PDF across-the-board in science - the x-ray total scattering portfolio at P07-DESY and P21.1 at PETRA III

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At the high-brilliance storage ring PETRA III at DESY, Hamburg, the two stations P07-DESY and P21.1 specialize in advanced x-ray total scattering (TS) techniques to study local disorder in a variety of sample types. Fast TS measurements on powdered, liquid or solid bulk samples is routinely available for traditional PDF analysis assuming fully random distribution of the scattering coherent domains. For in situ experiments, the beamlines offer spacious heavy-load sample stages for user-specific setups and access to standard sample environments e.g. for heating and cooling. The stations are equipped to apply the more recent 3d-ΔPDF method on single crystals as well as epitaxial thin films under ambient and non-ambient conditions. All thin film samples exhibiting a film thickness in the nanometer range are measured in grazing incidence to obtain high-quality PDFs on amorphous, nano- and polycrystalline layers as well as single-crystalline films. Owing to the high flux microfocused beams, the surface sensitivity reaches down to just a few nanometers in film thickness when using either amorphous or single-crystalline substrates. In addition, high-performance x-ray diffraction computed tomography (XRD-CT) scans are carried out in TS mode when PDF contrast is required. This presentation outlines the TS capabilities of the P21.1 and P07-DESY instruments to illustrate the wide range of opportunities for PDF-based structural studies at our facilities. [1]

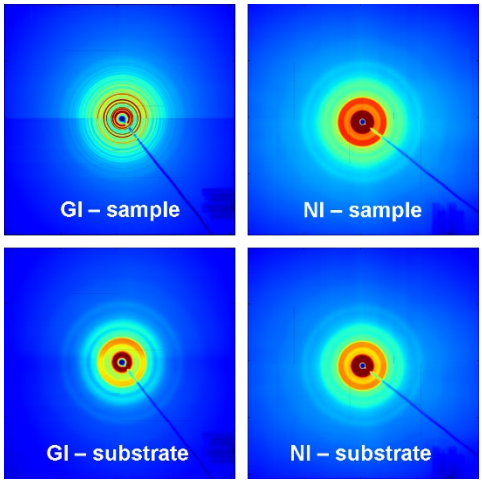


Figure 1. *The power of total scattering in grazing incidence (GI): 2D diffraction patterns of a ~30 nm ZrO_2 thin film (top) measured in GI [2] compared to transmission geometry (normal incidence NI as described in [3]) on 180 µm thick glass substrates (background patterns at the bottom).*

[1] M. v. Zimmermann, O. Ivashko, F. Igoa Saldaña, J Liu, P. Glaevecke, O. Gutowski, R. Nowak, K. Köhler, B. Winkler, A. Schöps, H. Schulte-Schrepping, A.-C. Dippel, J. Synchr. Rad. 32 (2025) 802-814.
[2] A.-C. Dippel, M. Roelsgaard, U. Boettger, T. Schneller, O. Gutowski, U. Ruett, IUCrJ 6 (2019) 290-298.
[3] K. M. Ø. Jensen, a. b. Blichfeld, S. R. Bauers, S. R. Wood, E. Dooryhée, D. C. Johnson, B. B. iversen, S. J. L. Billinge, IUCrJ 2 (2015) 481-489.