MS23-P03 | FROM A SINGLE SLIT TO PERIODIC, MODULATED AND QUASIPERIODIC CRYSTALS – A NEW APPROACH TO THE DIFFRACTION ANALYSIS OF APERIODIC SYSTEMS

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Over a hundred years old diffraction analysis of periodic crystals encountered serious difficulties when trying to describe diffraction patterns of aperiodic systems. In order to restore periodicity in the direct space, a multi-dimensional approach is commonly used. In the multidimensional description, both the periodic direct space lattice and the symmetrically equivalent periodic reciprocal space lattice are defined, which allows the use of well-known classical methods of crystallography. The problem is the lack of the universality of this approach. For each case, one needs to redefine both the dimension of the space used and the so-called atomic surface in additional dimensions. The problem is complicated even for simple model structures. In addition, there are many model structures which does not become periodic in any space with a finite number of dimensions. We encounter even greater difficulties when describing the dynamics of multidimensional systems. Thus, an attempt was made to describe any structure using only physical space (3D), abandoning the concept of a direct and reciprocal lattices with associated symmetry elements. This method uses the properties of the Fourier transform and is based on calculating the appropriate probability distributions of the positions of the atoms relative to the reference lattice. Ultimately, this leads to the expression of a structural factor in the form of a multimodal Fourier transform of probability distributions. The paper will present examples of the application of this method to describe diffraction patterns of selected systems: a single slit case, periodic and quasiperiodic crystals, including modulated structures.