordered structures; Average unit cell; Patterson function

The diffraction pattern of ideal crystals is discrete - consists of separated Bragg peaks. On the other hand it is known that diffraction of amorphous materials (as well as liquids) leads to continuous diffraction pattern due to structural disorder. In fact, diffraction always leads to this continuous component because of phonons, phasons and structural defects. Besides, there is a big class of materials that are not perfectly crystalline nor perfectly amorphous, e.g. polymers. Diffraction pattern of such materials consists of three components: background, crystalline and amorphous.

Classic crystallographic approach based on concept of unit cell and reciprocal lattice fails if unit cell doesn't exist. It has been shown that diffraction pattern of such structures may be described in average unit cell approach based on reference lattice concept. This approach has been used to calculate diffraction pattern of model one-dimensional disordered structures.

Inverse problem (i.e. determination of structure given its diffraction pattern) is still unsolved in general case. One can nevertheless obtain certain amount of information about structure calculating so-called average Patterson function. This approach has proven so far successful if used to describe perfect quasicrystals and modulated structures. Numerical calculations have been performed to check this approach when applied to disordered structures.

[1] Wolny, J., Philos. Mag. A 77, 395-412, (1998)