Type of presentation: Invited

IT-9-IN-1862 Multiple-scattering assisted electron crystallography

Koch C. T.[1]

[1]Institute for Experimental Physics, Ulm University, Ulm, Germany

Email of the presenting author: christoph.koch@uni-ulm.de

The ab-initio determination of crystal structures typically requires highly complete single-crystal diffraction data, i.e. diffraction intensities should have been measured for almost all unique reflections. The reason for this is that, if many more reflections have been measured, than there exist atoms within the structure, the sparseness (peaked nature) of the real-space representation of the charge density (in the case of X-rays) or potential (in the case of electrons) can be utilized to solve the crystallographic phase problem (e.g. by direct methods, or charge flipping, or similar kinematic scattering based techniques). While electron diffraction has the great advantage over X-ray or neutron diffraction, that very small crystallites are already sufficient to produce such single crystal patterns, multiple scattering of electrons within the material generally prevents electron diffraction data to be used in as quantitatively a manner as X-ray or neutron data. This limits the application of electron diffraction tomography [1] to samples that are small along at least two dimensions (e.g. rods), and makes the investigation of other geometries (e.g. platelets) generally more difficult.

It is a well-established truth that, if electron diffraction data corresponding to a few different dynamical diffraction conditions is available, the relative phases of the structure factors that correspond to this data are uniquely determined. This fact is being exploited in structure-factor refinement by quantitative convergent-beam electron diffraction (QCBED) [2,3]. Applying the same real-space constraints as are used for solving the crystallographic phase problem from kinematical diffraction data, a lot less properly phased structure factors are necessary to find the corresponding arrangement of atoms than would be the case if the phases were not known.

In this talk I will show that by applying the recently developed large-angle rocking-beam electron diffraction (LARBED) technique [4], as implemented in the QED plugin [5] for DigitalMicrograph (Gatan), highly quantitative dynamical electron diffraction data sufficient to solve the structure can be acquired from nanocrystals even without tilting the specimen at all.

[1] U. Kolb, E. Mugnaioli, T. E. Gorelik, Cryst. Res. Technol. **46** (2011) 542 – 554

[2] C. Deininger, G. Necker, J. Mayer, Ultramicroscopy **54** (1994) 15-30

[3] J.-M. Zuo, M. Kim, M. O'Keefe, J.C.H. Spence, Nature **401** (1999) 49

[4] C.T. Koch, Ultramicroscopy **111** (2011) 828 – 840

[5] http://www.hremresearch.com

[6] C.T. Koch and J.C.H. Spence, Journal of Physics A: Mathematical and General **36** (2003) 803-816

Acknowledgement: Financial support by the Carl Zeiss Foundation as well as the German Research Foundation (DFG, Grant No. KO 2911/7-1) is acknowledged.

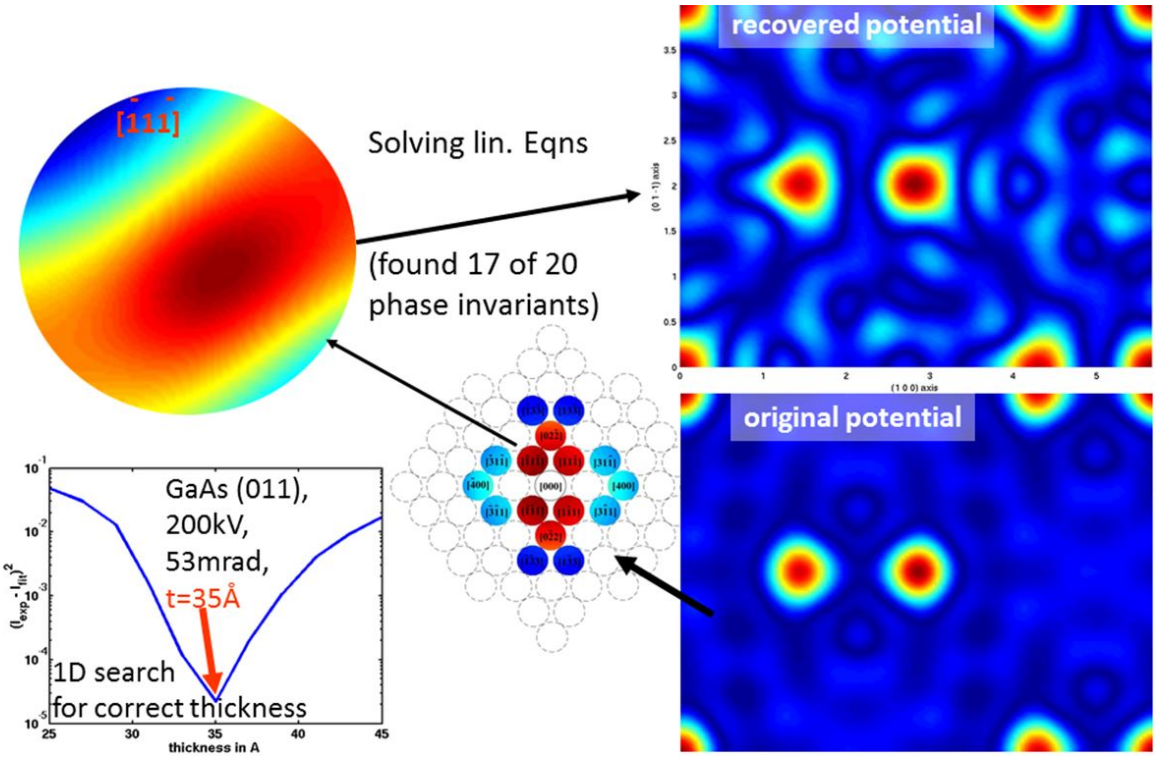

Fig. 1: Illustration of the recovery of structure factor phase triplets from a simulated 2D rocking curve (LACBED disc of radius 2°) for a single reflection of 3.5 nm thin GaAs by applying a recently developed scattering path expansion [6]. The structure factor phases can be further refined assuming sparseness of the potential in real-space.

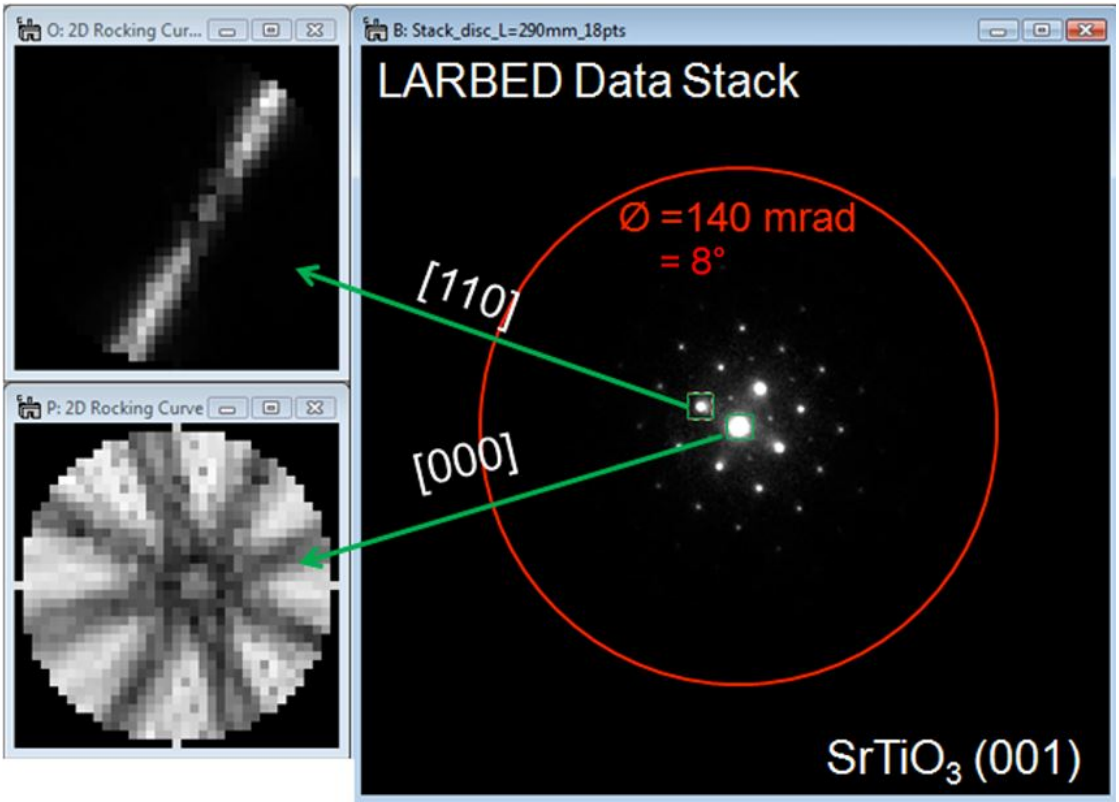

Fig. 2: (001) LARBED pattern of $SrTiO_3$. The range of beam tilts applied for acquiring this pattern spans the disc indicated by the red circle (diameter = 140 mrad). The beam tilt has been compensated by the diffraction shift coils to produce non-overlapping discs. Individual background-subtracted discs have been extracted and are shown as well.