Poster Presentation

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Indexation of grazing Incidence X-ray diffraction patterns

Josef Simbrunner[1], Roland Resel[2], Ingo Salzmann[3]
[1]*Dept. Of Neuroradiology, Vascular And Interventional Radiology, Graz, Austria,* [2]*Institute of Solid State Physics, Technical University Graz, Austria, Graz, Austria,* [3]*Department of Physics, Humboldt Universität, Berlin, Germany*
E-mail: josef.simbrunner@medunigraz.at

Crystal structure solution from thin films requires indexation of the diffraction pattern which means the assignment of Laue indices to the observed Bragg peaks. The focus of interest are molecular crystals at surfaces where usually low symmetry structures – either triclinic or monoclinic unit cells – are observed. The diffraction experiments for thin films are performed under grazing incidence condition of the primary x-ray beam which yields the reciprocal lattice vectors of the Bragg peaks split in two components: an in-plane part qxy and an out-of-plane part qz. Therefore, for this specific case two components of the reciprocal lattice vectors are available for the indexation process [1]. This is considerably different for the indexation procedure of single crystal diffraction pattern where all three components of the reciprocal lattice vectors are measured and powder diffraction on polycrystalline materials where only the lengths of the scattering vectors are detected. In a first step of our work analytical expressions were derived to calculate the lattice constants for a triclinic unit cell with the ab-plane parallel to the substrate Surface [2]. But in the general case the rotation matrix must be included which introduces additional unknown Parameters [3]. We use a mathematical formalism by including the specular diffraction peak so that the system of unknown parameters can be reduced from the 3- to the 2-dimensional space. Thus in the first part of the indexation routine the lattice parameters a, b, gamma and the Laue indices h and k are determined followed by the second part calculating the residual parameters c, alpha, beta and the Laue index l.

References:
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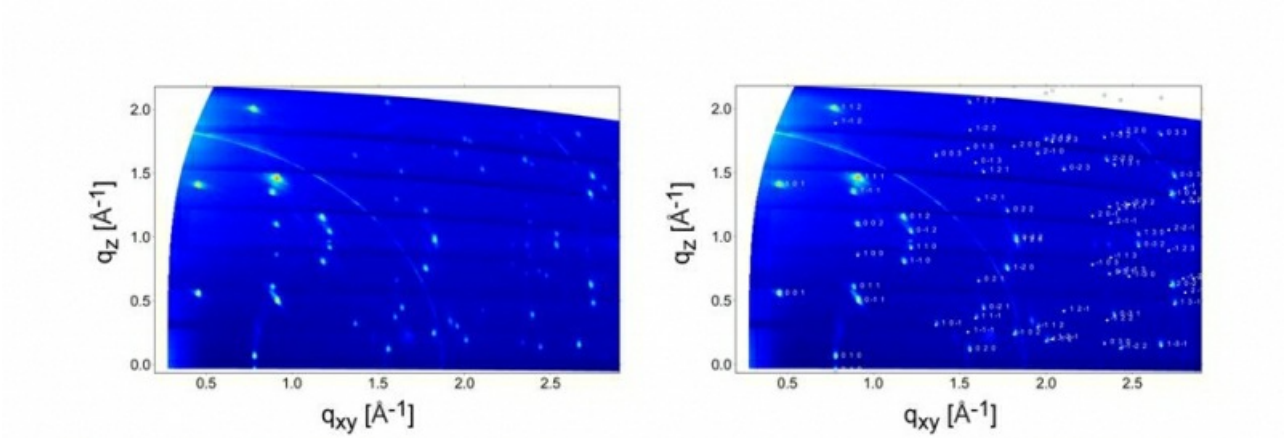

Figure: Grazing incidence diffraction pattern of pentacenequinone crystals on a graphite (0001) surface without indexation (left) and with indexation (right).

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