Structural Reconstruction of Organic Semiconductor Thin Films via Grazing-Incidence Diffraction Tomography

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The structural characterization of organic semiconductor thin films is essential for evaluating material processing outcomes and efficiency as well as establishing structure–performance relationships for applications in future. Grazing Incident X-ray Scattering technique in small- (GISAXS) and wide-angle (GIWAXS) regions is commonly used to reveal the in-general crystalline features, such as crystalline orientation, polymorphism, domain size and boundary, etc. However, the limited spatial resolution in grazing incident geometry constraints the investigation of structural features in localized area. Here, we introduce grazing-incidence diffraction tomography (GID tomography), a computational method based on in-plane diffraction signals that quantitatively determines the shape and orientation of crystalline domains. GID tomography combines the advantage of the GI measurement geometry and the resolving power of tomographic methods to reconstruct the spatial maps of crystalline orientations. The successful reconstruction shows the multiple domains of organic semiconductor thin films recognized by using in-plane diffraction signals. There are no restrictions on the beam coherence, substrate type, or film thickness for this method. In the future, with a rigorous intensity calibration, the method will provide not only quantitative orientation maps but also provide information on crystallinity. GID tomography has the potential to account for polymorphs or mixed materials by calculating the rotational angles between peak for each composition.