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REAL-SPACE IMAGING OF ATOMIC STRUCTURE

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The majority of x-ray methods for crystal structure investigations are based on diffraction phenomena and sample the information in the reciprocal space.

In this talk we will discuss the possibility of x-ray imaging of the atomic structure directly in the real-space [1]. This distinct and novel approach is possible by recording and analysing the absorption anisotropy of polychromatic, so called "white" x-rays. In this approach, the interference between the incident x-ray beam and the secondary waves coherently scattered inside the specimen modifies the x-ray wave field at the position of the absorbing atoms. Thus, the absorption cross-section is effectively modulated by the x-ray scattering. For a white x-ray beam, the wave field variations cancel out by energy integration for all directions, except for the near forward scattering components, coinciding with the incident beam. Therefore, a two-dimensional pattern of absorption anisotropy can be interpreted as a real-space projection of atomic structure. In this sense, the method lies aside from the traditional x-ray diffraction and closer to the forward scattering of electrons or ion beam channelling. However, its description can be made in the frame of a straightforward first Born approximation, which makes the data interpretation much easier.

We will present two algorithms for direct structure imaging from x-ray absorption anisotropy data. The first one allows for full three-dimensional imaging of crystal structure and it is similar to tomography [2]. The second one uses spherical wavelet transform to determine the bond directions in the local neighbourhood of the absorbing atoms.

Both approaches were tested on the experimental data recorded in HASYLAB for GaP(111) and InAs(001) samples, using a white x-ray radiation from a bending magnet [3]. In order to monitor the x-ray absorption anisotropy we measured total electron yield as the function of the orientation of the sample relative to the incident beam direction. Examples of the recorded data and the three-dimensional reconstruction of atomic structure are shown in Fig. 1.

In future experiments we plan to obtain chemically resolved x-ray anisotropy patterns for element specific imaging. This will be possible with a new experimental setup containing polycapillary optics for collimation of the secondary x-ray fluorescence.

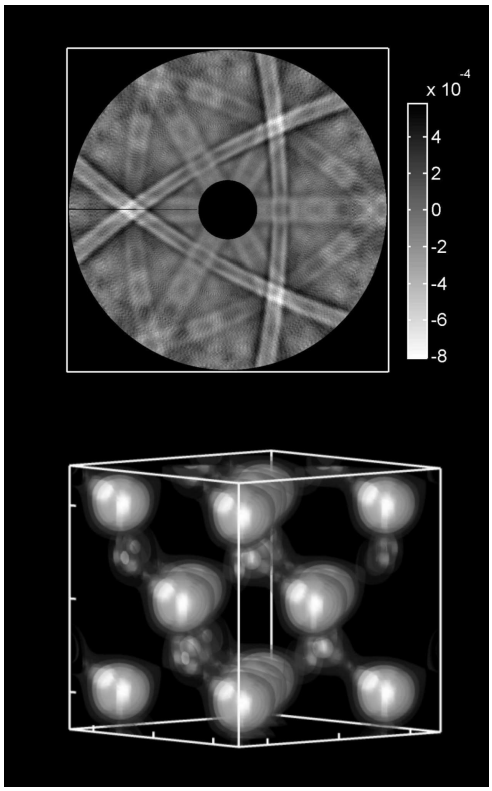

Figure 1. Top: white x-ray absorption anisotropy recorded for GaP(111) crystal. The visible bands correspond to real-space projections of atomic planes. Bottom: structure of GaP recovered with a tomographic algorithm form the data.

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