Keynote Lecture

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Application of Direct Methods to Inorganic Materials Characterization

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Although in the last years most attention has been paid to the development of direct methods (DM) in the macromolecular field, DM also play an important role in the characterization of inorganic materials. Very challenging is nowadays the structure solution of increasingly small crystals. Here the difficulty is not associated with the large number of atoms but with experimental limitations which may affect the data accuracy and the completeness of the data sets. It is obvious that DM have to adapt to this emerging scientific need. Particularly interesting has been the evolution of Patterson-function DM to cope with these objectives. The initial formulation based on the explicit use of triple-phase sums was modified to permit the calculation with Fourier transforms thus resulting in the more simple and accurate S-FFT algorithm [1]. Thanks to the resulting increased simplicity, this algorithm could be easily adapted to the treatment of powder diffraction data of complex inorganic materials [2]. The practical application of this algorithm is analyzed by using data of some synthetic and natural materials. Recently, the possibility of collecting good quality 3D intensity data from very small nanovolumes by new sophisticated electron diffraction (ED) techniques has become a reality. However, these data sets are often incomplete and, in addition, the intensities are not completely kinematical. The processing of these data sets represents a new challenge for DM. To this purpose a new (even more simple) Patterson-function DM (called delta-recycling) has been developed and tested on precession ED data from inorganic materials with variable degree of difficulty [3]. Phasing with delta-recycling proves to be highly efficient and from the interpretation of the results important practical conclusions can be drawn.

[1] *J. Rius, A. Crespi, X. Torrelles, Acta Cryst., 2007, A63, 131-134,* ***[2]*** *J. Rius, Acta Cryst., 2011, A67, 63-67,* ***[3]*** *J. Rius, E. Mugnaioli, O. Vallcorba, U. Kolb, Acta Cryst., 2013, A69, 396-407*

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