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**Keywords: electron diffraction, precession diffractometry, direct methods**

#### FA4-MS24-T04

**Structure of molecular crystals solved by automated electron diffraction.** Tatiana Gorelik, Enrico Mugnaioli, Andrew Stewart, Galina Matveeva, Ute Kolb. *Institute of Physical Chemistry, University of Mainz, Germany.*  
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Organic materials ranging from pharmaceuticals to pigments and polymers are essential part of everyday life. Molecular packing within these materials is a basis for understanding and controlling the functionality of the compound. Therefore structural investigations on molecular crystals are of great importance both for industrial applications and fundamental research.

Of particular interest is the structure of nano sized organic crystals; these crystals can either be confined in size on purpose (to suit better their applications) or exist only as nano crystalline domains. Crystal structure of nano phases often differ from that of larger crystals exhibiting different polymorphs [1]; a situation when a structure determined from a larger crystal via single crystal X-ray diffraction does not fit the X-ray powder profile of the nano material occurs much more often than is commonly perceived. Therefore techniques for structural analysis of molecular nano phases are of increasing importance in the age of nanotechnology.

Electron diffraction can provide structural information from a single crystal with a size down to 20 nm. Electron crystallography of organic materials has a long history going back to 50s [2]. Molecular crystals were always attractive for electron crystallography due to minimal effects associated with dynamical scattering. Nevertheless the method is not widely spread due to experimental difficulties connected with the beam damage. To overcome these limitations automated procedures for data collection optimizing the total electron dose distribution were created [3, 4].

The quality of automatically collected electron diffraction data sets turned out to be sufficient to perform ab-initio structure solution and even detect water molecules incorporated into molecular packing. Structure solution of organic crystals of various classes based on automatically collected electron diffraction data will be presented.

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**Keywords: electron crystallography, ab-initio structure determination, molecular crystals**

#### FA4-MS24-T05

**Measuring electron scattering factors by large angle rocking beam electron diffraction (LARBED).**

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The strong interaction of fast electrons with matter is viewed by many as both a blessing – the analysis of tiny volumes may yield excellent diffraction data – and a curse – even in thin samples dynamical scattering theory should be applied – at the same time.

Although it is, at least in principle and for moderately thin samples, possible to invert the dynamical scattering and extract scattering factor amplitudes and phases directly from diffraction data [1] it is common practice to treat electron diffraction data with kinematic scattering theory and use existing direct methods, iterative phasing algorithms, or information from HRTEM images to reconstruct the phase information. For this purpose the precession electron diffraction (PED) technique [2] has been of great help.

In contrast to PED, the LARBED technique [3] aims to preserve the information about the angle of incidence. Figure 1 shows first the LARBED acquisition principle, and also the benefit of having diffraction discs with a diameter much larger than the distance between two neighboring diffraction spots: The 2-dimensional rocking curves allow (a) all the symmetry information available from CBED patterns is available even for samples with very large unit cell and/ or very low thickness, (b) very accurate determination of structure factor amplitudes and sample thickness is made possible by fitting kinematical rocking curves to the data, (c) forbidden reflections may easily be identified [3], and (d) dynamical theory may be applied to retrieve the structure factor phases directly from the data [3].

In this presentation I will focus on aspects (a) and (b): the quantitative determination of structure factor amplitudes from LARBED patterns.

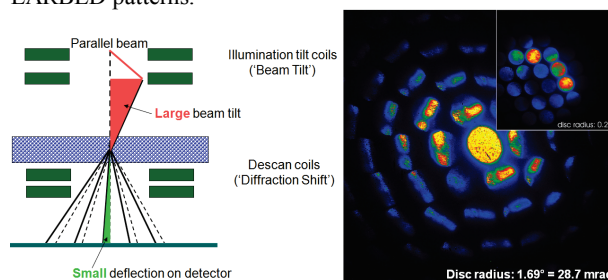


Figure 1 Left: diagram illustrating the LARBED experimental setup. The large beam tilt is above the sample is scaled down to a size avoiding overlapping diffraction discs. Right: LARBED pattern of Si (110). While the inset shows the diffraction discs without applying any de-scan, the scale of the diffraction discs in the large diffraction pattern has been reduced 6.25 fold to produce the same size discs.

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**Keywords: quantitative electron diffraction, CBED, dynamical electron scattering**