Adding a Second Dimension to Surface Diffraction: Reciprocal Space Mapping of Single-Crystal Scattering Rods

Detlef-M. Smilgies, Daniel R. Blasini, Shu Hotta, and Hisao Yanagi

[1)] CHESS Center, Cornell University
[2)] Cornell Department of Chemistry and Chemical Biology
[3)] Department of Polymer Science and Engineering, Kyoto Institute of Technology, Japan
[4)] Faculty of Engineering, Kobe University, Japan

Traditionally x-ray diffraction and grazing-incidence diffraction results are presented as simple line scans, because in most cases point detectors have been the working horses of x-ray diffraction, with the exception of oscillation camera methods used in protein crystallography. We have developed an intermediate approach suitable for weakly scattering systems such as surfaces, thin films, or, as in our case, molecular microcrystals on a substrate. Using the reciprocal space mapping system at CHESS G2 station, comprising a 100 mm linear gas detector with a matching Soller collimator, we studied microcrystallites of the boomerang-shaped molecule biphenyl thiophene (BP1T) which is interesting for its electro-optical properties and possible use in organic light-emitting diodes (OLEDs). The diffraction map obtained in a slice of reciprocal space parallel to the [110] high-symmetry direction of the substrate reveals a high degree of complexity of the orientation of BP1T microcrystals grown on an atomically well-defined KCl(001) substrate. This approach may also be of interest for studying proteins, of which only very small microcrystals can be obtained.

Reference: D.-M. Smilgies et al., J. Synchrotron Rad. 12, 807-811 (2005).

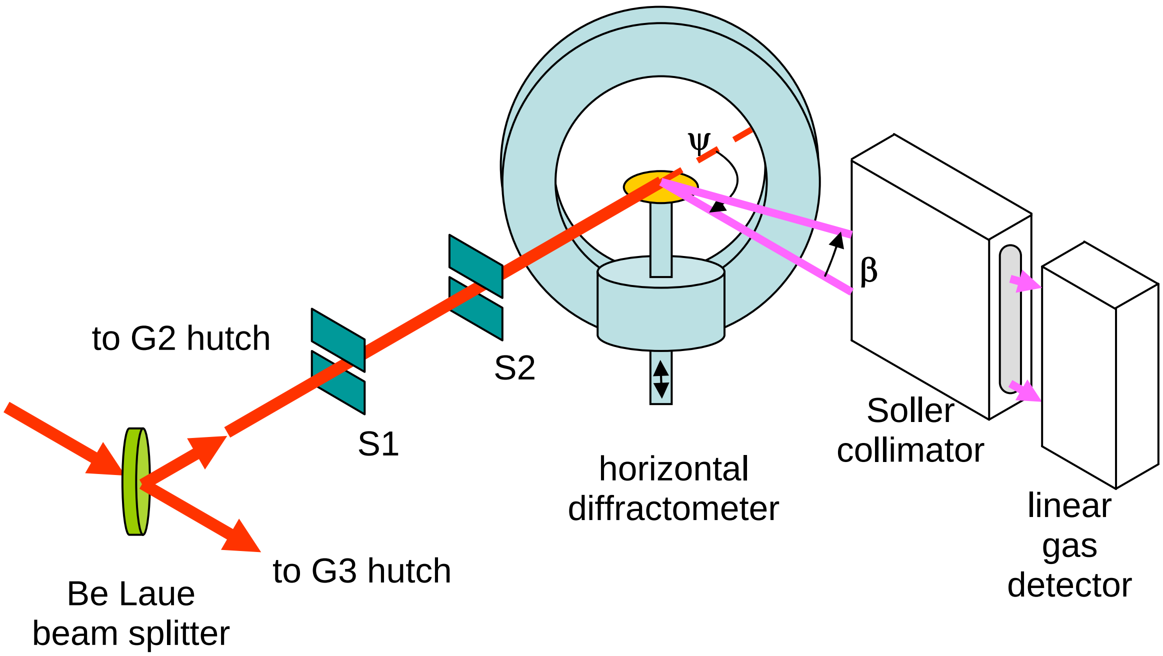

Fig. 1. Reciprocal Space Mapping set-up under grazing incidence at CHESS G2 station.

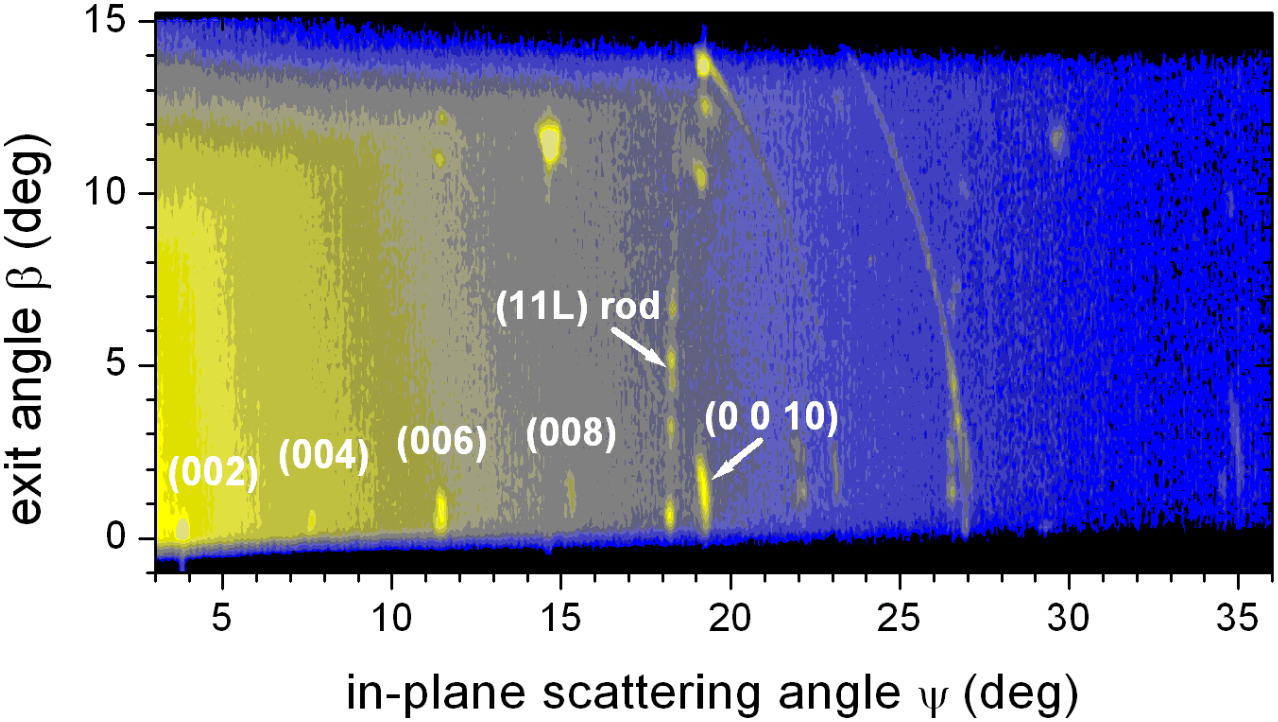

Fig.2 Map of BP1T diffraction intensities in a slice of reciprocal space parallel to the high-symmetry direction of the substrate. The (00L) family of reflections indicates microcrystals with the long molecular axis parallel to the substrate, while the (11L) scattering rod signifies microcrystals with the long axis perpendicular to the surface.