Contribution ID: **68** Type: **Oral**

Local atomic structure of highly ordered and highly disordered thin films: recent advances of in situ grazing incidence total x-ray scattering

Monday, 15 July 2024 17:30 (20 minutes)

Complementary to x-ray diffraction patterns that represent the crystal lattice in reciprocal space, the atomic pair distribution function (PDF) describes the structure of a material as a histogram of interatomic distances r in real space. The total scattering approach that enables PDF analysis requires that scattering data is collected over a wide Q range of the order of 20 Å⁻¹ and subsequent Fourier transformation of the entire scattering pattern into real space. While total scattering at high-energy x-ray beamlines has become a standard technique for bulk-type samples, the unfavorable thickness ratio of a thin film (nanometer regime) to its substrate (micro- to millimeter regime) limits the detectability of the film signal in simple transmission geometry as described *e.g.* in Ref. [1]. For the hard x-ray range, grazing-incidence (GI) geometry is well established for surface scattering. GI diffraction and total scattering at high photon energies >50 keV are advantageous as they enable direct access to a wide Q range in a single exposure on a large area detector, but are more demanding in terms of experimental prerequisites. At beamline P07 at PETRA III (DESY, Hamburg), high-energy surface diffraction [2] and, more recently, total scattering in GI geometry [3,4] have been developed into routine capabilities that benefit various research fields from catalysis to electronics and strongly correlated materials. This presentation reports on the latest progress at PETRA III beamlines P07 and P21.1 in applying GI total x-ray scattering to study the short-range order in epitaxial layers at non-ambient conditions and *in situ* processes like phase formation during post-deposition crystallization and electrochemical thin film growth. Such novel insights into the evolution of atomic structure on short to long-range scale in thin film systems demonstrate the expected huge gain for communities that have so far lacked a tool like PDF analysis to determine the local structure and disorder in thin layers.

[1] K. M. Ø. Jensen et al., IUCrJ 2 (2015) 481-489.
[2] J. Gustafson et al., Science 343 (2014) 758-762.
[3] A.-C. Dippel, et al., IUCrJ 6 (2019) 290-298.
[4] A.-C. Dippel et al., Nanoscale 12 (2020) 13103-13112.

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Instrumentation and methods

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Session Classification: Instrumentation and methods I