Session VII - Wednesday, September 2 - morning

S7-L1

CRYSALIS^{PRO} - DATA COLLECTION AND REDUCTION OF INCOMMENSURATE AND QUASI-CRYSTALS

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The origins of CrysAlis^{Pro} date back 20 years. At the 'Institut de cristallographie' in Lausanne (Switzerland) under the guidance of Prof. Gervais Chapuis we studied 1 and 2D incommensurate materials. As part of my PhD we developed a CCD detector and the software suited for incommensurate research.

Since that time CrysAlis^{Pro} underwent drastic changes, but the underlying data collection and data reduction engine is well suited for materials with up to 3 q-vectors.

The talk will describe all tools required for a successful experimentation and data reduction/analysis for incommensurate and quasi-crystals. It will explain the experimentation and data reduction workflow, comment on strategy, unit cell finding and optimization (reciprocal space visualization using Ewald^{Pro}), describe the data reduction and post correction issues, explain the binding to external programs (especially Jana2006). Furthermore the generation of 'Precession' reconstructions will be explained.

Examples will be taken from my personal research and our application work at Rigaku Oxford Diffraction.

S7-L2

IMPLEMENTATION OF MODULATED AND COMPOSITE STRUCTURES IN POWDER DIFFRACTION FILE™

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In recent years, modulated structures have attracted various scientists on account of their interesting structures and physical properties. The number of modulated structures being published is increasing steadily indicating the need

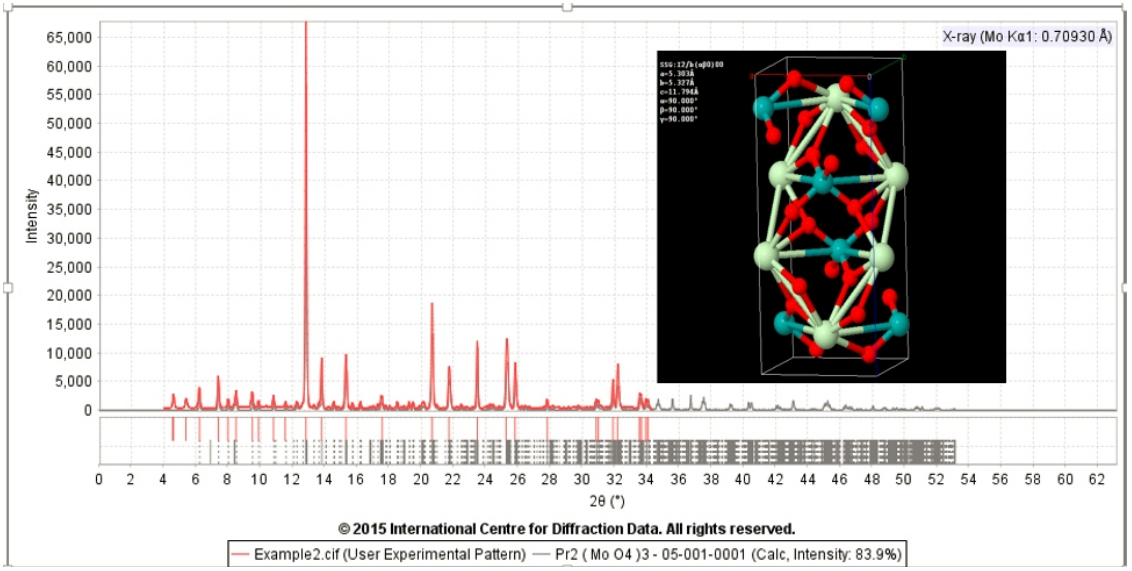

Figure 1. An example of phase identification of a modulated structure.

for a database to house them and describe them properly. International Centre for Diffraction Data's (ICDD) Powder Diffraction File™ is a powerful database for materials identification and is used extensively by the scientific community for seven decades. Starting in year 2010, ICDD took the initiative to develop a database to meet the requirement of growing scientific interest in this area of modulated structures. The number of modulated structural entries are steadily growing in the Powder Diffraction File™ since release 2011. For any quality database, a good editorial process involving stringent data validation is essential, which has been achieved by the JANA2006-ICDD suite. This presentation will emphasize the data validation procedure, exploring various type of modulated structures using the database and search/match methods. One such case study showing phase identification of a modulated structure is shown in Fig. 1.

S7-L3

SHORT AND LONG RANGE ORDER ANALYSIS (AMORPHOUS TO CRYSTALLINE) USING ELECTRON DIFFRACTION

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Understanding and possible prediction of interesting properties of a material depends upon heavily on the precise knowledge of the atomic structure of the material. The structural ordering of the material can vary from very short range ordering/no ordering (amorphous materials) to longer range ordering (crystalline materials). Transmission electron microscopy (TEM) allows to study materials with varying degree of order using Electron Diffraction (ED) techniques. Here we present how ED can be used to study materials from ordered nanoparticles to amorphous.

Materials having long range order will show always Bragg diffraction peaks. To solve their crystal structure, 3D diffraction tomography data (coupled with beam precession) can be collected on a single crystal of suitable size (40 nm -200 nm) and rotating the crystal around an arbitrary axis . Such 3D precession diffraction tomography data [1] can be analysed using software that allows semi-automatic unit cell determination and measure reflection intensities. Extracted intensities can be used to reveal all atomic coordinates in the structure.

On the other hand, any type of structural disorder/ defects may results in ED diffuse scattering and in many cases even complete disappearance of Bragg reflections (case of amorphous materials). In such cases Pair Distribution Function (PDF) analysis [2] calculated from ED data can be used very successfully to study local structural environment and the degree of long/short range order of the material (amorphous or nanocrystalline). In our work here we present two examples : one case considering NaYF4 nanoparticles where PDF analysis shows clearly existence of long range order (nanoparticle case) and in another case we consider amorphous Opal mineral where using PDF analysis only short range order is visible (until 0.8 nm). In addition, ED related techniques like ASTAR (orientation imaging in TEM) allows to analyse at nm scale precise amorphous and crystalline areas, revealing the true order of complex materials [3].

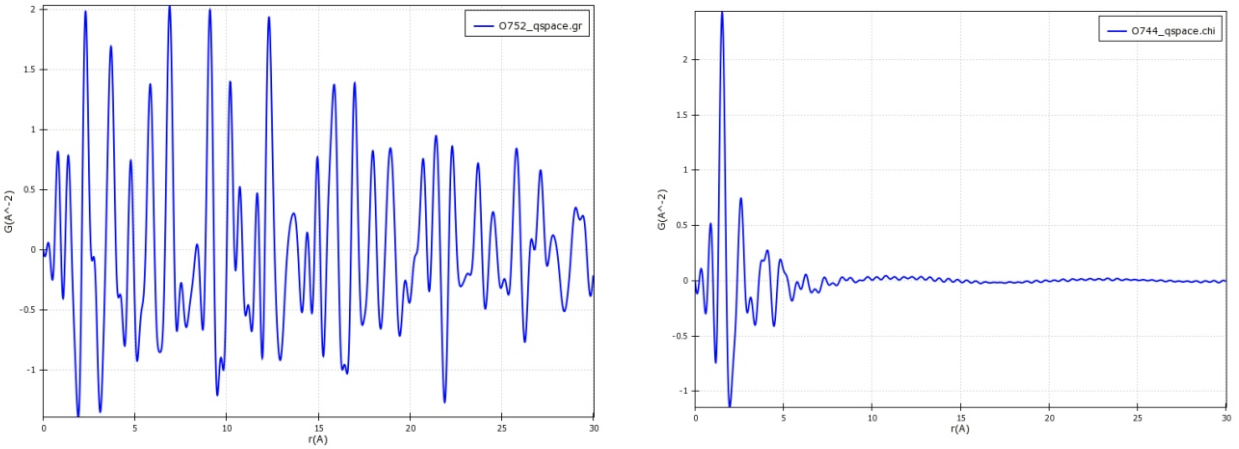

Figure 1. Pair Distribution Function for a Nanoparticle (long range order) (left image) and an amorphous opal (right image) mineral which shows only short range ordering < 0.8 nm.

1. E. Mugnaiolo, T. Gorelik, U. Kolb, *Ultramicroscopy*, **109**, (2009), 758.
2. G. R. Anstis, Z. Liu, M. Lake, *Ultramicroscopy*, **26**, (1988), 65.
3. E. F. Rauch, M. Veron, J. Portillo, D. Bultreys, Y. Maniette, S. Nicolopupos, *Microsc. and Anal.*, 93, (**2008**), S5.

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S7-L4

1D QUASICRYSTALS, RANDOM MATRICES, AND THE MODULAR GROUP

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Many aperiodic tilings can be generated in two different ways: either by the cut-and-project method or by an iterated-substitution scheme. What exactly is the relationship between these two approaches? I begin by sorting out this question explicitly in the simplest case -- i.e. for 1-dimensional quasicrystals "of order 2" (i.e. obtained from a 2D lattice by the cut-and-project method) -- in which case there is a beautiful answer, controlled by the modular group. I then discuss how the results extend to the more general case of n-dimensional quasicrystals of order N. In particular, I consider the limit as N goes to infinity, and discuss the relationship with large random matrices.