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Real time structural of thin films on the local atomic scale: capabilities of the grazing incidence pair distribution function technique

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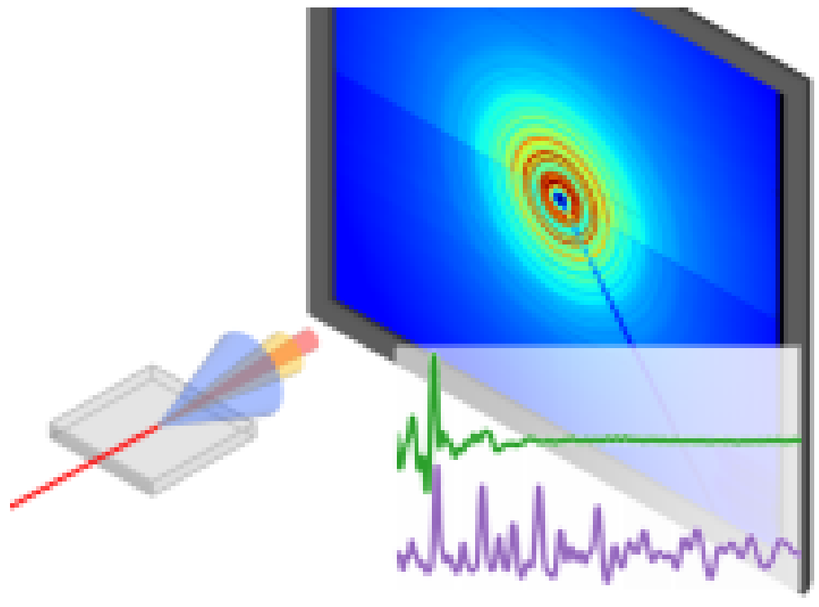
Abstract: Pair distribution function (PDF) analysis has become a widely used and most effective tool to study the local structure of materials that exhibit some degree of disorder. With the increasing availability of high-energy x-ray sources equipped with large and fast area detectors, PDF has advanced into the field of in situ and operando studies. Nowadays, PDF is indispensable to follow processes in manifold bulk-type and nanostructured systems such as chemical reactors, electrochemical cells, mechanical testing setups, etc. In particular for nanomaterials that generally lack any long-range ordering, the PDF technique has largely contributed to obtaining insight into the structure-property relationship of which is often dominated by the quantum confinement. Since many applications require processing of nanoparticles to thin films and complex hetero-structures, the conventional bulk approach of PDF reaches its limits. Recently, different approaches to thin film PDF have been applied, including (i) the exfoliation of the film from the substrate to grind it up into a powder [1], as well as measuring the film on the substrate in transmission under normal incidence on the surface [2]. While both of these methods are experimentally similar to bulk measurements with respect to the data collection and evaluation, they have particular drawbacks: for method (i), film-specific features such as preferred orientation may be lost and the structure modified by the mechanical treatment, and case (ii) provides an unfavorable signal to background ratio, given that the scattering from both the film and the substrate is collected and the thickness ratio is typically of the order of a factor 1000 (nanometer vs. micrometer range). In this presentation, we demonstrate the advantages of surface diffraction type PDF measurements under grazing incidence (GIPDF) to quantitatively analyze thin films with thicknesses down to a few nanometers [3]. In contrast to previous GIPDF studies, we use microfocused high energy x-rays (>60 keV) and a fast area detector to obtain high quality PDF data on the time scale of seconds to enable in situ and operando studies of thin films in real time. In a first in situ PDF analysis of thin film deposition [4], we followed the growth and strain evolution of sputtered platinum layers. This presentation highlights perspectives and challenges for future benefits from GIPDF in research on e.g. solar fuel cells, smart windows, thermoelekctric devices, microelectronics, and manifold other thin film applications.



[1] S. R. Bauers et al., J. Am. Chem. Soc. 137 (2015), 9652.
[2] K. M. Ø. Jensen et al, IUCrJ 2 (2015), 481.
[3] A.-C. Dippel et al., IUCrJ 6 (2019) 290.
[4] M. Roelsgaard et al., IUCrJ 6 (2019), 299.

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