TOF reflectometry at PSI:
from an optical bench set-up
to a new instrument concept
with a focus on small samples

JCNS instrumentation workshop
04. – 07. 10. 2011, Tutzing
pre-history

scientific case: liquid-air-interface

⇒ ○ vertical scattering geometry
  ○ (variable) inclination of the beam
  ○ TOF operation (double-blind-chopper)

variable resolution

⇒ ○ optical bench set-up
  ○ high flexibility
the optical bench

8 m granite block

maximum length chopper to detector = 10 m

$2\theta \in [-3^\circ, 12^\circ]$

$\lambda \in [2 \text{ Å}, 18 \text{ Å}]$

detectors: $^3$He single and area (180 × 180 mm$^2$)
options

trough  polarisation  cryomagnet
polarisation analysis (horizontal, 6 T)

1T electromagnet
large gap
actual usage of Amor

(Amor is the only reflectometer at SINQ)

- liquid/air interfaces < 10%
- liquid/solid interfaces < 30%
- magnetic samples > 50%
- non-magnetic solid samples > 10%

majority of the samples is < 2 cm²
some are < 5 × 5 mm²

⇒ adaption of Amor for small magnetic samples
innovations:

non-magnetic sample table for 1t load

\( \omega \in [\pm 4^\circ] \) for heavy set-up

\( \omega \in [\pm 15^\circ] \) else
innovations:

shielding of the detector and flight tube

⇒ background from sample(environment) only
innovations:

focusing guide element for small samples
focusing in the sample plane
including the guide field

McStas simulation of the beam spot:

measured gain for samples of < 10 mm width ≈ 3
innovations:

2D focusing elliptic guide
- to combine $\theta$ and $\lambda$-dispersive operation
- to allow for $\lambda/\theta$ encoding

Selene
Selene: principle

Convergent beam:

Slit-defined beam:

Sample: Ni/Ti multilayer
Selene: realisation

- Chopper housing
- 1st slit
- Elliptic reflector (SwissNeutronics)
- Sample (hidden by diaphragm)
- Detector

Guide
Slit
Focusing guide

Chopper
Knife-edge collimator
Sample
Detector

x/mm: -622 0 880 1880 3880 4880 8663
Selene measurements: 1000 Å Ni film on glass, 9 × 9 mm²
Selene

measurements: 1000 Å Ni film on glass, $9 \times 9 \text{ mm}^2$

measured

simulated with geometrical errors

4 guide elements à 500 mm
Selene measurements: 1000 Å Ni film on glass, 9 × 9 mm²

Measurement time:

- **Conventional set-up**
  - Horizontal focusing
  - 1500 rpm
  - 5 h

- **Selene set-up**
  - No horizontal focusing
  - 750 rpm
  - 45 min

Gain-factor: 6.7
Selene

focusing in the sample plane
+ counting time reduced by 60%

focusing in the scattering plane
+ counting time reduced by 90%

± off-specular & incoherent scattering set limits
– high-precision guide and careful alignment needed
  → improvements under development
– coma aberration
  → correction possible
Selene as an instrument concept  (TOF)

cut in the scattering plane
stretched by 10 normal to incident beam

initial slit \(\approx\) projected sample size

1\textsuperscript{st} elliptic reflector

2\textsuperscript{nd} elliptic reflector
detector

shielding

biological shielding
no direct line of sight

cold source

intermediate image:

beam manipulation

\begin{itemize}
  \item polarising reflector
  \item small chopper
  \item deflector (to bend beam)
\end{itemize}
why 2 ellipses?

- convenient beam manipulation
- guide dimensions not too large
- correction for aberration
mode: almost conventional

- beam is still convergent
- off-specular measurements are feasible
mode: high-intensity specular reflectivity

- energy- and angle-dispersive ⇒ gain > 10
- for fast scanning (T, H, E...)
- or if off-specular scattering is no problem
**mode: low-divergent beam**

- uses the focusing due to coma aberration
- corresponds to Montel optics used at synchrotrons
- for high $q_z$ resolution
**mode: small spot size**

- uses the focusing due to coma aberration
- scanning mode possible

point source off focal point: image is a function of $\theta$
**mode: wide $q$-range**

- shift diaphragm (chopper) between pulses
- vary $\theta$ with fixed sample position
- suited for liquid surfaces

\[
\begin{array}{c|c}
\theta & q_z/\text{Å}^{-1} \\
\hline
0.5^\circ & 0.014 \ldots 0.055 \\
1.5^\circ & 0.042 \ldots 0.165 \\
2.5^\circ & 0.070 \ldots 0.275 \\
\end{array}
\]

e.g. $\lambda = 2\text{ Å} \ldots 8\text{ Å}$
**mode: angle/energy encoding**

- use a ml-monochromator at the intermediate image
- spectral analysis of the beam: $\lambda / \theta$ encoding
- large $\lambda$ on small $\theta \Rightarrow$ wide $q_z$-range

\[\begin{align*}
\text{e.g. } & \lambda = 2\,\text{Å} \ldots 8\,\text{Å} \\
& \theta = 0.5^\circ \ldots 2.5^\circ \\
\Rightarrow & \quad q_z = 0.014\,\text{Å}^{-1} \ldots 0.275\,\text{Å}^{-1}
\end{align*}\]
mode: high $q_z$-resolution

- double PG-monochromator at the intermediate image
- high resolution for $\Delta \lambda / \lambda$, i.e. specular reflectivity
- moderate resolution for $q_x$

- convergent beam is used to recover losses due to the combination of TOF and monochromator
mode: pure TOF

- free choice where to put the choppers

e.g. chopper behind 1\textsuperscript{st} slit at $x = 2\text{ m}$

$\Rightarrow \Delta \lambda / \lambda = \text{const.} = 5\%$
Selene is a guide concept...

- prevents direct line of sight
  - reduces radiation in the guide
  - allows for convenient beam manipulation
- reduces illumination of the sample environment
  - allows for a convergent beam set-up
  \[ \Rightarrow \text{flux gain} > 10 \]

combination with focusing in the sample plane
- beam spot of the order of \( 0.1 \times 1 \text{ mm}^2 \) reachable
- flux gain \( > 100 \) for high-intensity specular reflectometry
tests: \([\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3/\text{SrTiO}_3]_4/\text{NGO}, 4 \times 5 \text{ mm}^2\]

- no focusing in sample plane
- TOF mode, \(\lambda \in [2 \ldots 18 \text{ Å}]\)

- measurement time:
  - conventional: 6.5 h
  - Selene: 45 min
  - gain-factor: 8.3

\[
\log_{10}[R(q_z)]
\]

by courtesy of C. Aruta and F. Miletto