Poster

On the Lorentz correction for grazing incidence X-ray diffraction

F. Gasser[1], J. Simbrunner[2], M. Fratschko[1], H.-G. Steinrück[3], R. Resel[1]

[1]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria, [2]Department of Neuroradiology, Vascular and Interventional Radiology, Medical University Graz, Auenbruggerplatz 9, 8036 Graz, Austria, [3]Institute for Sustainable Hydrogen Economy, Forschungszentrum Jülich GmbH, Am Brainergy Park 4, 52428 Jülich, Germany

fabian.gasser@tugraz.at

Grazing incidence X-ray diffraction (GIXD) is the method of choice for the characterization of crystallographic order in thin films [1]. An essential part of the analysis of GIXD maps is the determination of accurate Bragg peak intensities, as they are directly related to the position of individual atoms within the unit cell. To correct for different measurement parameters a variety of intensity corrections are applied to measured GIXD data. These include the polarization of the incident beam [2], solid angle variation [3], absorption effects [3,4] and transmissivity [5]. Particularly interesting is the so-called Lorentz correction, a geometrical factor reported to correct for the velocity at which a Bragg peak moves through the Ewald sphere. While initially described for single crystal and powder diffraction experiments, multiple adaptations of the Lorentz correction for GIXD experiments are reported in literature with varying mathematical derivations [2]. Such Lorentz corrections are then typically applied to measured data without further considerations.

In this work we want to show how modern data treatment simplifies the Lorentz correction substantially. After transforming measured GIXD data to reciprocal space coordinates using well established software tools [6] the Lorentz correction turns out to be a simple Jacobian. Examples for the Lorentz correction for cylindrical or spherical reciprocal space coordinates are shown in Fig. 1. To verify and benchmark this novel approach, GIXD measurements were performed on model systems utilizing a two-dimensional area detector at beamline XRD1, Elettra Trieste. The investigated systems include classical powders, uniaxial textured thin films and single crystals. After applying all the required intensity corrections, we demonstrate how integrated peak intensities can be obtained for the various systems taking advantage of their respective symmetries. The obtained results are compared to the already known crystal structure solutions from these systems.

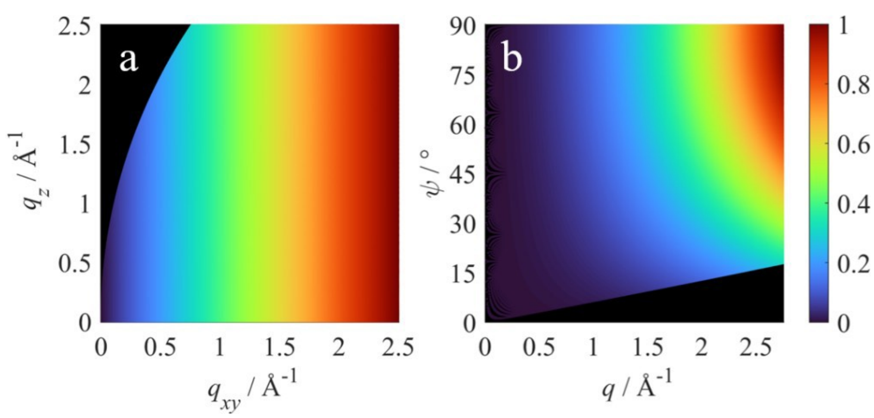

Figure 1. Colormap of the inverse Lorentz correction for (a) cylindrical and (b) spherical reciprocal space coordinates.

Reliable peak intensities from GIXD measurements are essential for the determination of crystal structure solutions. Further applications involve quantitative texture and phase analysis on thin films. This work aims to clarify the concept of the Lorentz correction for GIXD measurements. At the same time, it is expected that the same principles can be applied beyond the limits of grazing incidence conditions, i.e. for single crystal and powder diffraction as well as wide and small angle x-ray scattering.

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