

Finding crystal orientation in uniplanar textures

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The crystallization of molecular materials on isotropic substrates typically results in a so-called fiber or uniplanar texture which comprises crystallites that share a common fiber axis perpendicular to the substrate surface, but which are azimuthally randomly oriented. The crystallographic characterization of such films is commonly performed by grazing-incidence X-ray diffraction (GIXD) [1]. Two-dimensional reciprocal space maps are obtained, which incorporate the in-plane component q_{xy} and the out-of-plane component q_z for each diffraction peak. The exact position of each diffraction peak depends on the crystallographic lattice and on the orientation of the unit cell relative to the substrate surface. The unit cell orientation can be characterized either by two rotation angles or by the Miller indices of the crystallographic plane parallel to the substrate surface [2,3,4]. Here, equations are derived that allow the calculation of the orientation parameters and describe the relations between them. Depending on the underlying unit cell, a manifoldness of possible orientations exists. Examples based on molecular crystals of pentacenequinone, diindenoperylene and binaphthalene (cf. Fig. 1) are given which are illustrative examples comprising triclinic, monoclinic and tetragonal unit cells having two, four and 16 possible crystal orientations, respectively [5].

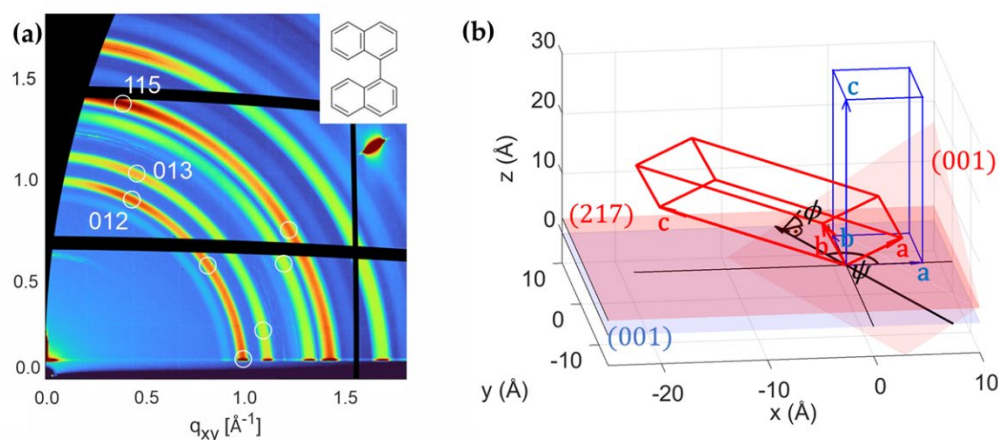


Figure 1. (a) GIXD pattern of binaphthalene (BNP) crystals. For clarity, Laue indices are given only for selected Bragg peaks, specified for the contact plane (217). The chemical structure of the molecule is given as inset. (b) Schematic sketch of the tetragonal unit cell BNP with its lattice vectors \mathbf{a} , \mathbf{b} and \mathbf{c} . The new crystal orientation (colored in red) is obtained by rotation around the axis depicted as black vector. Also shown are the rotation angles ψ and ϕ . Blue: unit cell with its contact plane (001), identical to the xy plane, also colored in blue. Red: rotated unit cell with its crystallographic planes (001) and (217) which is parallel to the xy plane.

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