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## Grazing Incidence Total Scattering at PETRA III: Extending Local Structure Analysis to Ultrathin Films on Single-Crystal Substrates

### Content

Grazing incidence scattering is a technique that takes advantage of the total external reflection of X-ray photons as they shine on a flat surface below the material's critical angle. When this condition is met, the X-ray photons only penetrate the material some 1-10 nm as an evanescent wave. Hence, surface scattering is amplified with respect to the bulk. If combined with high energy photons and high-angle data collection, then surface sensitive grazing incidence total-scattering (GI-TS) and pair distribution function (pdf) analysis can be achieved.

The critical angle depends on the photon energies, such that it lies around (10 - 60) milidegrees, which imposes strict boundary conditions for alignment, sample flatness and roughness. As a matter of fact, empirically, always a certain degree of bulk penetration is observed, which contributes to background scattering. Therefore, well-behaved, i.e. isotropic scattering, substrates have been historically chosen to perform GITS, neglecting the more application relevant options, such as single-crystalline silicon.

Single-crystalline silicon exhibits an anisotropic scattering that combines discrete Bragg reflections and distributed diffuse scattering. Azimuthal averaging is out of question in this case, for which its use in GITS has long been considered a dead-end. We recently optimized a 2D-background correction and subtraction strategy that successfully allows to eliminate the anisotropic background contribution, and hence isolate thin film scattering that can be transformed to pdf. This strategy is based on using the substrate Bragg reflections as a reference to correct and subtract 2D images prior to azimuthal integration.

In this presentation, the grazing incidence total scattering capabilities at P21.1 at PETRA III will be discussed, along with recent advancements that enable the use of anisotropic substrates.

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