SEMINAIRE DE LA MATIERE CONDENSEE

Laboratoire Léon Brillouin

Professor Jordi RIUS
jordi.rius@icmab.es

Institut de Cienca de Materials de Barcelona [ICMAB]

Advances in Patterson-function direct methods and recent applications for Powder & Single-Crystal Diffraction

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Part I: 14h30 Séminaire
Part II : 16h30 Démonstration / Tutoriel de logiciels libres écrits par J.R.
Salle de conférence 15 – Bâtiment 563

Conventional direct methods are the simplest way of exploring the observed Patterson function in terms of the phases. However, the close connection between direct methods and Patterson function had remained hidden for many years probably due to the fact that individual phase relationships were used as starting point in the development of direct methods. However, this connection became evident when it was demonstrated that the incidence of the wrong *uranium-atom* solution in direct methods disappeared when the origin-peak of the observed Patterson-type function was removed[1]. Further progress in Patterson-function direct methods was later achieved by replacing the individual phase relationships by Fourier transforms, since the resulting S-FFT algorithm was more accurate and less time consuming for large structures[2]. In 2011, it was shown that S-FFT is especially well-suited for handling powder diffraction data according to a conceptually new strategy called “Cluster-based Direct Methods” which allows the active use of high resolution powder diffraction data during the phase refinement process[3]. A necessary preliminary step is the accurate decomposition of the observed pattern in intensity clusters. In this way a number of new complex inorganic, hybrid and even organic crystal structures have been routinely solved. More recently, further progress in Patterson-function direct methods has been achieved by introducing the so called delta-recycling phase refinement algorithm[4]. As the name indicates it is based on the properties of the delta function which allow expressing the (electron) density function in an uncorrelated alternate manner and hence establishing a phasing residual which can be minimized by means of the iterative delta-recycling algorithm[4]. This simple procedure was worked out using single-crystal X-ray diffraction data. To test its phasing power when intensity data are not ideal, delta recycling has been applied to electron diffraction data from nanovolumes of some selected inorganic compounds[5]. The data used had been collected with the *Automated Diffraction Technique* at the Univ. Mainz by Prof. Kolb’s group. Besides confirming the suitability of the delta recycling algorithm, other important aspects like the accuracy of the intensity data and the effect of missing reflections are also analyzed.

1 Acta Cryst (1993) A49, 406-409.
2 Acta Cryst (2007) A63, 131-134.
3 Acta Cryst (2011) A67, 63-67.
4 Acta Cryst (2012) A68, 77-81.
5 Acta Cryst (2013) A69, 396-407.

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