orso

file formats

definitions

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June 14, 2021

1 nomenclature and definitions

Here bold lower case letters are used for vectors, e.g. $\mathbf{x}$ or $\mathbf{q}_z$, where its magnitude is given by lower case italics, x or q_z.

1.1 coordinate systems

(taken from a discussion in 2020)

Jochen: I suggest to use a right-handed coordinate system based on the sample with the x axis the projection of the incoming beam onto the sample and the z axis normal to the sample surface.

This seems straight forward, but it can still be controversial: It remains the question if we favour a local coordinate system where $\mathbf{z}$ varies along the sample surface for a non-flat surface, or if we use the *average* sample surface orientation and plane. Let's call this the *macroscopic* coordinate system.

Andrew N: The local coordinate system will reduce to the macroscopic coordinate system when the sample is flat. My preference would be to use the macroscopic coordinate system. This is because we know the location of instrument components such as direct beam paths, reflected beam paths, detectors. α_i and α_f are then calculated from the macroscopic location of the instrument (they have to be, that's the purpose of a sample alignment).
If there are any corrections for non-flat surfaces they are then applied on top of the values derived from the macroscopic coordinate system.

Brian: When you refer to a non-flat sample, are you talking about macroscopically curved samples, or just local roughness? For local variations I would argue that the average z is the only one that matters, but for a curved sample we might need another coordinate system definition (rather than complicating the default coordinate system, why not define a new one?)

Jochen: Also, for an incoming beam with a divergence in y direction, $\mathbf{x}$ is no longer well defined and we have to agree on a way to do so.

The origin of the coordinate system is the centre of gravity of the beam footprint on the sample? or the intensity-weighted centre of gravity of the footprint? or just the centre of the sample? or does it matter anyhow?

1.2 names, symbols, units

Table of quantities with their definitions, recommended (tolerated) units and the notation to be used in the data file.

(orso2020 S3.2) The dictionary is meant for the reduced data file and explicitly not for the raw data file. The reason being, that the later is very technical and very specific for each instrument.

We suggest to

- use the Nexus or canSAS definitions whenever they also apply to reflectometry.
- adapt and modify canSAS definitions for reflectometry whenever they do not exactly match. The names should not be the same, though!

It was also recommended to start with a small set of definitions essential to all / a lot of cases, and to expand if necessary. E.g. sample coordinate system and basic beam characteristics are important, while the detector coordinate system might not be necessary at all because it should be *eliminated* during the data reduction process.

Brian: *I would tolerate as many units for a quantity as are in common use. There's no cost in providing definitions that cover all the use cases.*
For the ORSO standard names, should we stick with the ASCII character set? Is a name like 'alpha_i' going to rub people the wrong way? If we use the more descriptive labels as the ORSO standard identifier, e.g. "incident_angle" we could provide a list of common aliases or "display labels" which could include extended characters or LaTeX or ...?
Agreed with AN that we should provide a way of specifying the probe (neutron vs X-ray). Should polarization state of the probe be included in this definition?

Andrew N: Is it necessary to define specular scattering angle, or specular angle of incidence? I'm happy with α_i, α_f. The specular angles can be worked out from those, and are therefore redundant.

Jochen: some remarks about the seemingly similar angles α_i, θ and ω: I use ω as an instrument degree of freedom. The ω stage tilts the sample to realise the wanted angle of incidence of the beam on the sample surface, α_i. Often, but not necessarily ω is then redefined to have the same value as α_i.
In the case of a converging beam ($\Delta\alpha = 1.5°$ on Amor) there is only one ω (tilt of the sample surface), but a wide range of α_i.
θ comes in as the special case of specular reflectivity. Its use implies that the data are specular data.

	symbol(s)	definition	unit(s)		orso
surface normal	$\hat{\mathbf{z}}$	unit vector	nm	(Å)	
	$\mathbf{z}$	$= z\,\hat{\mathbf{z}}$	nm	(Å)	
	z	$= \lvert\mathbf{z}\rvert$	nm	(Å)	
scattering plane normal	$\hat{\mathbf{y}}$	$= \hat{\mathbf{z}} \times \mathbf{k}_i / k_i$	nm	(Å)	
	$\mathbf{y}$	$= y\,\hat{\mathbf{y}}$	nm	(Å)	
	y	$= \lvert\mathbf{y}\rvert$	nm	(Å)	
	$\hat{\mathbf{x}}$	$= \hat{\mathbf{y}} \times \hat{\mathbf{z}}$	nm	(Å)	
	$\mathbf{x}$	$= x\,\hat{\mathbf{x}}$	nm	(Å)	
	x	$= \lvert\mathbf{x}\rvert$	nm	(Å)	
wave vector	$\mathbf{k}$		nm^{-1}	($\mathrm{Å}^{-1}$)	
	k	$= \lvert\mathbf{k}\rvert = 2\pi/\lambda$	nm^{-1}	($\mathrm{Å}^{-1}$)	
incident angle	α_i	$= \angle(\mathbf{k}_i, \hat{\mathbf{x}})$	rad	(deg)	
final angle	α_f	$= \angle(\hat{\mathbf{x}}, \mathbf{k}_f)$	rad	(deg)	
specular scattering angle	2θ	$= \alpha_i + \alpha_f$	rad	(deg)	
specular angle of incidence	θ	$= \frac{1}{2}2\theta = \frac{1}{2}(\alpha_i + \alpha_f)$	rad	(deg)	
or?		$= \frac{1}{2}2\theta = \alpha_i$ if $\alpha_i = \alpha_f$	rad	(deg)	
scattering vector	$\mathbf{q}$	$= \mathbf{k}_f - \mathbf{k}_i$	nm^{-1}	($\mathrm{Å}^{-1}$)	
normal scattering vector	$\mathbf{q}_z$	$= (\mathbf{q} \cdot \hat{\mathbf{z}})\,\hat{\mathbf{z}}$	nm^{-1}	($\mathrm{Å}^{-1}$)	`Qz`
	q_z	$= \frac{2\pi}{\lambda}(\sin\alpha_i + \sin\alpha_f)$	nm^{-1}	($\mathrm{Å}^{-1}$)	
in-pane scattering vector	$\mathbf{q}_x$	$= (\mathbf{q} \cdot \hat{\mathbf{x}})\,\hat{\mathbf{x}}$	nm^{-1}	($\mathrm{Å}^{-1}$)	
	q_x	$= \frac{2\pi}{\lambda}(\cos\alpha_i - \cos\alpha_f)$	nm^{-1}	($\mathrm{Å}^{-1}$)	
⋮					
wavelength	λ		nm	(Å)	
⋮					
incident intensity	I_0		$\mathrm{s}^{-1}\mathrm{mm}^{-2}$		
neutron beam polarisation	P	$= \frac{I_0^+ - I_0^-}{I_0^+ + I_0^-}$			
reflectivity	R				
density					
scattering length density	ρ^b				

1.2.1 definition of vocabulary

proposals/examples:

reflectivity (to be discussed!) normalised intensity reflected from a sample surface. The *reflectivity* is dimensionless, but might still contain experimental influences and is thus not identical to the sample property reflectivity, solely based on the laterally averaged density depth profile.

angle of incidence

bin, binning

resolution

1.3 dictionary of data reduction steps

proposals/examples:

footprint correction based on geometry The incident intensity on the sample I^0_{sample} is calculated from the total incident intensity I^0_{total}, the beam width d_{beam}, the sample length l_{sample} and the angle of incidence α_i.

$$\begin{aligned} I^0_{\text{sample}} = & \quad I^0_{\text{total}} \cdot \tfrac{l_{\text{sample}} \sin \alpha_i}{d_{\text{beam}}} & \text{for } \alpha_i < \arcsin \frac{d_{\text{beam}}}{l_{\text{sample}}} \\ = & \quad I^0_{\text{total}} & \text{for } \alpha_i \geq \arcsin \frac{d_{\text{beam}}}{l_{\text{sample}}} \end{aligned}$$

(missing: non-flat intensity distribution, convolution with geometrical resolution)

footprint correction using reference sample The footprint is intrinsically corrected by normalisation using a reference measurement: reflected intensity of a supermirror sample $I^r_{\text{reference}}$ with known reflectivity $R_{\text{reference}}(q_z)$ and the same surface shape as the sample.

$$R_{\text{sample}} = \frac{I^r_{\text{sample}}}{I^r_{\text{reference}}} R_{\text{reference}}$$

(incomplete! high angles)