MS44-P10 | INDEXING GRAZING INCIDENCE X-RAY DIFFRACTION PATTERNS OF THIN FILMS

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Grazing incidence X-ray diffraction (GIXD) studies on organic thin films are often performed on systems showing fibre-textured growth. However, indexing their experimental diffraction patterns is generally challenging, especially if low-symmetry lattices are involved. Recently, analytical mathematical expressions for indexing experimental diffraction patterns of triclinic lattices were provided. In the present work, we provide a unifying framework for the indexing reciprocal-space maps obtained by GIXD for monoclinic lattices and lattices of higher symmetry. Our approach of including the Bragg peak from a specular X-ray diffraction experiment into the mathematical formalism is of considerable help for indexing of GIXD pattern, where the spatial orientation of the unit cell must be considered. Mathematical expressions with a significantly reduced number of unit cell parameters are derived, which facilitates the computational efforts. For crystallographic lattices of higher symmetry, where the set of unit cell parameters is reduced, the specular diffraction peak is still important for determining the orientation of the crystallographic unit cell relative to the sample surface. Procedures are described in detail for how to use the derived mathematical expressions. Two examples are presented to demonstrate the feasibility of our indexing method. For layered crystals of the prototypical organic semiconductors diindenoperylene and (*ortho*-difluoro) sexiphenyl, as grown on highly oriented pyrolytic graphite, their yet unknown unit-cell parameters are determined and their crystallographic lattices are identified as monoclinic and orthorhombic, respectively.