Estia DMSC Software Requirements

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September 17, 2015

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2.1. Currently used software for data analysis (AMOR@SINQ/BL4A@SNS)

2.1.1. Basic data analysis concept for reflectometry

For most neutron reflectometers the data analysis consists of three basic steps:

Raw data view The instrument and reduction software must allow to view raw data of the measurements in different sensible projections. The basic functionality includes a time-of-flight vs. horizontal detector pixel and horizontal vs. vertical detector pixel map. Further helpful views include a translation of the axes mentioned to wavelength λ and angle θ as well as viewing normalized datasets.

Reduction The raw neutron event data needs to be converted from angle/time-of-flight coordinates into wave vector transfer (q_z), binned, properly normalized and combined to produce a reflectivity curve R(q_z). This reduction step strongly depends on the mode of operation of the instrument and is therefore often done with instrument specific programs. To generate correct reflectivity curves several parameters of the instrument geometry need to be taken into account.

For *Estia* the normalization and binning can become much more complicated than for other time-of-flight machines due to the additional complexity of the high intensity mode described in section 3.2.3.

Modeling Sample models are used to simulate reflectivity curves and refine sample parameters. These simulations mostly use the Parratt[2] recursion or matrix[3–5] formalisms to self-consistently model the refraction and reflection of the wave at the various interfaces in the sample. There is a variety of tools available that implement these models, see a list in section A.1.

2.1.2. Data reduction at beamline 4A of SNS

The magnetism reflectometer uses the python based QuickNXS[1] reduction program with graphical user interface. It allows the normalization and stitching of several time-of-flight based measurements and is optimized for easy usability. The program does reduction of reflectivity, off-specular scattering and GISANS measurements for polarized measurements. Scripting options are limited and there is no support for more than one θ value per file. The raw data views of the GUI mimic the ones used in the instrument control software (dcomclient).

ISIS and SNS are planning to incorporate a QuickNXS based interface into the Mantid framework. In the current stage the program is not instrument independent.

2.1.3. Data reduction of Selene measurements at AMOR of SINQ

At the AMOR instrument at SINQ user experiments are already employing the Selene guide prototype for many measurements. Right now the data reduction is performed with pearl scripts (amorreducer, selenereducer), which perform the normalization of datasets. The output data can be used to look at the raw data against various axes and with different normalization stages.

The scripts are limited to command line operation and the current SINQ data acquisition model does not allow event mode operation or treatment of polarization states. As the mode of operation is very new the analysis script is still under active development and testing. It can be expected that several aspects of the data treatment algorithm needs to be changed during the *Estia* development phase and beyond.

2.2. Missing analysis tools

As the important steps for data reduction is the only analysis tool necessary for reflectometry there is no need for additional tools, only improvement of the currently used procedures.

2.3. Points for improvement in currently used software

2.3.1. Live data reduction

Especially with the decreased measurement times expected at ESS it is essential to quickly generate reflectivity curves to be able to decide on future experimental steps. The currently used data reduction at SNS and SINQ do not allow access to live data and therefore lead to unnecessary delays of such decisions.

2.3.2. Synergy between instrument planning and data reduction

Many parameters necessary for the data reduction are already known during the planning of the experimental script. One example would be the mapping of run numbers to individual reflectivity measurements. This aspect could be used to speed up the reduction process by recording such information to the data files during acquisition.

2.3.3. Connection to modeling software

Some of the reflectivity programs allow expansion through plugins (e.g. GenX), which could be used to form a connection to the data reduction software. This could be used to quickly refine the recorded spectra, especially in combination with live data. This

way the refinement could be improved while data is recorded and after the measurement is finished the results would instantly be available.

2.3.4. Refinement servers

Large amounts of measurement data necessitates quick refinement. Although reflectivity data generally can be fitted with a normal personal computer, a dedicated refinement server would be necessary for sets of e.g. parameter dependent reflectivity measurements.

2.3.5. Error estimation

Least squares refinement of reflectivities is often done with non-linear weighting as the information about the sample structure is within oscillations that drop after the cricical edge of total reflection with $\approx q_z^{-4}$. Up to now it has been hard to estimate actual errors on the retrieved model parameters/scattering length density profiles. Mathieu Doucet at SNS data analysis is investigating a Monte-Carlo based method of varying starting parameters and data points to help with this estimation. This effort could be picked up for ESS reflectometer, as well, as it is instrument independent.

2.4. Instrument specific aspects

2.4.1. Data normalization

Especially *Estia*'s high intensity mode requires a more complicated treatment during data reduction. The 2D data needs to be binned into q_z ranges and normalized by some kind of incident spectrum measurement. This incident spectrum could be a direct beam or super-mirror measurement. Depending on the measurement conditions of these reference spectra the data normalization is performed differently (a direct beam measurement has inverse θ direction on the detector, super-mirrors have a q_z dependent intensity).

The software needs to be flexible enough to allow certain instrument parameters to be overwritten (e.g. wrong θ calibration during measurement) while at the same time allowing quick reduction of standard measurements for users.

2.4.2. Resolution function

The resolution of individual points on the reflectivity will be λ and θ dependent. The reduction process must be able to correctly calculate these resolutions as they are used in the simulation programs and can considerably change the model.

2.4.3. Flexible q-binning

As reflectivity datasets span a large intensity range and the same q_z will be measured with different wavelengths and angles in the high intensity mode, a constant $\frac{\Delta q_z}{q_z}$

binning will not produce the optimal results possible. A flexible binning based on measured intensity would allow to have the best point resolution while keeping the statistics as necessary.

Another option would be to directly model the measured data using the known resolution function. This option would approximately square the number of necessary calculation points and therefore have considerable performance impact.

3. Concepts of Operation

3.1. Geometry

«Filled in later.»

3.2. Estia operation modes

3.2.1. Almost conventional reflectivity

measurement scheme   This mode corresponds to the conventional TOF reflectometry, where the beam divergence and footprint size are defined by slits. The angle of incidence and the divergence are constant for the duration of one pulse. Using the *Selene* guide the footprint is defined by the virtual source. For adjusting the divergence one slit (the aperture) behind the last guide element is sufficient.

Due to the analogy with conventional TOF reflectometers, the data collection, normalisation and further treatment for one angle of incidence follow exactly the procedure used there.

An additional feature when using a wide divergence cut down by a narrow aperture is that by moving this aperture in between measurements, one can change θ without rotating the sample.

Figure 3.1.: Sketch to illustrate the operation scheme: the beam (gold) is transported with the full divergence and without chopping to the end of the guide system. There an aperture (black) defines $\Delta\theta$, and its position together with the sample orientation ω also the angle of incidence θ. The beam footprint on the sample is defined by size and orientation of the virtual source.

Data acquisition

The width of the q_z-range covered in one measurement with constant θ is rather small (given by $\lambda_{\max}/\lambda_{\min} = 1.88$). Thus in most cases several sample orientations are needed, which results in longer measurement times due to the movement of the detector. A possible combination of angles of incidence θ with 4% overlap is given in table 3.1.

The wide divergence of the incoming beam opens the opportunity to cover the first 4 angles by moving the aperture rather than by rocking sample and detector. The

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$\frac{q_z}{{}^{-1}}$	$\frac{\theta}{\deg}$	$\frac{\omega}{\deg}$	$\frac{\omega}{\deg}$	$\frac{\text{offset}}{\deg}$
$0.005 \rightarrow 0.009$	0.21	−1.04	−0.40	−0.64
$0.009 \rightarrow 0.017$	0.39	−0.86		−0.46
$0.016 \rightarrow 0.030$	0.69	−0.56		−0.16
$0.029 \rightarrow 0.055$	1.25	0.00		+0.40
$0.052 \rightarrow 0.099$	2.25	1.00		
$0.094 \rightarrow 0.178$	4.05	2.80		
$0.170 \rightarrow 0.320$	7.29	6.04		
$0.306 \rightarrow 0.575$	13.12	11.87		
$0.551 \rightarrow 1.036$	23.62	22.37		

Table 3.1.: q_z-ranges covered with one sample orientation. The third column gives the corresponding angle of incidence θ and the forth column the sample tilting with respect to the long half axis of the *Selene* guide, ω. The wide divergence of the beam incident on the aperture allows within limits for changing θ by moving the aperture. This is illustrated in columns 5 (ω) and 6 (offset of the aperture). The limit for the offset is $\pm 0.75°$.

actual counting times will stay the same, but the switching between the settings is much faster (a few pulses might be lost by repositioning the aperture).

Discussion

This is the method of choice if off-specular scattering is to be measured, or in cases when the background caused by off-specular or diffuse scattering has to be separated or reduced.

The performance of *Estia* in this mode is expected to be very close to other concepts since the beam intensity and thus the measurement times are essentially given by the brilliance transfer of the guide.

The instrument-intrinsic resolution $\Delta\lambda/\lambda$ varying from 2% to 4% between 9.4 and 5 leads to a saw-tooth-like shape of the resolution function of the full measurement (see figure **??** d). For all measurements requiring moderate to low resolution (which is the by far largest fraction) this is completely fine **??**. For higher resolution the λ-θ-encoding mode described in the next section has to be chosen.

3.2.2. λ-θ-encoding

The strengths of the λ-θ-encoding are the wider q_z-range accessible with one angular setting, a possible constant $\Delta q/q$, and eventually the *nicer* off-specular area, compared to the almost conventional mode.

the measurement scheme There are (at least) two possibilities to obtain a λ-θ-encoding: either by using the pulsed structure and varying the angle of incidence θ with time - and thus with λ. Or to spectraly analyse the beam (no pulsed beam is needed) e.g. by reflecting on a multilayer monochromator, or by refraction using a prism [**?**].

Figure 3.2.: Sketch to illustrate the operation scheme: the beam (gold) is transported with the full divergence and without chopping to the end of the guide system. As in the conventional mode **??**, a slit (black) defines $\Delta\theta$ and together with the sample orientation ω also the angle of incidence θ. But the opening and position change during the passing of each pulse. This way high θ can be related to low λ and vice versa.

scanning aperture The divergence-defining aperture behind the guide exit scans across the convergent beam in the direction of the sample normal for each pulse and thus creates a λ-θ-encoding. Figure 3.2 shows the principle. The aperture position defines $\theta(\lambda \propto t)$. For covering a wide q_z-range it should be located at the high-θ edge at the time the 5 neutrons arrive and at the low-θ edge for 9.4. The aperture opening defines $\Delta\theta$. Thus a variation of the slit-width Δy with time can be used to realise $\Delta\theta/\theta = \text{const}$, or more sophisticated, $\Delta q/q = \sqrt{(\Delta\lambda/\lambda)^2 + (\Delta\theta/\theta)^2} = \text{const}$, where $\Delta\lambda = \text{const} \approx 0.2$ here.[1]

As long as both blades forming the aperture are in one plane, the resolution $\Delta\lambda/\lambda$ is not affected. By separating the blades along the flight direction x one can realise a set-up analogue to the blind double chopper concept by Ad van Well [**?**]. Looking at one neutron trajectory (and assuming a continuous beam for the beginning), the two blades create a pulse with $\Delta\lambda/\lambda = \Delta x_a/x_{ad} = \text{const}$, where x_{ad} is the distance from the aperture mid-point to the detector, and Δx_a is the separation of the blades. The same is true for any trajectory as long as the edges of the blades are exactly in line with the sample at all times. I.e. they move with slightly different speeds. With the continuous beam this is a TOF set-up with time-zero varying with angle of incidence θ. With the pulsed beam and coupling θ to λ the band-width of the beam arriving at the aperture is restricted to $\Delta\lambda = 0.2$, which is the resolution of the encoding. The latter affects only the off-specular resolution of the measurement.

Given the intrinsic resolution of $\leq 4\%$, a constant $\Delta\lambda/\lambda$ is only useful for 1% or 2%, which corresponds to a separation $\Delta x_a = 84\,\text{mm}$, or $168\,\text{mm}$, respectively.

spectral analysis using a multilayer A ML monochromator at or before the virtual source encodes the wavelengths of the neutrons in the final angle of the monochroma-

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[1]Solving this equation for $\Delta\theta$ gives (l is the slit-sample distance):

$$
\begin{aligned}
\Delta\theta(t) &= \theta(t)\sqrt{\left(\frac{\Delta q}{q}\right)^2 - \frac{\Delta\lambda^2}{(\lambda_{\min} + (\lambda_{\max} - \lambda_{\min})(\theta(t) - \omega + \epsilon)/\Delta\theta_{\text{beam}})^2}} \\
&\approx \arctan\frac{\Delta y(t)}{l} \\
\theta(t) &= \omega + \epsilon + \frac{\Delta\theta_{\text{beam}}}{2} + \frac{\lambda(t) - \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}}\Delta\theta_{\text{beam}} \\
&= \omega + \arctan\frac{y(t)}{l}
\end{aligned}
$$

Figure 3.3.: Illustration of the principle of the λ-θ-encoding. A convergent white (pulsed) beam is spectral analysed by a ML monochromator (a). The beam then propagates to the sample keeping the relation between λ and θ (b). For a pulsed beam at any time an almost monochromatic beam is impinging on the sample, where θ and $\lambda \sim \theta$ vary with time. The sketches (c) to (e) show snap-shots of the beam within the *Selene* guide system and after the sample. In (f) to (i) the corresponding situation on the sample is shown.

tor.[2] For small θ one gets $\theta \propto \lambda$. The specular reflectivity from the sample then leads to a diagonal streak in $I(\lambda, \theta)$ on the detector, so that off-specular scattering can be measured. Figure 3.3 shows *snap-shots* of the beam-distribution within the guide and at the sample.

The resolution in q_z is essentially given by the ML monochromator and can reach 2%, while the TOF resolution influences Δq_x. So this mode could be realised without any chopper.

The guide geometry, its coating and the wavelength-range define $\Delta \theta$ **??**, i.e. for $\lambda \in [5, 9.4]$ and $\Delta \theta = 1.5°$ one gets $m \approx 3.4$ with $\theta \in [1.7°, 3.2°]$. A plateau of total reflection ($m \leq 1$) results in $\theta \leq 1°$ for the same λ-range. Thus totally reflected neutrons do not reach the guide.

A ML monochromator leads to an illumination of the *off-specular region* on the detector by diffuse and off-specular scattering at the multilayer, but also by specular scattering away from the Bragg condition. This can be seen in figure **??**. The off-specular contribution can be suppressed by the virtual source diaphragm if the monochromator is located before it. An additional scanning aperture the sample (see above) can be used to filter the unwanted specular intensity from the monochromator. This combination allows for a clean beam and a high and constant resolution.

Data acquisition

Also the data acquisition follows the scheme of the almost conventional reflectometry. Only the number of q_z-ranges is reduced, and the counting times are increased. Table 3.2 gives a set of possible orientations ω and the related θ- and q_z-ranges.

Figure 3.4 shows a simulated $I(\lambda, \theta)$-map for $\omega = 5°$. The sample is a Ni/Ti multilayer with artificial off-specular scattering[3] The diagonal specular streak is clearly

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[2] In principle one could use the monochromator itself as the virtual source: It has to have the shape and orientation of the sample or smaller for under-illumination. But in this case all scattering from the monochromator, specular and off-specular, is focused to the sample and results in background in the off-specular signal from the sample.

[3] The specular reflectivity was simulated with EDXR [**?**] The off-specular signal is *generated* by convolution of the specular reflectivity $R(q_z)$ with 2 Gaussian functions $R(q_x, q_z) = R(q_z) * (g_1(q_x) + g_2(q_x))$. with a cut-off at the sample horizon. A bending of the Bragg sheets, Yoneda wings and the low-intensity region between Yoneda and horizon are not produced this way. Within McStas this folding is achieved by randomly adding a q_{xy} component, but with a Gaussian probability distribution centred at $q_{xy} = 0$.

ω	$\theta_{\min}$	$\theta_{\max}$	$q_{z\,\min}$	$q_{z\,\max}$
deg	deg	deg	$^{-1}$	$^{-1}$
-0.4	0.1	1.6	0.003	0.068
1.7	2.2	3.7	0.052	0.160
5.0	5.5	7.0	0.128	0.305
10.0	10.5	12.0	0.253	0.522

Table 3.2.: Sample orientations ω and related θ- and q_z-ranges as used for the simulations shown below.

visible. Its width is given by the opening of the scanning aperture. The Bragg peaks show the resolution for the specular intensity to be oriented along lines originating from $(\lambda = 0, \theta = 0)$. The visible off-specular Bragg-sheets are inclined with respect to these.

Figure 3.4.: Intensity-map $\log_{10}[I(\lambda, \theta)]$ of the NiTi multilayer for $\omega = 5°$. The map is already corrected for $I(\lambda)$ of the incoming beam.

Normalisation and integration

Normalisation for the off-specular region is a bit more complicated than discussed in the general part for specular reflectometry because there is no reference sample with a well-known high-intensity off-specular scattering.

Most likely one has to use the specular reference to also scale the off-specular region, taking inhomogeneities of the detector into account. An alternative, but time-consuming approach is to perform an ω-scan with the reference sample. After illumination correction this mimics an off-specular signal with specular intensity, and the latter is known.

Here, for normalising the simulations a perfect reference sample was assumed, and the *measurement* was repeated without the scanning aperture. Figure 3.5 shows the $I(q_x, q_z)$-maps obtained for the four ω orientations, and figure 3.6 the resulting $R(q_z)$ curves.

Discussion

The λ-θ-encoding mode allows to cover the most often used q_z-ranges with 2 to 4 sample orientations. With the encoding performed by a co-planar scanning aperture the off-specular region up to $q_x \approx \pm 3 \cdot 10^{-3}\ ^{-1}$ is accessible. The varying resolution from 2% to 4% for each range results in a mismatch in the overlapping regions. For a consistent data treatment the individual measurements should be convoluted to constant 4% before merging and comparison to a simulated curve.

The main outcome of the simulation is that a good separation of specular and off-specular reflectivity can be reached with the λ-θ-encoding. The number of angular

Figure 3.5.: Intensity-maps $\log_{10}[I(q_x, q_z)]$ of the NiTi multilayer for $\omega = 5°$ (top), and for all sample orientations given in table 3.2, obtained by summation over the individual maps (left). There is no total reflection plateau visible, here. This is a result of the insufficient computing statistics of the presented map.

Figure 3.6.: $R(q_z)$ of the NiTi multilayer, obtained from the maps shown in figure 3.5 with a binning of $\Delta q/q = 1\%$. The green line is the initial reflectivity convoluted to $\Delta q/q = 2\%$. The data set for $\omega = -0.4°$ clearly shows the insufficient computational statistics. The other data points show a systematic tilt to lower intensities for small q_z. This originates from an improper choice of the Gaussian, widening the specular intensity in q_x direction. This width is larger than the 2% resolution used for data analysis, and thus part of the specular intensity is missing.

settings to cover $q_z \in [0.01, 0.5]^{-1}$ is reduced to 4 relative to the conventional mode needing 7 settings (with 10% overlap).

The next step will be to use an aperture with shifted blades, allowing for a constant high resolution (for the cost of longer counting time).

3.2.3. High intensity mode

the measurement scheme The full beam leaving the *Selene* guide is directed to the sample. The reflected beam is measured with an area-sensitive detector, who's distance and resolution defines the angular resolution $\Delta\theta$ (see figure 3.7). Each intensity curve obtained by integrating over the detector normal to the scattering plane for a given position along the scattering vector (i.e. a certain θ) corresponds to one TOF measurement. This is illustrated in figure **??**.

The increase of specularly reflected intensity is about an order of magnitude with respect to the conventional set-up, or with the λ-θ-encoding. The price to be payed

is that the off-specular resolution gets completely lost. The off-specular scattering corresponding to one θ-channel forms a background for all other channels. Most likely there is no way to de-convolve the specular and the off-specular signals.

Figure 3.7.: Sketch to illustrate the high-intensity specular reflectivity operation mode.

Simulation

Data acquisition and reduction is shown below for a simulated experiment. The corresponding real life experiment is discussed in section ??.

the sample The sample used for this simulations is a multilayer of the composition

$Si(179\,) / Fe(12\,) / Cu(462\,) / \text{Si-substrate}$

The ideal reflectivity was simulated using EDXR [?], where the SLD for magnetic Fe was chosen to be $14.096 \cdot 10^{-6}\,^{-2}$ for $Fe^{|+\rangle}$, and $2.096 \cdot 10^{-6}\,^{-2}$ for $Fe^{|-\rangle}$, respectively. No off-specular or incoherent scattering was assumed. The binning is $\Delta q = 4.4 \cdot 10^{-4}\,^{-1}$. The substrate area is $5 \times 5\,\text{mm}^2$.

The sample for this example was inspired by work of B. Wiedemann, TUM, who investigates the magnetic behaviour of thin iron films during growth. According in-situ measurements were performed at REFSANS, MLZ, and on Amor, PSI, using the *Selene* prototype ??. Feasibility studies for the latter were performed with a sample similar to the one used in these simulations, but with a larger area.[4] Figures ?? and ?? show the experimental raw-data, the reduced $I(\lambda, \theta)$-map and the resulting reflectivity curves.

Data acquisition

To cover $q_z \in [0.01, 1]\,^{-1}$ there are 6 angular settings necessary (with a large overlap of 20%). The following table gives the sample tilt ω, and the corresponding θ-range and q_z-range.

Figure 3.8 (a) shows the $I(\lambda, \theta)$-map for $\omega = -0.3°$. For normalisation here an ideal supermirror ($R(q_z) = 1 \forall q_z$) was assumed. The corresponding intensity map is shown in figure 3.8. It can be seen there that the highest intensity occurs at low λ and high θ. The first finding results from the choice of the λ-range ??. The second finding results from the increasing projected sample area for larger θ.

Figure 3.8 (e) shows the simulated $R(q_z)$ data points obtained by projection of $\mathbf{R}(\lambda, \theta)$ onto q_z.

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[4]For the off-situ experiments the Fe-layer was prevented from oxidation by covering it with the Si-layer.

ω	$\theta_{\min}$	$\theta_{\max}$	$q_{z\,\min}$	$q_{z\,\max}$
deg	deg	deg	$^{-1}$	$^{-1}$
−0.3	0.2	1.7	0.005	0.074
1.8	2.3	3.8	0.054	0.166
5.0	5.5	7.0	0.128	0.305
10.0	10.5	12.0	0.253	0.522
17.5	18.0	19.5	0.412	0.834
30.0	30.5	32.0	0.677	1.102

Table 3.3.: Sample orientations ω and related θ- and q_z-ranges for the simulations. The time t is determined by the highest relative error of 14% after re-binning to 2.5%.

Figure 3.8.: Simulated intensity-maps $I(\lambda,\theta)$ for a sample with the composition (a) $Si\,(179\,)\,/\,Fe\,(12\,)\,/Cu\,(462\,)\,/\,Si$ and a size of $5\times5\,\mathrm{mm}^2$, and for a perfect supermirror with the sample shape (b), respectively. Map (c) is obtained by pixel-wise division of maps (a) and (b). For map (d) λ was converted to q_z. Integration along θ and re-binning to $\Delta q/q = 2.5\%$ lead to the red marks in diagram (e). The green line is obtained by convolving the initial $R(q_z)$ used for the simulations with $\Delta q/q = 2.5\%$.

The complete procedure was repeated for all ω settings mentioned in table 3.3, and the resulting individual reflectivity curves as well as the merged curve are shown in figure 3.9.

Discussion

counting time The gain of the high-intensity mode over the λ-θ-encoding mode in the present case is a factor 20 for the lowest ω and decreases for increasing ω. The reason is that in the encoding mode $\Delta\theta$ and thus the slit-opening are proportional to θ. At $\omega \approx 30°$ ($\theta \in [30,5°,32°]$) the aperture opening corresponds to half the full divergence. The time-gain there is only about a factor 2.

The average reduction in counting time for a moderate q_z-range (up to $\approx 0.5\,^{-1}$) is one order of magnitude.

For larger samples, relaxed resolution (binning) requirements, or lower counting statistics it is possible to reach the split-second time-scale for time-resolved measurements. The q_z-range one can cover in one shot e.g. spans from $0.01\,^{-1}$ to $0.085\,^{-1}$.

resolution Even though the resolution function is quite complex, the final $R(q_z)$ curve follows the simulated curve convoluted with 2.5% resolution up to high q_z. So even without a data treatment as suggested in section ?? a reasonable result is achievable in the high-intensity mode. This is in agreement with the experimental findings obtained with the *Selene* prototype.

dynamic range The dynamic range of 8 orders of magnitude obtained in the simulations is not realistic. The simulations ignored all background from the sample itself,

Figure 3.9.:   Specular   reflectivity $R(q_z)$ of   the   multilayer
$Si\,(179\,)\,/\,Fe\,(12\,)\,/\,Cu\,(462\,)\,/\,Si$.   The   green   curves   correspond   to
the ideal reflectivity, convoluted with $\Delta q/q = 2.5\%$, the upper red and
blue data points were obtained by simulations in the high-intensity
specular mode for various sample orientations ω 3.2.3. These are scaled
by 10 for clarity. The lower red data points were obtained by merging the
individual *measurements*. The binning has a width of $\Delta q/q = 2.5\%$. The
gray curve gives the relative error of the merged $R(q_z)$, the straight gray
line is at 0.14.

from the sample environment, and from the detector. And the sample was assumed
to show no off-specular or diffuse scattering.

3.3. Measurement examples

«Filled in later.»

A. Appendix 1

A.1. List of reflectivity simulation software

AFIT -

drydoc http://material.fysik.uu.se/Group_members/adrian/drydoc.htm

GenX http://genx.sourceforge.net

lprof Adrian.Rennie@fysik.uu.se

Motofit http://motofit.sourceforge.net/wiki/index.php/Main_Page

Parratt http://www.hmi.de/bensc/software/index2.html

Reflpak http://www.ncnr.nist.gov/reflpak

slab_fit cubitt@ill.fr

wetdoc/wetlay Adrian.Rennie@fysik.uu.se

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