Intensity Corrections in Grazing Incidence X-ray Diffraction

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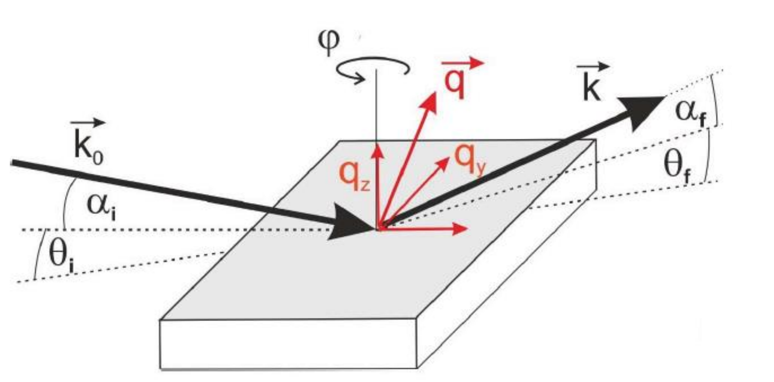
Motivation

measured intensity ~ calculated intensity · correction factors

radiation, measurement type, sample texture ↵

Grazing Incidence X-ray Diffraction

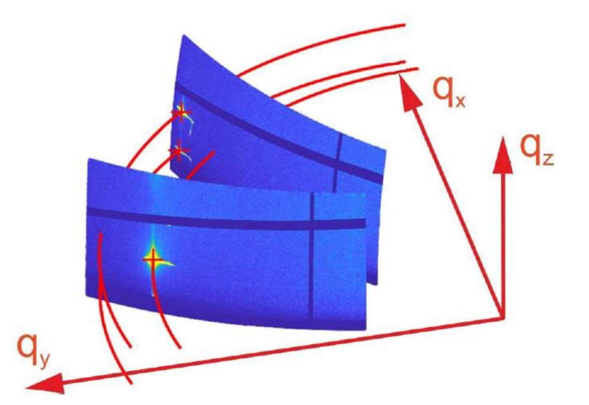


Performance of x-ray diffraction under very small incidence angles $\alpha_i \sim \alpha_c$. An evanescent wavefield is formed at the surface. This is particularly useful for the investigation of thin films.

GIXD with sample rotation

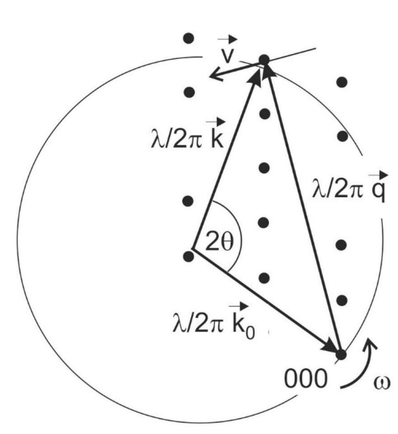
access to 3D reciprocal space

⟶ investigation of textured samples
⟶ improve statistics by averaging over 360° rotation



Lorentz Correction

Describes how quick a reciprocal lattice point moves through the Ewald sphere. In literature different corrections are reported:



In-plane Diffraction[1]: $1/L = \cos(\alpha_i)\sin(\theta_f)\cos(\alpha_f)$

Rotating Single-Crystal[2]: $1/L = \sin(2\theta)$

3D Powder[2]: $1/L = \sin^2(\theta)\cos(\theta)$

None of these factors lead to good agreement between measurement and calculations. Therefore we present a different approach where the Lorentz correction is only a Jacobian[3]:

3D Powder

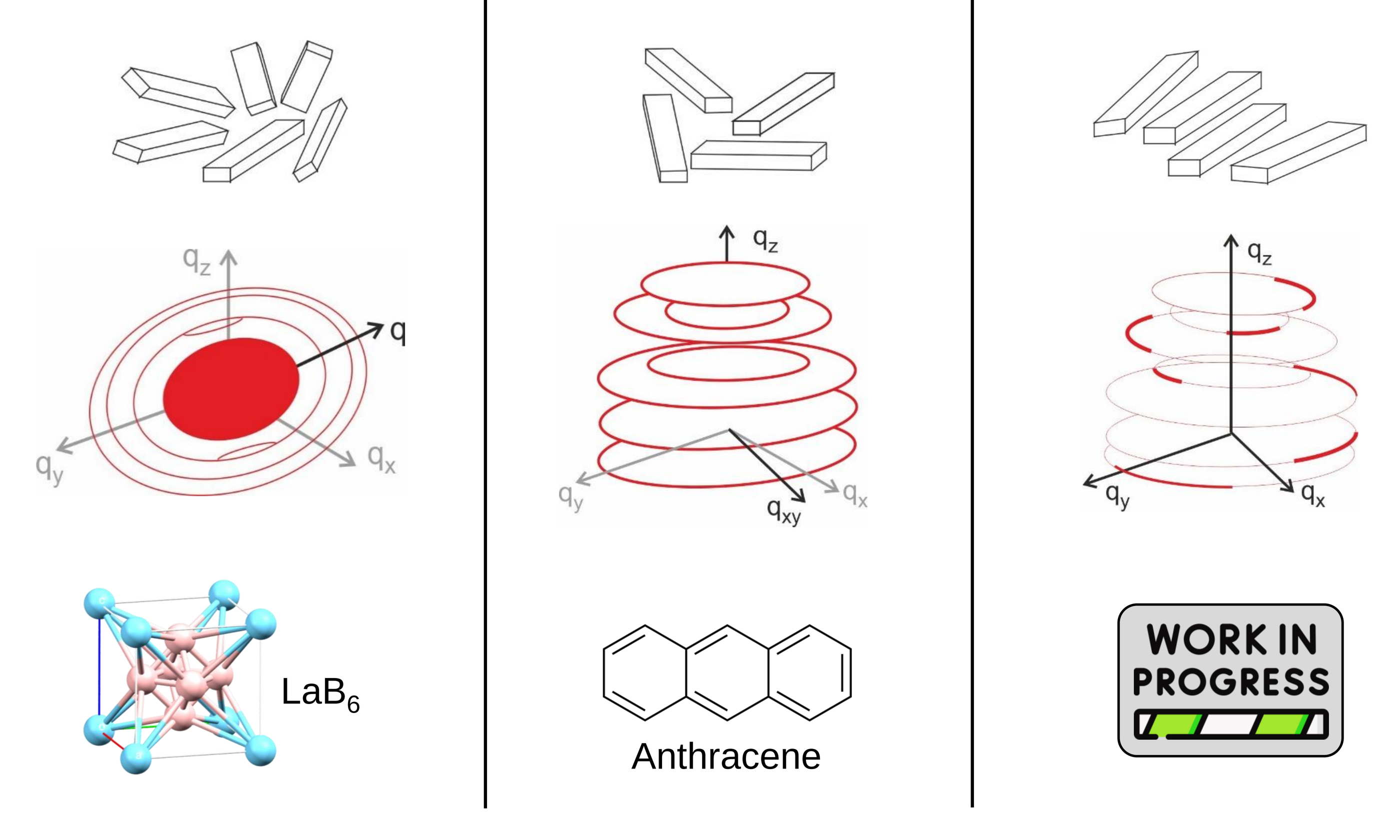
$$I_{int} = \iiint I(q_x, q_y, q_z)\, dq_x dq_y dq_z =$$
$$= \iiint I(q,\psi,\phi)\, q^2 \sin\psi \, dq d\psi d\phi =$$
$$= 2\pi \int_{q_{min}}^{q_{max}} I(q)\, q^2 \, dq$$

2D Powder

$$I_{int} = \iiint I(q_x, q_y, q_z)\, dq_x dq_y dq_z =$$
$$= \iiint I(q,\psi,\phi)\, q^2 \sin\psi \, dq d\psi d\phi =$$
$$= 2\pi \int_{\psi_{min}}^{\psi_{max}} \int_{q_{min}}^{q_{max}} I(q,\psi)\, q^2 \sin\psi \, dq d\psi$$

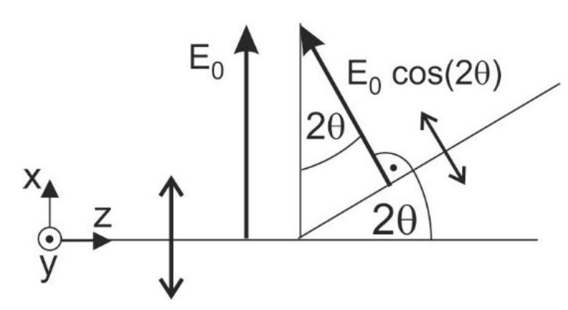
Sample Textures

3D Powder | 2D Powder | Biaxial Texture

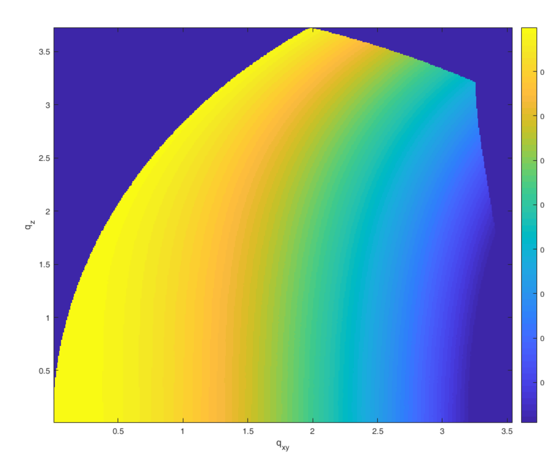


Polarization Correction

Required since only the field component perpendicular to the scattering direction contributes[1].



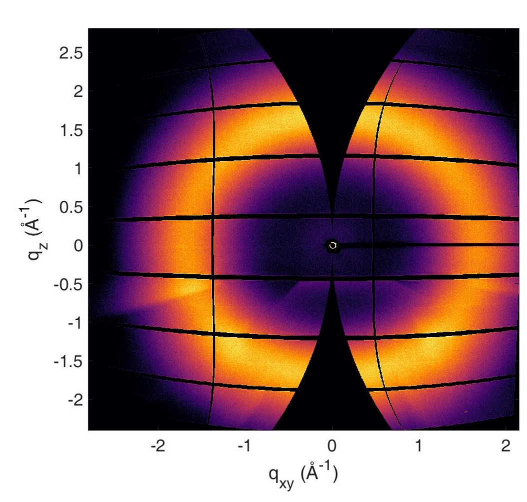
$$P = \xi P_H + (1-\xi) P_V$$
$$P_H = \|\vec{p}_H \cdot \vec{k}\|^2$$
$$P_V = \|\vec{p}_V \cdot \vec{k}\|^2$$

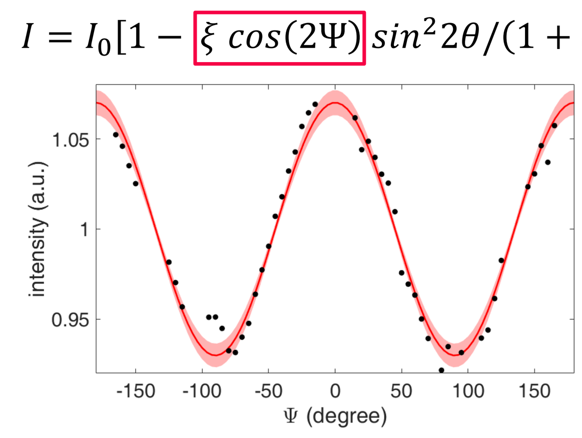


Measurement of the Polarization Coefficient

Transmission measurement through 2 glass slides (0.30 mm). The maximum intensity along the amorphous ring follows[4]:

$$I = I_0[1 - \xi \cos(2\Psi) \sin^2 2\theta/(1+\cos^2 2\theta)]$$

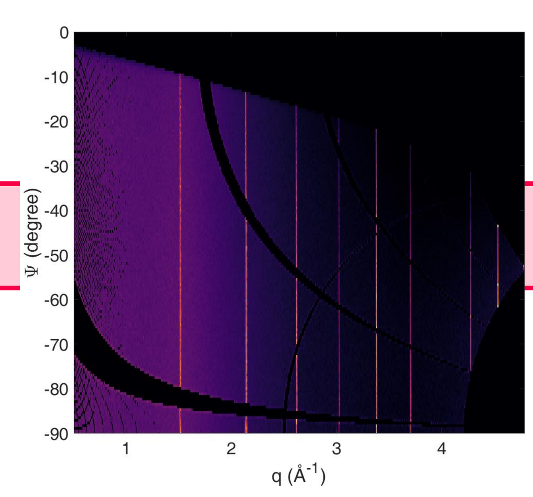




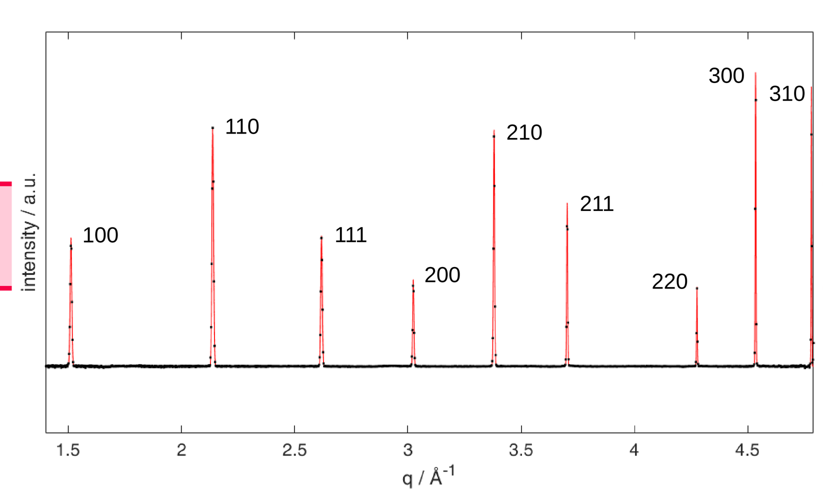
⟶ $\xi > 94.7\%$

Measurements to Investigate the Lorentz Correction

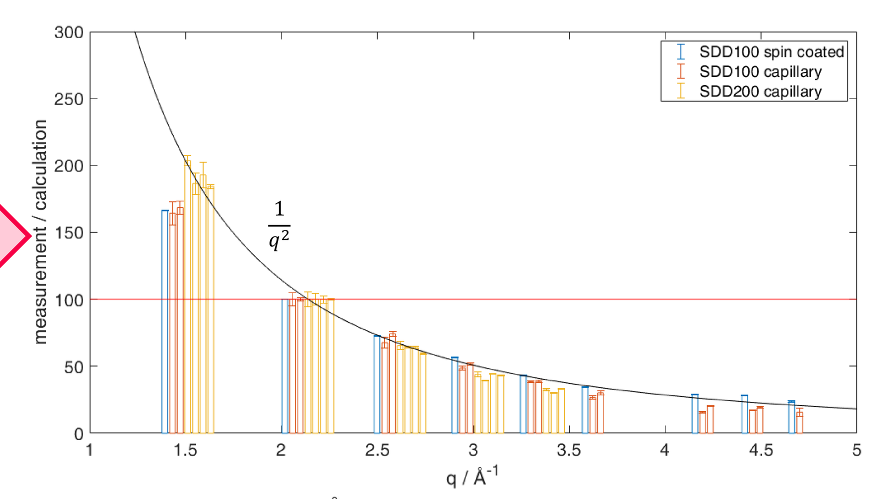
3D Powder



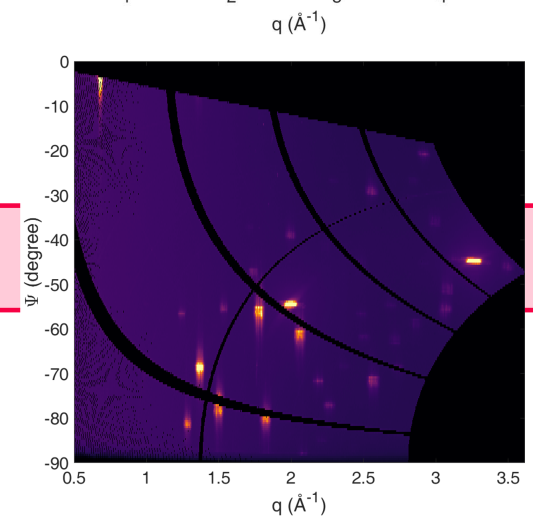
Summation[5] over Ψ



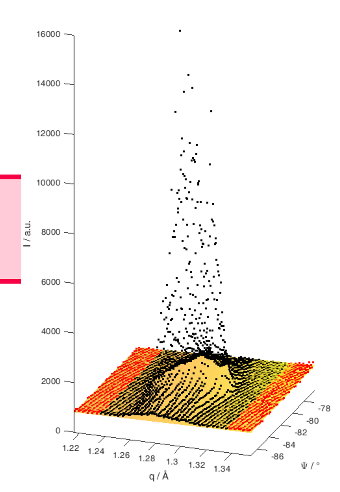
Comparison with calculation



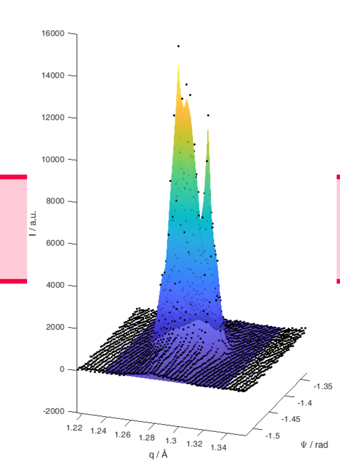
2D Powder



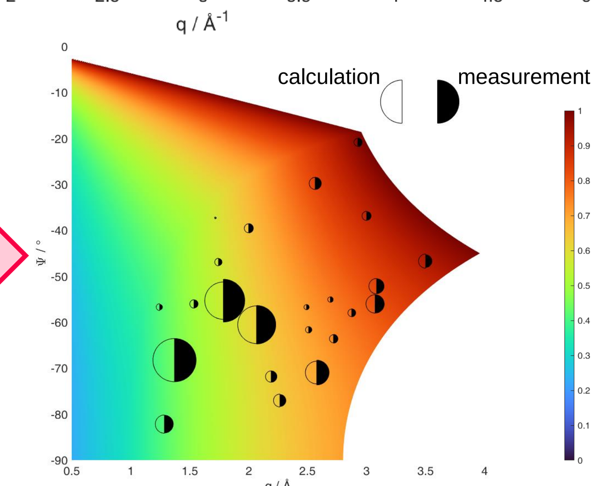
Extraction of data points



2D numerical integration



Comparison with calculation



Conclusion

With knowledge on the polarization coefficient of $\xi > 94.7\%$ an effective polarization correction can be performed. Measurements show that the Lorentz correction strongly depends on the sample texture. For both 3D and 2D powder performing a proper peak integration in spherical coordinates (with a corresponding Jacobian) leads to very good agreement between measured and calculated peak intensity.

Literature

1 Smilgies, D.-M. Geometry-independent intensity correction factors for grazing-incidence diffraction. *Review of Scientific Instruments* **73**, 1706–1710 (2002).
2 Cullity B. D., Stock S. R. in Elements of X-Ray Diffraction (Pearson, 2014)
3 http://gisaxs.com/index.php/Integrated_intensity
4 Sulyanov, S., Dorovatovskii, P. & Boysen, H. A simple approach to determine the polarization coefficient at synchrotron radiation stations. *Journal of Applied Crystallography* **47**, 1449–1451 (2014).
5 Schrode, B. et al. GIDVis: a comprehensive software tool for geometry-independent grazing-incidence X-ray diffraction data analysis and pole-figure calculations. *Journal of Applied Crystallography* **52**, 683–689 (2019).

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