Jochen Stahn Laboratory for Neutron Scattering Paul Scherrer Institut

specular reflectomety

on small samples using a convergent beam

outline amor at PSI

refocus concept

selene@amor

design study for a reflectometer



amor – polarised reflectometer in TOF mode



double disk chopper $\Delta q_Z/q_Z \approx 7 \%$

optical bench: $~\approx 9\,m$ long

diaphragms frame overlap mirror polariser sample stage area or single detector



reflectometer amor

amor – polarised reflectometer in TOF mode



highly flexible

 \Rightarrow tests of new concepts

allows for liquid surfaces

 \Rightarrow can do everything — but nothing really good!



ideas to reduce measurement time for small samples (few mm²)

- dynamic range: 5 orders of magnitude in a reasonable time, only
- off-specular scattering hardly accessible
- \Rightarrow trade more intensity against off-specular scattering
 - prism analyser (\rightarrow Bob Cubitt's talk)

spectral analysis of the reflected white beam

- convergent beam (Frédéric Ott)

focusing to the sample

- angle/wavelength encoding





convergent beam

- $\bullet~\lambda/\omega$ encoding of the incomming / reflected beam
- dispersive set-up:

 \Rightarrow broad q_Z range



 $\begin{array}{ll} \mbox{example:} & 0.5^\circ < \omega < 2^\circ \\ & 4\,\mbox{\AA} < \lambda < 12\,\mbox{\AA} \end{array} \qquad \Rightarrow 0.01\,\mbox{\AA}^{-1} < q_Z < 0.11\,\mbox{\AA}^{-1} \end{array}$



convergent beam

- $\bullet~\lambda/\omega$ encoding of the incomming / reflected beam
- weakly dispersive set-up:

 \Rightarrow narrow q_Z range



example: $0.5^{\circ} < \omega < 2^{\circ}$ $4 \text{ Å} < \lambda < 12 \text{ Å}$

 $\Rightarrow 0.03 \text{ Å}^{-1} < q_z < 0.04 \text{ Å}^{-1}$



convergent beam

- resolution defined by detector $(\Delta \alpha_f)$
- gain $\propto \Delta \omega$

e.g. $1.5^{\circ}/0.05^{\circ} = 30$



• but: signal per channel $\propto \Delta \alpha_f$ background per channel $\propto \Delta \alpha_f \cdot \Delta \omega$ \Rightarrow limit at $\approx 10^{-5}$



convergent beam — how to create it?

define the beam, starting at the sample, by:

- size at the sample position
- divergence
- wavelength, $\Delta\lambda/\lambda$

and avoid everything else!



⇒ focusing optics
dispersive monochromator
filtering / beam-profiling far from the sample



convergent beam — how to create it?

define the beam, starting at the sample and avoid everything else!



 \Rightarrow focusing optics

dispersive monochromator filtering / beam-profiling far from the sample



beam defined by • required beam divergence





beam defined by • finite source size





beam defined by • filtering (polarisation / monochromatisation)





beam defined by • background / radiation issues



focusing

focusing

focusing optics

background / radiation issues







aperture

sample

realisation





focusing optics — a name





coma aberration (distortion of the image of an off-axis point source)



inhomogeneous ilumination



	large α	small α	
coma effect:	amplification	reduction	of preimage (slit)
divergence intensity	low high	high Iow	at the sample position



focusing optics — aberration



aberration of a staight guide





amor – polarised reflectometer in TOF mode



losses between guide ($50 \times 50 \text{ mm}^2$) and sample:

	96%	chopper:
use more flux	> 80%	first diaphragm:
&	pprox 5%	frame overlap filter:
avoid the rest	> 60%	polariser:
	20%	sample $(10 \times 10 \text{ mm}^2)$:
	> 99.75%	П:

amor with selene in TOF mode



horizontal focusing gain factor ≈ 6

enables high-intensity specular reflectivity gain factor ≈ 20



amor with selene in monochromator mode



chopper stopped double monochromator (ml or PG)

same flux, but different q_z -range

polarising ml possible



_







selene





McStas simulations for selene — reflectometer using a double **ml monochromator** (m = 3)

incident angle on the ml: $0 \dots 2^{\circ}$ with $\lambda \propto \sin \alpha_i$

acceptance of the guide: $\Delta \alpha = 1.3^{\circ}$

 $\Rightarrow \lambda$ vs. α_i at sample position:





McStas simulations for selene — reflectometer using a double ml monochromator m = 6, $\Delta q_Z/q_Z \approx 1\%$



no off-specular scattering included, yet



McStas simulations for selene — reflectometer using a double ml monochromator m = 5, $\Delta q_Z/q_Z = 7\%$





McStas simulations for selene — reflectometer using a double PG monochromator ($\Delta \alpha = 0.16^{\circ}$)



no illumination correction applied yet



McStas simulations for selene — reflectometer using a double PG monochromator

comparison: mosaicity of PG





selene reflectometer — resumee

maximum flux on the sample fo a given $\Delta \alpha_i$

allows for high-intensity reflectometry:

- ml monochromator: q_z -range e.g. 0.01 to 0.1 Å⁻¹
- PG monochromator: q_z -range $\propto \Delta \alpha_i$

reduction of $\Delta \alpha_i$ leads to a *conventional* angle-dispersive reflectometer

- ⇒ off-specular measurements are possible
- \Rightarrow a diaphragm-scan results in a q_z -scan





filter first:

- + reduction of radiation entering the guide to < 1%
- + reduced n-background: saves shielding material
- + reduced radiation level: saves life!
- no gain in flux!
- mechanical parts close to source

focusing guide:

- + reduces illumination of sample sourroundings
- + no direct view to source
- + allows for small monochromators . . .
- \circ no gain in flux!
- + allows for q_z/α_i encoding
- (coma) aberration
- does not work for *large* samples

applies for

- source
- filter
- guide
- . . .



thanks to

T. Panzner and U. Filges

for the McStas programmig and simulation work

C. Marcelot and L. Holitzner

for support in the test and design process

F. Ott

for the ReFOCUS concept — which triggered this work

P. Böni, U. Stuhr and C. Niedermayer

for long discussions

nmi3, MaNEP, SNF and SwissNeutronics

for financial and technical support

YOU