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Next Level Grazing Incidence: Let the Standardization Begin

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Reproducibility of experiments is something most natural scientists would consider important. However, how do we know experiments are comparable between instruments without explicitly disclosing, tracking and discussing instrument calibration and data processing methods? At SXNS17 we would like to introduce our standardization initiative to the Grazing Incidence Small-Angle Scattering (GISAS) community and gather initial feedback and perhaps contributors before we proceed further.

From the point of view of development of a new lab GISAXS setup at BAM (Berlin, Germany), we propose a draft autoalignment and calibration routine. Together with the GISAS community, we would like to further develop this routine into a standard. On that basis, agreed-upon methods for data treatment could be the next step for the future and perhaps an organization like the Open Reflectometry Standards Organisation (1).

We begin with a survey of hardware in use around the world, an area we are not planning to address in terms of standardization but which nonetheless provides the practical background for our efforts. We assume availability of pitch, roll, y and z motions, those may be present in the form of a stack of stages, a hexapod, or even a robot arm. All of these can be used for GISAS, but specifications such as backlash direction and minimum incremental motion need to be considered when it comes to resolution and repeatability of experiments. We ask for your help in gathering information on sample stages and holders and would like to present the results at the International Small-Angle Scattering Conference (SAS2024) in November 2024. We believe this an important step to ensure any developed standard can work for everyone in the end.

With the setup in place we can align a sample (cf. Fig. 1). While a step function for z scans is a typical feature of instrument control software, we suggest to implement a functional form for the expected transmission during a pitch angle scan as well (Fig. 1, steps 3 and 5).

Inspired by work for Grazing Incidence X-ray Diffraction (2) one of our goals is to estimate and propagate uncertainties from stage motions to scattering vector q (compare (3) for Small-Angle X-ray Scattering). Further ideas for standardization include the use of reflectometry in choosing angles of incidence and, perhaps more importantly, data corrections.

References

1. www.reflectometry.org
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Instrumentation and methods

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