



ReMagX^{V1.1}

(x-ray magnetic reflectivity tool)



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Documentation for ReMagX V1.1.0(build4) and dbEditor V1.0

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ReMagX is a simulation and fitting tool for X-ray reflectometry (XRR) data and especially for X-ray resonant magnetic scattering (XRMR). XRMR is a technique which extends standard X-ray reflectometry by the additional contrast from X-ray magnetic circular dichroism. It provides chemical and magnetic depth profiles of thin layered samples. ReMagX was developed by the group of Dr. E. Goering in the dept. of Prof. G. Schütz at the Max Planck Institute for Metals Research in Stuttgart, Germany. The project started in 2004 as part of the Diploma thesis of Max Harlander. Later, several extensions and improvements were added and in the meantime ReMagX has evolved into a powerful and highly versatile tool for XRMR and also XRR. For further reading and theoretical background of most features refer to:

Max Harlander Diploma thesis, University of Stuttgart 2005.

Untersuchung über die Grenzflächenmagnetisierung an (FM) Kobalt- und (AFM) Eisen-Mangan-Schichten.

Sebastian Brück PhD thesis, University of Stuttgart 2009

Resonant Magnetic Reflectometry on Exchange Bias Systems.

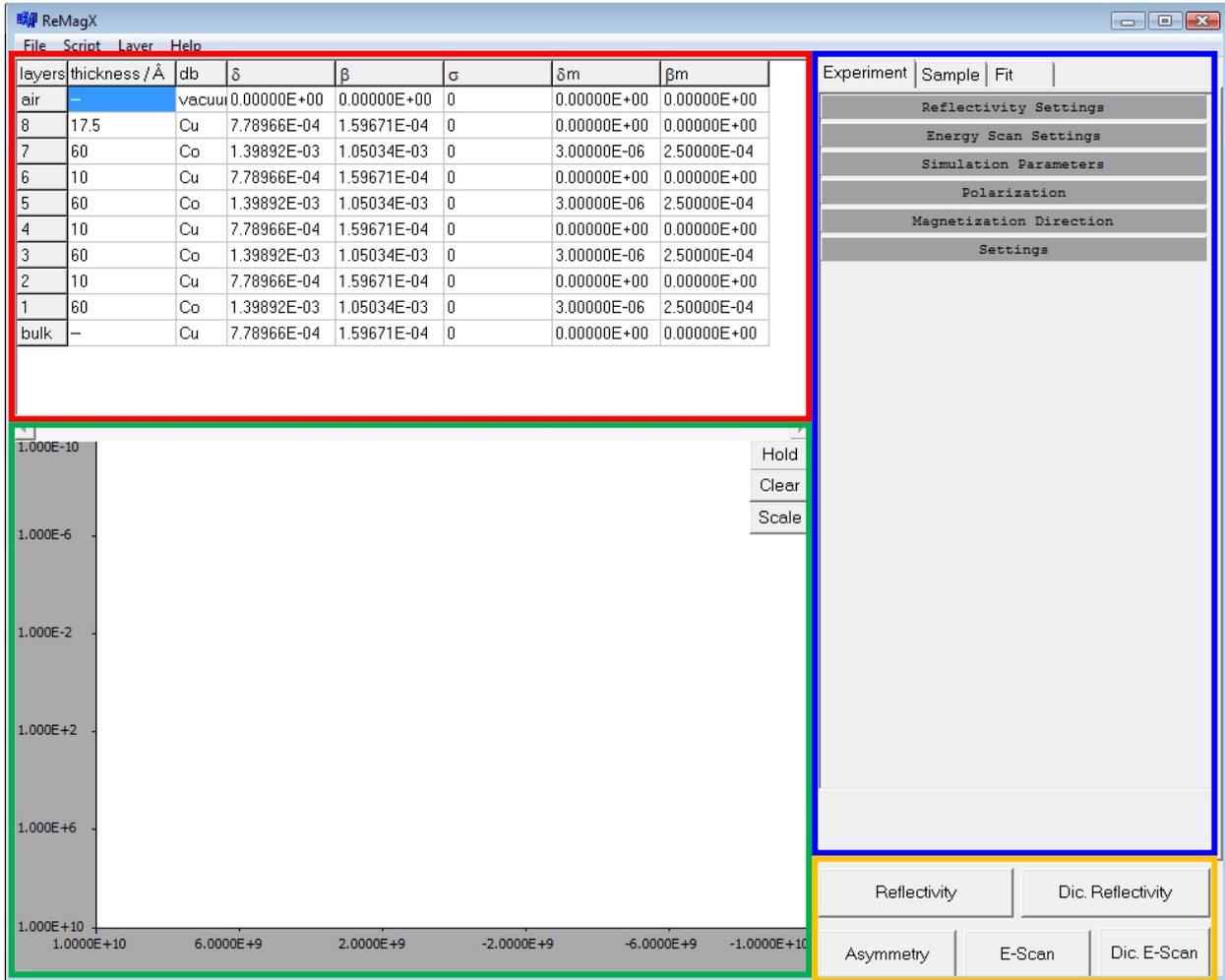
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I. Getting Started

A – Overview and Startscreen

Start ReMagX either from the start menu or directly double clicking the .exe file. After the start-up screen, you will see the following window:



It consists of four different sections:

Layer Input Table – contains all parameters for the individual layers

Plot Window – graph window for plotting curves

Settings Tabs – control of the simulation, experiment, fit etc. parameters

Buttons – buttons for starting a simulation

B – Layer Input Table – defining the sample...

The layer input table defines the sample layer-by-layer:

edit	thickness / Å	db	δ	β	σ	δ_m	β_m
air	--	vacuum	0.00000E+00	0.00000E+00	0	0.00000E+00	0.00000E+00
1	60	Co	1.33000E-03	1.09753E-03	0	-2.74280E-04	-1.82470E-05
2	10	Cu	7.30049E-04	1.78421E-04	0	0.00000E+00	0.00000E+00
3	60	Co	1.33000E-03	1.09753E-03	0	-2.74280E-04	-1.82470E-05
4	10	Cu	7.30049E-04	1.78421E-04	0	0.00000E+00	0.00000E+00
5	60	Co	1.33000E-03	1.09753E-03	0	-2.74280E-04	-1.82470E-05
6	10	Cu	7.30049E-04	1.78421E-04	0	0.00000E+00	0.00000E+00
7	60	Co	1.33000E-03	1.09753E-03	0	-2.74280E-04	-1.82470E-05
8	10	Cu	7.30049E-04	1.78421E-04	0	0.00000E+00	0.00000E+00
bulk	--	Cu	7.30049E-04	1.78421E-04	0	0.00000E+00	0.00000E+00

1
2
3
4
5
6
7
8

- 1 - **The index of the layer**...this index is used to reference its parameters, e.g thickness[2] for the thickness value.
- 2 - **Thickness of the layer** in Ångström (10^{-10} m)
- 3 - **Filename of the optical constants database file** without ending (here Co.db, Cu.db, and vacuum.db). Files have to be in the ReMagX.
- 4 - Optical constant **Delta**, for the given energy (either from .db file or entered manually)
- 5 - Optical constant **Beta**, same as Delta
- 6 - **Sigma**, RMS roughness in Å between the layer and the one above!
- 7 - **Magnetic Delta**, magneto optical constant (see remarks below)
- 8 - **Magnetic Beta**, see *Magnetic Delta*

The example system is a multilayer consisting of 4x[Cu (10Å) / Co (60Å)] on a Cu substrate. The optical constants provided correspond to a X-ray energy of 900eV and the .db filenames to the files shipped with this version of ReMagX (check the installation directory).

Remarks:

Delta (δ) and Beta (β) are the optical constants (dispersive and absorptive part) of the material according to the standard notation of a complex index of refraction: $N = 1 - (\delta + i\beta)$.

Sigma (σ) is the RMS roughness according to standard notation in surface science.

Magnetic delta (δ_m) and beta (β_m) are the variation of the optical constants due to magnetism. **NOTE: the values are added/subtracted to the normal optical constants!**

Note:

- Select a cell on the "layer input table" by left mouse click

Layer	δ	β
vacuum	0.00000E+00	0.000
Cu	7.78966E-04	1.596
Co	1.39892E-03	1.050
Cu	7.78966E-04	1.596

- Change a parameter by double clicking it

Layer	δ	β
vacuum	0.00000E+00	0.000
Cu	7.78966E-04	1.596
Co	1.39892E-03	1.050
Cu	7.78966E-04	1.596

- Select a cell and right click for additional options

Layer	δ	β	δ_m	β_m
vacuum	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
Cu	7.78966E-04	1.59671E-04	0	0.00000E+00
Co	1.39892E-03	1.05045E-03	0	0.00000E+00
Cu	7.78966E-04	1.59671E-04	0	0.00000E+00
Co	1.39892E-03	1.05045E-03	0	0.00000E+00
Cu	7.78966E-04	1.59671E-04	0	0.00000E+00
Co	1.39892E-03	1.05045E-03	0	0.00000E+00
Cu	7.78966E-04	1.59671E-04	0	0.00000E+00
Co	1.39892E-03	1.05045E-03	0	0.00000E+00
Cu	7.78966E-04	1.59671E-04	0	0.00000E+00

The additional options available from the dropdown menu are:

Fit	
UnFit	
Show Delta and Beta spectrum	
Add Layer	Ctrl+A
Remove Layer	Ctrl+R
Get delta/beta from database	
Get deltam/betam from database	

Fit

...select this parameter for fitting

UnFit

...de-selects fit parameter

Show Delta and...

...plots δ & β from the .db file

Add Layer

...adds a layer by duplicating the selected one

Remove Layer

...obvious.

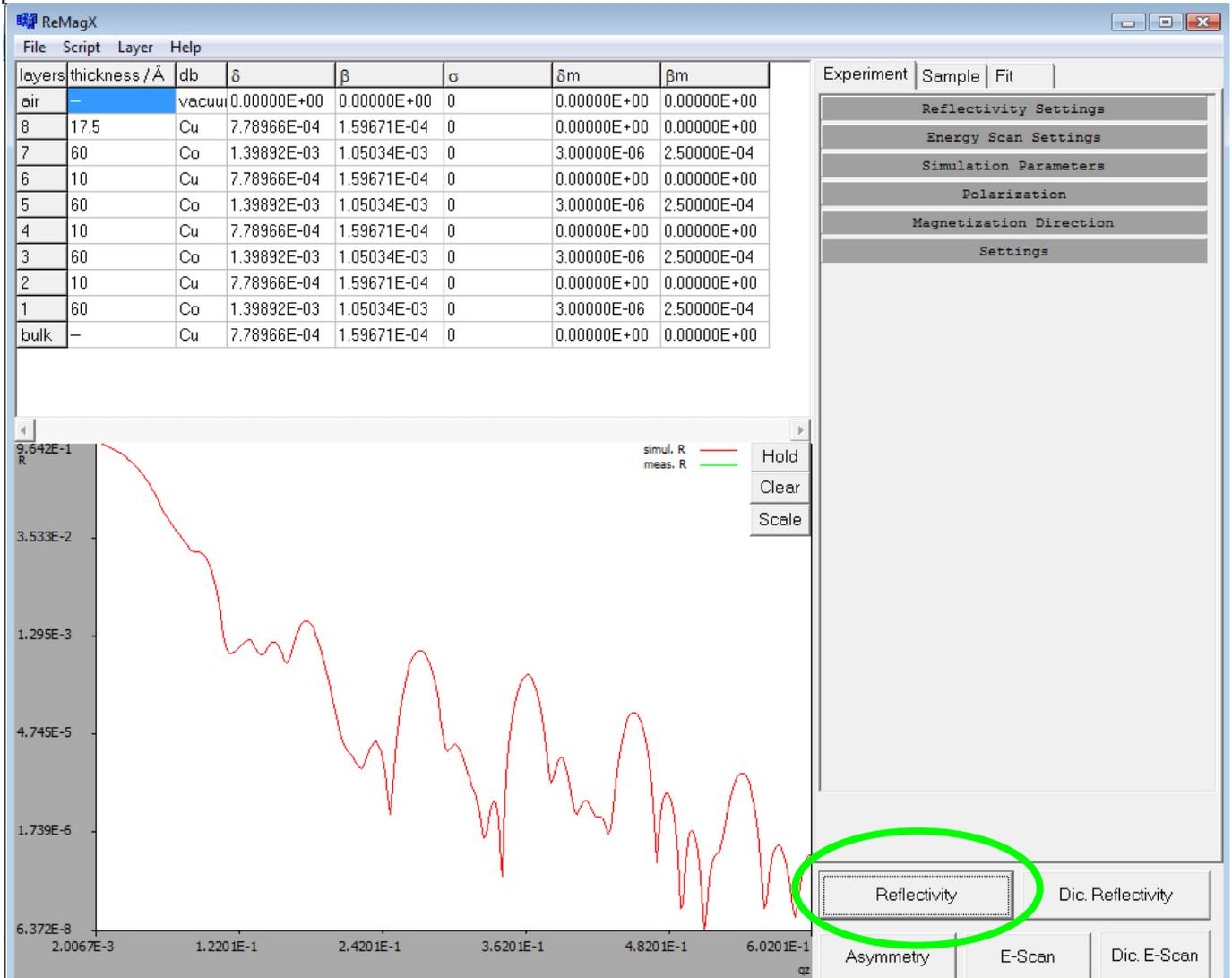
Get delta/beta from database

Loads δ, β from **.db file** for all layers

Loads δ_m & β_m from a **.m database file** for all layers.

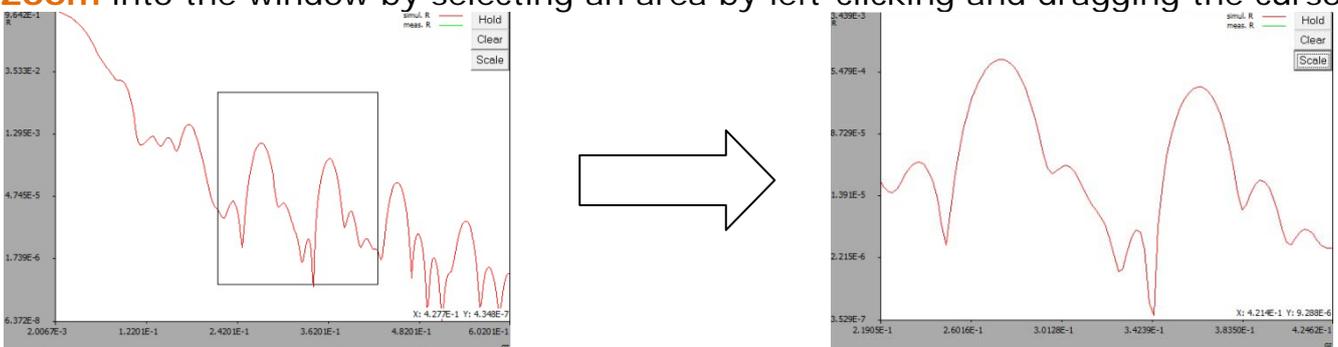
C – Plotting Curves

After starting ReMagX you can immediately use the default example to simulate reflectivity and also magnetic reflectivity. Press the **"Reflectivity"** button on the lower right. The reflectivity, for the given energy and sample-parameters, is then plotted in the lower window and the screen will look like this:



The plot window has several additional features:

Zoom into the window by selecting an area by left-clicking and dragging the cursor



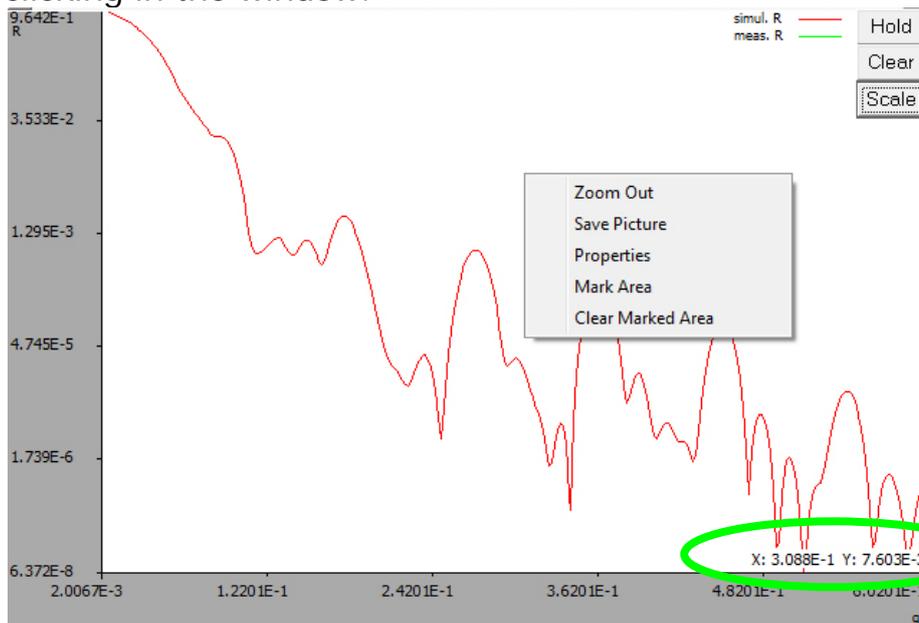
Buttons:

Hold ...locks the currently plotted curves. This allows comparing curves directly.

Clear...clears the plot window.

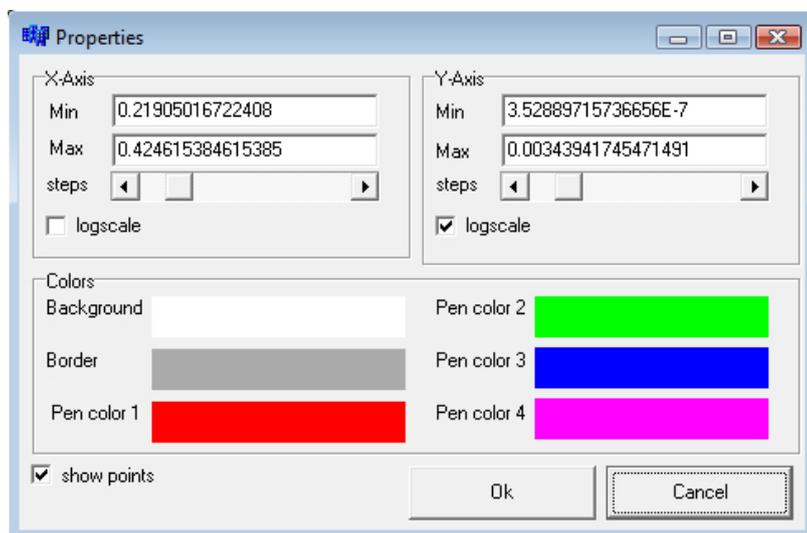
Scale...scales the plot to min./max. x- and y-values (replots curve).

More options are available from a dropdown menu which is accessed by right-clicking in the window:



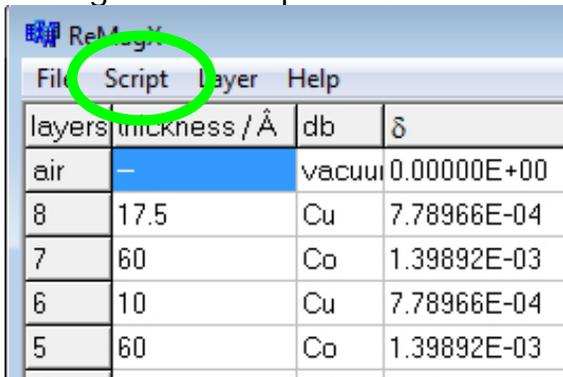
Note: When moving the cursor into the plot window, the x and y position of the cursor (tip of arrow) is plotted on the lower right of the window.

- Zoom out** ...self explaining.
- Save Picture** ...saves the plot window as .bmp image.
- Properties** ...curve colour, manual x- and y- scaling, logarithmic scaling etc.:



D – The Script Window

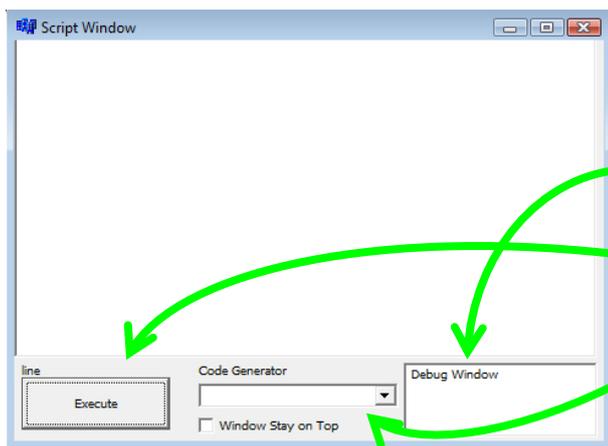
A new feature of ReMagX is the script feature which allows using LUA scripts in ReMagX. The script window which is accessible from the menu:



layers	thickness / Å	db	δ
air	–	vacuum	0.00000E+00
8	17.5	Cu	7.78966E-04
7	60	Co	1.39892E-03
6	10	Cu	7.78966E-04
5	60	Co	1.39892E-03

Note: Scripts are executed as the last step before calculating reflectivity.

The script window has four main items:



The window itself is for entering scripts. These are stored in the .all files of ReMagX.

The output (or **Debug**) window.

Press the **execute** button to manually launch your script.

Code Generator contains several script templates for ReMagX.

You can use the script window for example to define boundary conditions (which overrule the ReMagX internal boundaries), constraints, couplings etc. The script window uses the scripting language LUA (see: <http://www.lua.org/> or <http://de.wikipedia.org/wiki/Lua>) and therefore provides a large function pool (mathematical functions, control structures etc.).

ReMagX provides access to some of its parameters from the script window. The following list contains all ReMagX specific script variables:

Variable	Description	Type
<code>thickness[i]</code>	Thickness of layer i	Array of Decimals
<code>delta[i]</code>	Optical constant delta for layer i	Array of Decimals
<code>beta[i]</code>	Optical constant beta for layer i	Array of Decimals
<code>sigma[i]</code>	RMS roughness of layer i	Array of Decimals
<code>deltam[i]</code>	$\Delta\delta$ – magnetic change of δ of layer i	Array of Decimals
<code>betam[i]</code>	$\Delta\beta$ – magnetic change of β of layer i	Array of Decimals

<code>gauss_delta[i]</code>	Optical constant δ for Gaussian i	Array of Decimals
<code>gauss_delta[i]</code>	Optical constant δ for Gaussian i	Array of Decimals
<code>gauss_variance[i]</code>	Variance of Gaussian i	Array of Decimals
<code>gauss_z[i]</code>	Position z of Gaussian i	Array of Decimals
<code>Energy</code>	Energy	Decimal
<code>resolution</code>	Resolution	Decimal
<code>nlayers</code>	Number of layers	Integer

Note: the index i is the layer index according to the layer input table.

Examples

Imagine you want to fit a multilayer sample where every second layer has the same thickness...select `thickness[1]` for fitting (on the layer input table) and then define the following script in the script window:

```
for i = 3, 7, 2 do
    thickness[i] = thickness[1]
end
```

...the script window defines the `thickness[3]`, `[5]` and `[7]` to be equal to `[1]`. Another example could be a hardcoded constraint of the roughness like:

```
sigma[3] = sigma[1];
sigma[5] = sigma[1];
sigma[7] = sigma[6];
```

the Code Generator in the script window has even more examples for ReMagX specific problems.

But LUA can of course do more, for example (see the Debug window!):

```
function PrintBottleNumber(n)
    local bs
    if n == 0 then
        bs = "No more bottles"
    elseif n == 1 then
        bs = "One bottle"
    else
        bs = n .. " bottles"
    end
    return bs .. " of beer"
end

for bn = 99, 1, -1 do
    write(PrintBottleNumber(bn), " on the wall,")
    write(PrintBottleNumber(bn), "")
    write("Take one down and pass it around,")
    write(PrintBottleNumber(bn-1), " on the wall, ")
    write("")
end
```

```
write("No more bottles of beer on the wall,No more bottles of beer")  
write("Go to the store, buy some more!")
```

E – Importing measurement data

If you want to use experimental results with ReMagX they have to be in an ASCII text file with column like organization. An example might look like:

```
#qz R0 R+ R-
0.00 1 1 1
0.01 0.98 0.99 0.97
0.02 0.94 0.96 ...
```

Note: The default separator is a tab between the columns.

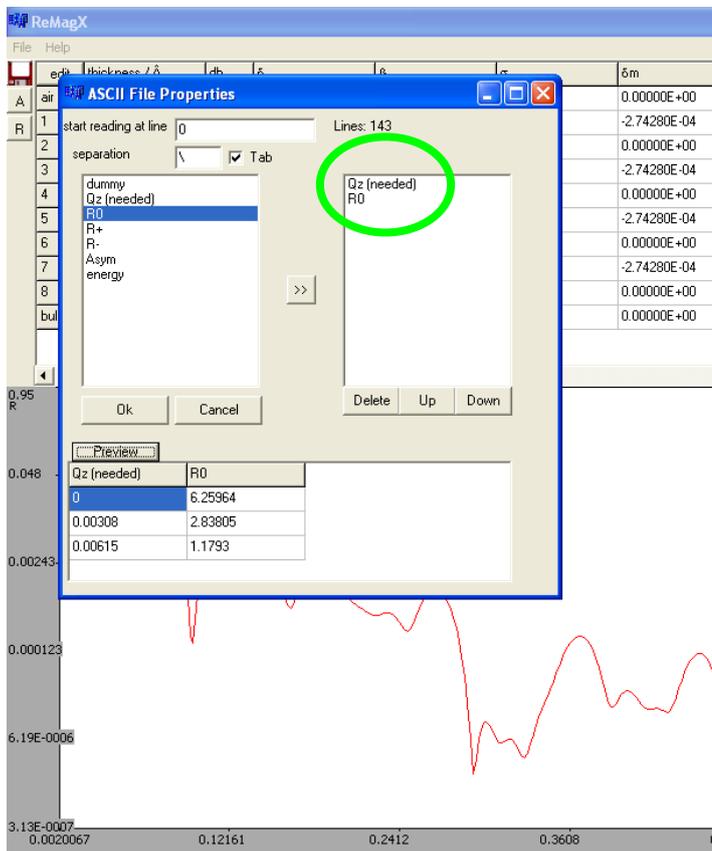
The columns are the non-magnetic reflectivity **R0**, the dichroic reflectivity with positive field **R+** and the dichroic reflectivity with negative field direction of the magnetic field **R-**.

Note: the file has to use the **momentum transfer in z-direction, q_z** , as x values. The q_z for a given angle θ and energy E can be calculated using the following formula:

$$q_z = 0.001013546247 \cdot \text{Energy [eV]} \cdot \sin \theta \quad \text{or} \quad \frac{4 \cdot \pi \cdot e}{c \cdot h} \cdot 10^{-10} \cdot E[\text{eV}] \cdot \sin \theta$$

Here, c is the speed of light, h Plancks constant and e the elementary charge quantum.

If you have prepared your data file go to “**File**” in ReMagX and choose “**Load Dataset**”. A file dialog appears where the position of the data file can be chosen.

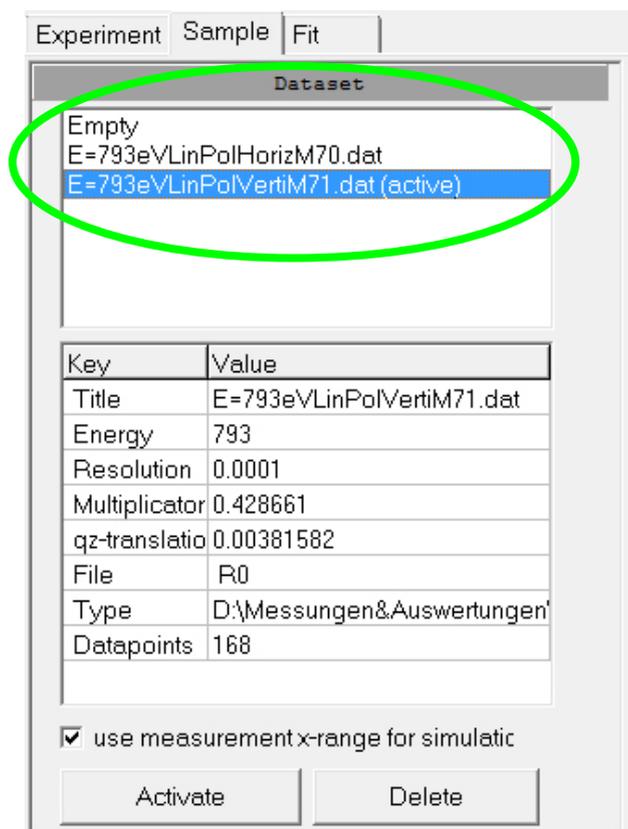


The next window is the data selector: This dialog lets you choose the columns and their order in the data file. In the example to the left already two columns have been chosen, q_z as first and **R0** as second column.

Note: The order has to be correct. If there are columns which you don't want to import in between place a “**dummy**” at their position.

You can check your selection by pressing “**Preview**”. If there is an error or some discrepancy between file and selection ReMagX will produce an error.

After successfully importing the dataset into ReMagX it is necessary to activate it. Therefore choose the "**Dataset**" section of the "**Sample**" tab. In the list you will find a new entry for the imported data. It is activated by **double-clicking** on it.



You have to provide some additional information for the dataset so it can be handled properly by ReMagX.

Refer to:
Dataset in the **B – Sample Tab** section on page **19**.
...for additional information

F – Using the fit function of ReMagX

The main task for ReMagX is to fit the simulated reflectivity, dichroic reflectivity or asymmetry to experimental data. The following steps will exemplify the fitting process using the Evolution algorithm:

The first step is selecting the free parameters of the fit. Select a parameter or several of them from the layer input table (for special parameters like e.g. the measurement multiplicator see the **Additional Fit Parameters** section of the **C – Fit Tab**). Right click on the layer input table and select **Fit** from the drop-down menu:

air	–	vacuum	0.00000E+00	0.00000E+00	0
8	17.5	Cu	7.78966E-04	1.59671E-04	0
7	60	Co	1.39892E-03	1.05034E-03	0
6	10	Cu	7.78966E-04	1.59671E-04	0
5	60	Co	1.39892E-03	1.05034E-03	0
4	10	Cu	7.78966E-04	1.59671E-04	0
3	60	Co	1.39892E-03	1.05034E-03	0
2	10	Cu	7.78966E-04	1.59671E-04	0
1	60	Co	1.39892E-03	1.05034E-03	0
bulk	–				

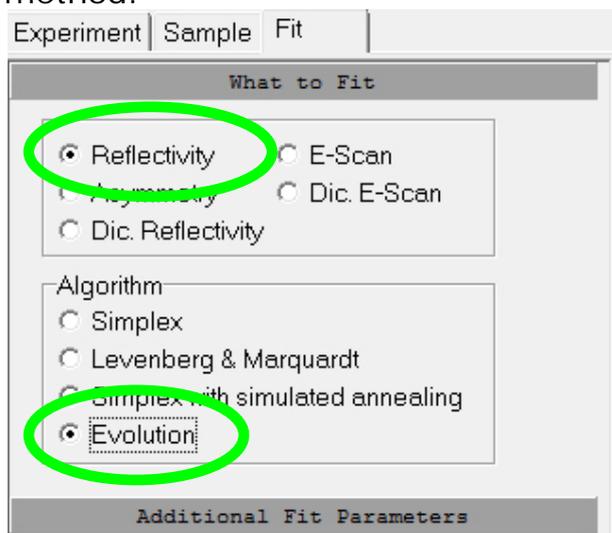
Parameters selected for fitting are marked red in the table:

layers	thickness / Å	db	δ
air	–	vacuum	0.00000E
8	17.5	Cu	7.78966E
7	60	Co	1.39892E
6	10	Cu	7.78966E
5	60	Co	1.39892E
4	10	Cu	7.78966E
3	60	Co	1.39892E

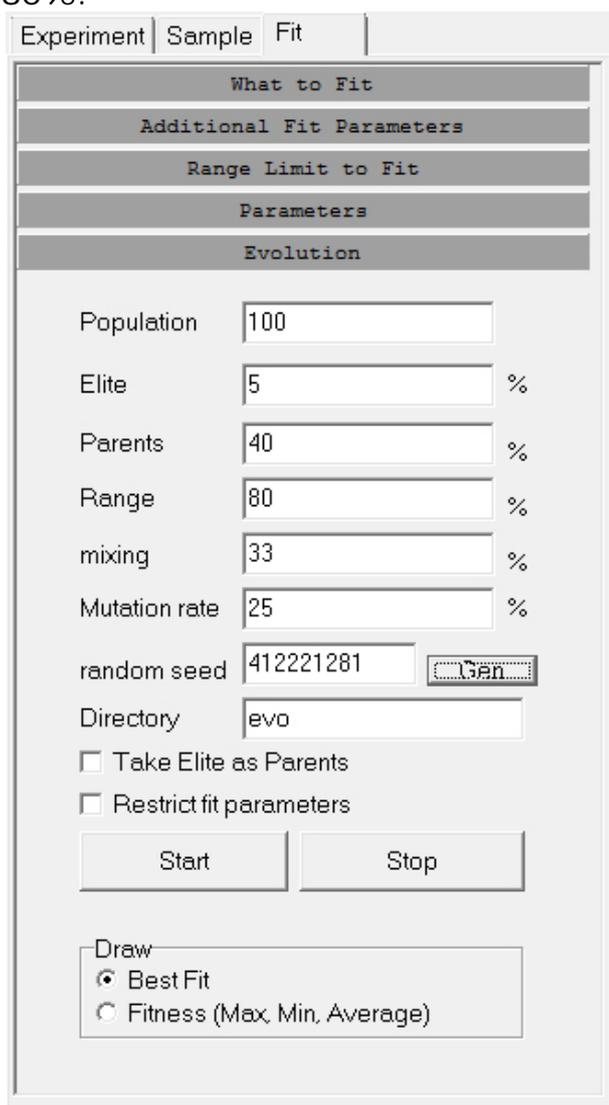
Next, go to the **C – Fit Tab** and choose **Parameters**. All free parameters of the fit are listed here. Define the upper and lower limit for each of them.

Parameters			
Name	value	lo. bound.	up. bound.
thickness 7	60	50	70
thickness 6	10	5	15

The next step is selecting what kind of data you want to fit and what algorithm you want to use. Here we select Reflectivity for fitting and Evolution algorithm as fit method:



Finally some parameters for the evolution have to be defined. Note how the **population** size is set to 100 and the **Range** (for mutating a parameter) is set to 80%.

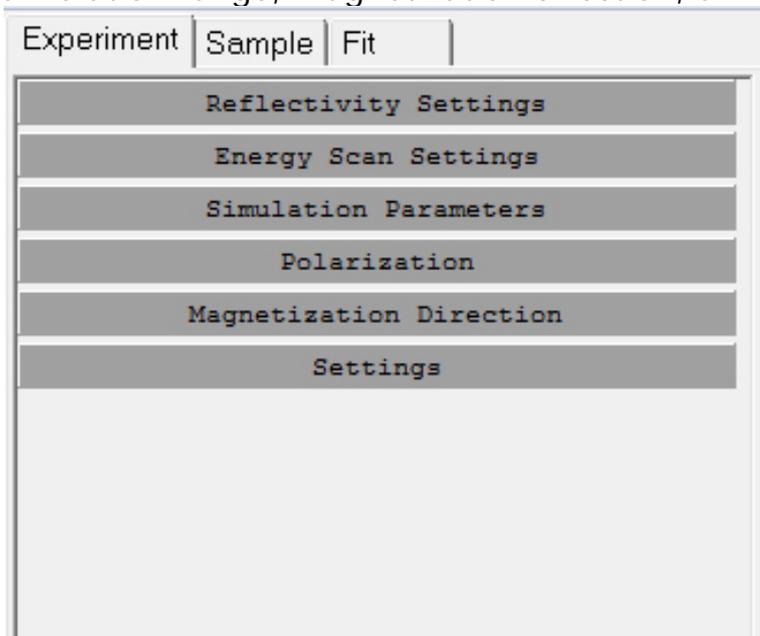


Now press **Start**...and let's go!

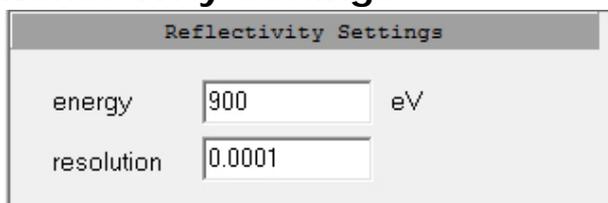
II. Settings Tabs

A – Experiment Tab

This tab defines basic parameters of the experiment like X-ray energy, polarization, simulation range, magnetization direction, simulation algorithm etc.



Reflectivity Settings



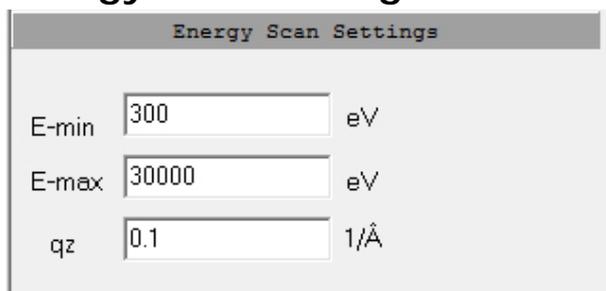
energy

...defines the energy of the incident X-rays in eV. Overwritten if a dataset is activated.

resolution

...angular resolution of the simulation to account for experimental resolution. This setting is overwritten if measurement data is activated.

Energy Scan Settings



E-min

...

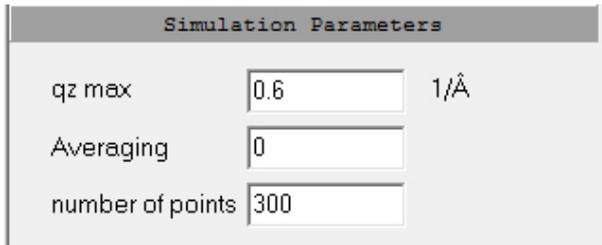
E-max

...

qz

...q_z value of the E-Scan

Simulation Parameters



Simulation Parameters	
qz max	0.6 1/Å
Averaging	0
number of points	300

qz max

...maximal q_z range for the simulation (this is overruled by the x-range of the experimental data if the "use measurement x-range for simulation" checkbox is selected)

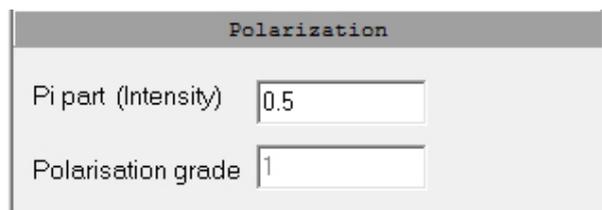
Averaging

...averages over # of points. This is an option to get potentially better fit results. **The averaging smoothes your measurement data as well as the simulation data.** Noise as well as small fast oscillations can be eliminated. Effectively the parameter averaging and (fast)-resolution does some averaging over neighbour solutions. The main difference here is that the resolution parameter is physically motivated while the averaging is numerically motivated.

number of pints

...number of x points for the simulation (this is overruled by the measurement x-values if the "use measurement x-range for simulation" checkbox is selected)

Polarization



Polarization	
Pi part (Intensity)	0.5
Polarisation grade	1

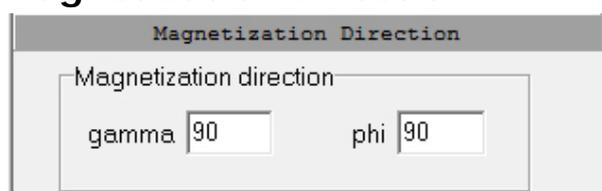
Pi part

... describes the degree of polarization of the incident X-rays by the π (parallel) part of the light. A value of $\pi = 0.5$ corresponds to 100% circular light. $\pi = 1$ corresponds to linear horizontal polarized light.

Polarisation grade

...not implemented

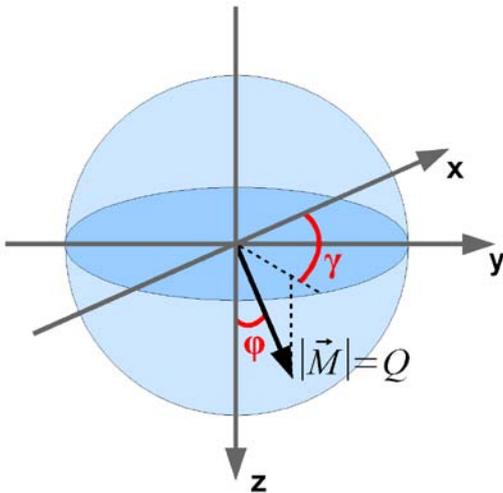
Magnetization Direction



Magnetization Direction	
Magnetization direction	
gamma	90
phi	90

gamma/phi

...angles of the magnetization with respect to the incident beam direction (y-axis). See the following drawing (y-axis=beam direction!):



Note: The magnetization direction only works with the matrix formalism!!

Settings

x-Axis

qz alpha [°]

algorithm

Parratt

matrix formalism

calculation mode

roughness by Nevot & Croce

layer segmentation

layer segmentation with M(z)

Precision

single precision

double precision

fast resolution

Settings

x-Axis (qz/alpha)

...this changes the x-axis presentation from q_z (1/Å) to angle (degree). Depends on the given energy.

algorithm (Parratt/matrix formalism)

...choose the algorithm, i.e. physics, ReMagX uses to calculate the reflectivity. The **Parratt** algorithm is much faster but the magnetic contribution is not 100% physically correct. The **matrix formalism** is based on the matrix multiplication of boundary and damping matrices and describes magneto-optical properties correctly.

Please note: Sometimes Parratt can be used to simulate magnetic reflectivity as well since the error might be small. However a final test with the matrix formalism is always necessary.

calculation mode

...determines how ReMagX simulates the sample to account for roughness and local variations of δ , β , δ_m , and β_m . The **Nevot & Croce** approach simulates roughness by an exponential damping and does only work with the Parratt algorithm! Furthermore it cannot be used to simulate local variations of the magnetism.

When **layer segmentation** or **layer segmentation with M(z)** is chosen, the sample is subdivided into slices (automatically). This allows simulating

roughness with the matrix formalism. The $M(z)$ option allows local variations of the magnetization with the Parratt and the matrix formalism. See also: [Adaptive Layer Segmentation](#)

Precision (single/double)

...choose the internal variable format for all calculations (affects CPU time and memory usage)

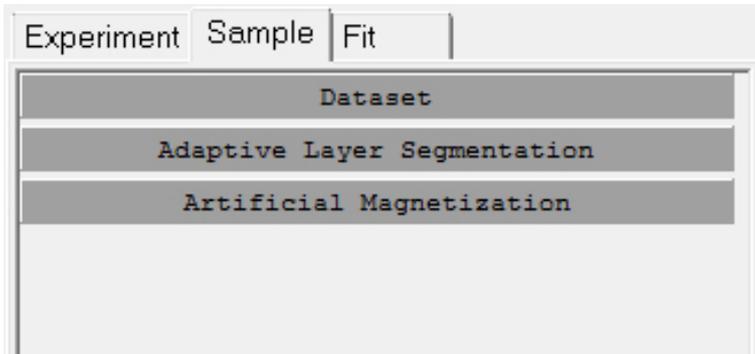
fast resolution

...the incident ray normally has a small angle distribution which can be declared by the resolution parameter. However to simulate this distribution ReMagX calculates for each point in the reflectivity solution eight further reflectivity points by a variation of the angle of the incident ray.

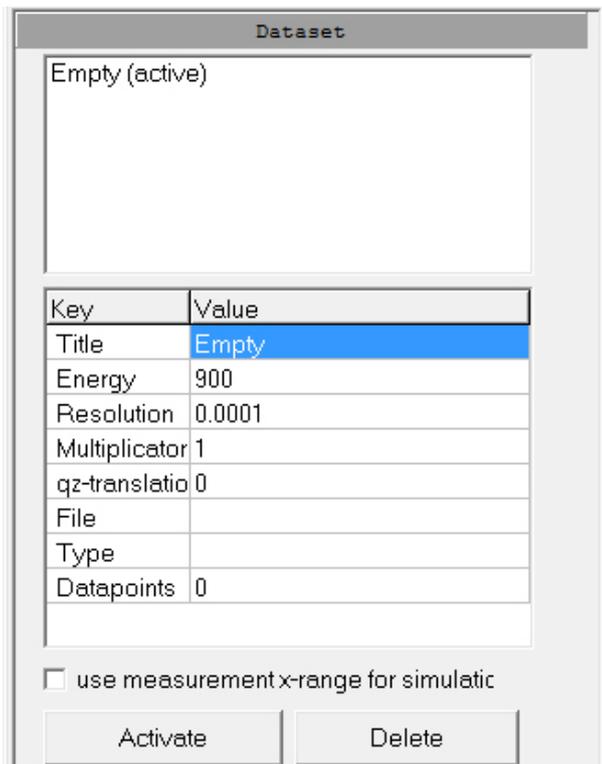
This takes much CPU time. To avoid this computational cost the eight points can be taken by linear interpolating of the neighbour reflectivity solutions.

B – Sample Tab

All sample relevant parameters like the dataset, the layer segmentation and any artificial magnetization are defined here.



Dataset



Key	Value
Title	Empty
Energy	900
Resolution	0.0001
Multiplicator	1
qz-translatio	0
File	
Type	
Datapoints	0

use measurement x-range for simulatic

Activate Delete

Title

...title of the measurement (default is filename)

Energy

...energy in electronvolts of the used X-rays

Resolution

...angular resolution of the experiment. This value is used for simulating curves.

Multiplicator

...moves the measurement (not the simu) vertically. Can be used to normalize the data to 1.

Qz-translation

...moves the measurement curve horizontally. Allows correcting angle offsets.

File

...filename of the measurement data file.

Type

...type of data (R0, R+, R-, Asymmetry) provided by the datafile

Datapoints

...number of datapoints

Note:

The dataset is selected by double clicking it in the list.

Adaptive Layer Segmentation

Settings for the adaptive (automatic) layer segmentation. These parameters are only relevant if the corresponding calculation mode is chosen.

Adaptive Layer Segmentation

Adaptive layer segmentation

minimal layer thickness Å

maximal layer thickness Å

gradient scale

Illustrate Segmentation

with $M(z)$

Show current profile in left table
(no roughness, no segmentation)

model

DM1 DM2 parratt

Show Profile

Magnetic profile

to layer list

minimal/maximal layer thickness

... minimal/maximal layer thickness in Å used for slicing the sample.

gradient scale

...defines how fast the slice thickness changes between min. and max. value at interfaces.

Illustrate segmentation

...uncheck here to plot only the optical/magneto-optical profile without slices when pressing **Show Profile/Magnetic profile**.

with $M(z)$

...check this box to show localized moments defined by **Artificial Magnetization** in the illustration.

model (DM1/DM2/parratt)

...model used to calculate the transition of the index of refraction between two layers. The default is Parratt which means the method used in the Parratt32 software from the HMI. The two other models are described in the diploma thesis of M.Harlander. If the thickness is smaller than σ all models describe the interface almost like the roughness approximation by Nevot&Croce. However there are differences for the case $\sigma >$ thickness. The density models DM1 and DM2 should give you physical more feasible results which cannot be modelled by the analytical approximation.

Show Profile/Magnetic profile

...plots the profile in the graph window.

to layer list

...this copies the internally sliced sample to the layer list. BE CAREFUL WHEN USING THIS BUTTON!

Artificial Magnetization

This section defines artificial variations of the sample magnetization like for example induced magnetism in non-magnetic layers or reduced magnetization at an interface.

Note: The “layer segmentation with $M(z)$ ” calculation mode from **Settings** and the “with $M(z)$ ” checkbox from **Adaptive Layer Segmentation** have to be selected to use this feature!

	Gauss	Fit
delta	0	<input type="checkbox"/>
beta	0	<input type="checkbox"/>
variance	1	<input type="checkbox"/>
z	0	<input type="checkbox"/>
amplitude coupling	none	
variance coupling	none	
bind to layer	all	

$M(z)$ uses two different methods of introducing local variations of the magnetic contributions:

+ $M1(z)$ + $M2(z)$ +...

...introduces the given delta and beta values as absolute values. This method can be used to introduce completely new magnetic signals (without the need of an existing δ_m/β_m in the layer).

* $(1+M1(z))$ * $(1+M2(z))$...

...this mode introduces a variation of the existing magnetic signal as defined by δ_m and β_m . This option can be used to alter an existing magnetization at e.g. the interface.
Note: the values delta and beta are relative numbers here!!

delta/beta

...variation of the optical constants induced by the Gaussian (either absolute or relative numbers).

variance

...width of the Gaussian.

z

...z-position of the Gaussian in Å with respect to the layer input table (substrate surface is $z=0!$).

bind to layer

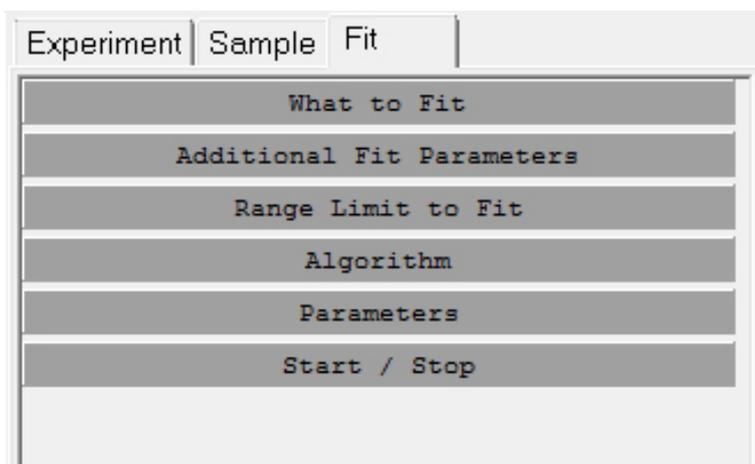
...this binds the Gaussian to the optical thickness of a layer. Imagine you want to introduce some moment at an interface but only for the element of layer 5, just put here 5 and the effect scales with the atomic density of layer 5. The density of one layer is calculated like in the density model 2 (DM2).

$$d(z) = \frac{1}{4} \left(1 - \operatorname{erf}\left(\frac{z_t - z}{\sigma_t}\right)\right) \left(1 + \operatorname{erf}\left(\frac{z_b - z}{\sigma_b}\right)\right)$$

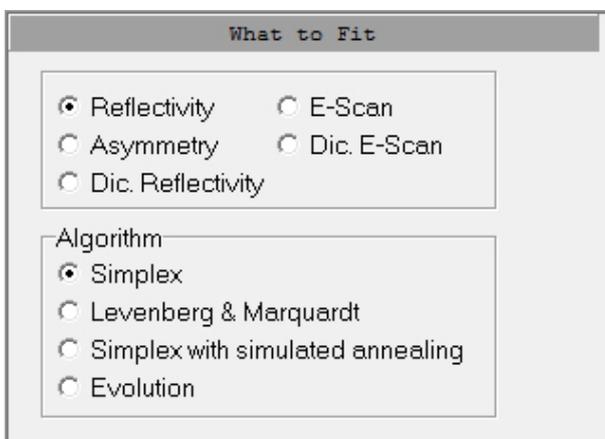
z_t, z_b are the top and bottom positions of the layer with the corresponding RMS roughness σ_t and σ_b .

C – Fit Tab

Contains all relevant fit settings: The fit algorithm, additional fit parameters and the ranges for all fit parameters.



What to Fit



Choose what kind of curve to fit.

Algorithm

...choose the fit algorithm. Simplex, Levenberg & Marquardt are down-hill optimization techniques which means they always converge into the next minimum (not necessarily the global one). Simplex with simulated annealing is an improved simplex which does not converge into the next minimum. Evolution is an advanced fitting routine based on a genetic algorithm. This method is especially suited for reflectometry fits with many free parameters.

Additional Fit Parameters

Additional Fit Parameters

resolution

measurement multiplier

qz measurement movement

choose here which experimental parameters you want to fit.

Range Limit to Fit

Range Limit to Fit

qz: - 1/Å

Range limit for the fit. Can be used to restrict the fitting process to a special qz range.

Algorithm (only available for Simplex/Levenberg-Marquardt)

Algorithm

Simplex with simulated annealing

temperature

delta temperature per iteration

temperature

...initial temperature for the simulated annealing. A fluctuation based on the temperature is added to the fit parameters.

delta temperature per iteration

...decrease of the temperature in dT per iteration for the simulated annealing. If the temperature is zero the simplex annealing algorithm is the standard simplex algorithm.

Parameters

Parameters

Name	value	lo. bound.	up. bound.
thickness 7	60	50	70
thickness 6	10	5	15

This list shows all parameters selected for fitting.

Name

...name of the parameter referenced by the variable name. Here, the thickness of layer 7 and 8 is selected for fitting.

value

...initial parameter values given to the fit algorithms. Right click the list to copy the values in or out of the layer list.

lo.bound.

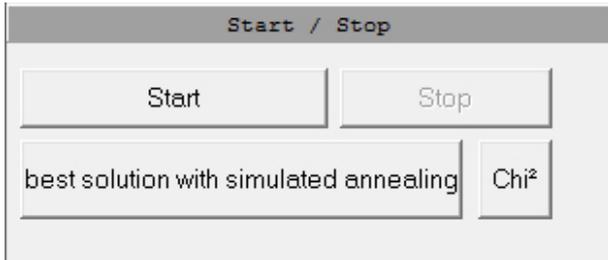
...lower boundary for the fit of the parameter. Note that this boundaries are only strict for Simplex/L&M and for evolution

if "Restrict fit parameters" is checked. Initial boundaries are set to physical feasible values.

up.bound.

...upper boundary (details see above)

Start / Stop (only available for Simplex/Levenberg-Marquardt)



Start/Stop

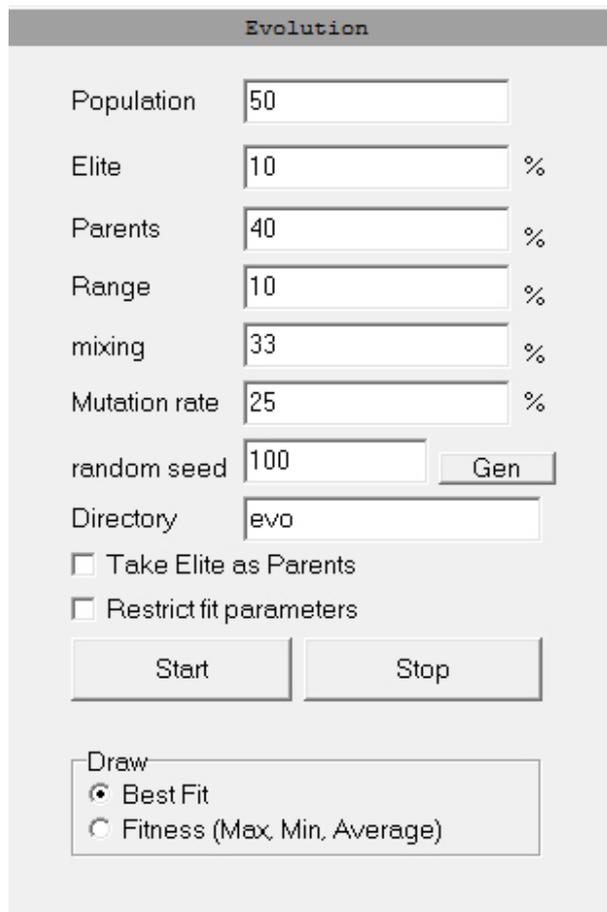
...start/stop the fit algorithm

Best solution with simulated annealing

...plot the best solution of a "simplex with simulated annealing" fit.

Evolution (only available for the Evolution fit algorithm)

Controls for the Evolution (Genetic Algorithm) fit routine. A genetic algorithm is a special optimization technique for non-linear curve fitting. The evolution fit routine used here can be outlined as follows: First an initial population of N curves (individuals) is created by using random parameter values (within the parameter boundaries). Then the population is sorted by fitness (weighted mean square) and the elite (top x% of the list) is moved on to the next generation. Next the Parents fraction from the remaining population is used to create children from each pair by either mixing or swapping parameters. Finally the parameters of the children are mutated by a factor (e.g. range=10 → factor 0.1) according to the mutation rate.



either mixing or swapping parameters. Finally the parameters of the children are mutated by a factor (e.g. range=10 → factor 0.1) according to the mutation rate.

Population

...number of individuals (curves) in the population.

Elite

...defines the size x of the "elite", the top x% individuals (curves).

Parents

...top x% individuals (in percent of the whole population) who will be parents for the children of the generation.

Range

...defines the mutation factor for the children.
For example: a range of 60% is used to
mutate thickness=5. The mutated thickness
is then in the range of $5 \pm 0.6 * 5$.

mixing

...setting for the mutation process (mixing or
swapping parameters).

Mutation rate

...mutation probability per parameter
(25%=every fourth parameter is mutated by
the factor "**Range**").

Random seed

...seed for the random number generator.

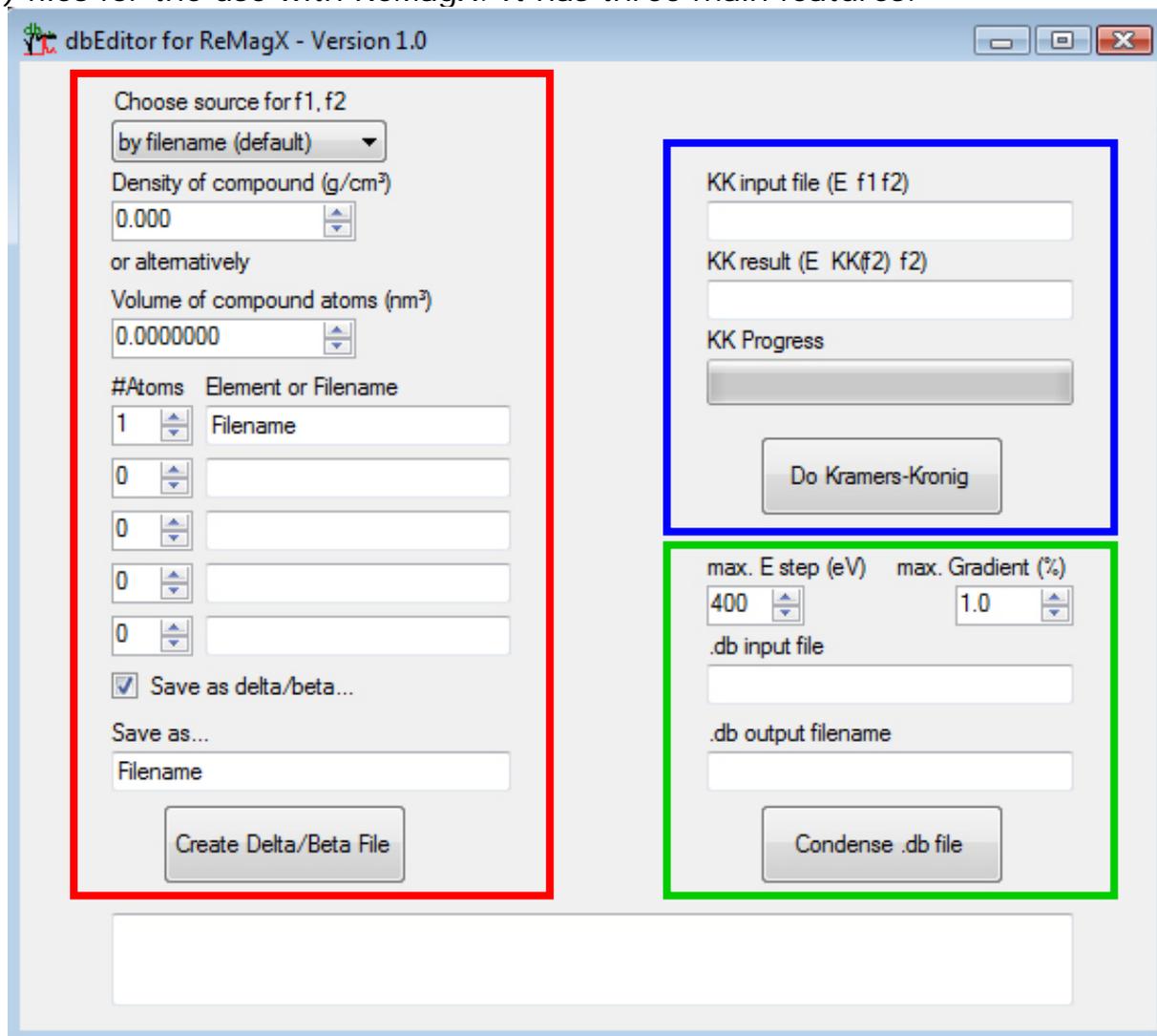
Directory

...directory for the results (only elite stored).

III. dbEditor for ReMagX

Programmed by Sebastian Brück with contributions from Sebastian Macke.

dbEditor is a small piece of software which can be used to prepare optical database (.db) files for the use with ReMagX. It has three main features:



.db creator

– create .db files from atomic scattering factor files.

Kramers-Kronig

– perform a KK transformation of the dataset.

Reduce .db file size

– reduce the file size

Remarks:

dbEditor does not automatically interpolate data points nor does it permit any change to the header layout!

...therefore any file processed by dbEditor has to stick to the format, number of points, x-range scaling etc. of the reference datasets which ship with dbEditor!

.db Creator

Two large compilations of atomic scattering factors exist for the X-ray energy range: The Henke tables by B.L. Henke, E.M. Gullikson and J.C. Davis (see: <http://dx.doi.org/10.1006/adnd.1993.1013>) and the Chantler tables by C. T. Chantler (see <http://dx.doi.org/10.1063/1.1321055>). From these datasets, non resonant scattering factors for any alloy or compound can be calculated.

The .db creator can help you preparing a .db file from either the reference tables or from a custom file (which may contain measured values for example). In the following, an example will illustrate this feature:

A .db file for Al_2O_3 based on the reference data from the Chantler table will be created. Al_2O_3 has a density of 3.69 g/cm^3 and since we will use Chantler reference data shipped with dbEditor it is sufficient to provide only the element names. The screen should then look like:

dbEditor for ReMagX - Version 1.0

Choose source for f1, f2
Chantler Table

Density of compound (g/cm³)
3.690

or alternatively
Volume of compound atoms (nm³)
0.0000000

#Atoms	Element or Filename
2	Al
3	O
0	
0	
0	

Save as delta/beta...

Save as...
Al2O3.db

Create Delta/Beta File

The top most drop-down menu lets you choose the source of the f1,f2 files

Density of compound (g/cm³)

...self explaining

Volume of compound atoms (nm³)

...if the density is omitted (is set to 0.0) dbEditor uses this value. This is the volume the atoms defined below occupy.

Important: This is not necessarily the unit cell volume!

#Atoms & Element/Filename

dbEditor can handle a maximum of 5 elements for the creation of an compound .db file. If you use Chantler/Henke from the dropdown menu on top, the element is sufficient. If "by filename" is chosen, provide full filenames (with ending).

Save as delta/beta

...if you uncheck this box, the compounds f1, f2 factors are saved instead.

Save as

...define the filename for the result.

The output window will show the following string if the file is successfully created:

```
Result written to System.IO.StreamWriter
```

Kramers-Kronig

This section performs a Kramers-Kronig transform of a given atomic scattering factor dataset. You can only KK transform atomic scattering factors, i.e. a file containing f1 and f2 data. The KK will then overwrite the f1 values. The file format (and especially the header) for the KK has to look like:

```
#Mn from Chantler
#Z   A(g/mol)  rho(g/cm3)  frel(e/atom)
#   25   54.938   7.43 -0.0612
# E(eV)  f1    f2
10   4.88252  0.7957
10.1 4.88125  0.81023
10.2 4.87999  0.82477
10.3 4.87872  0.8393
10.4 4.87746  0.85384
10.5 4.87619  0.86837
10.6 4.87493  0.88291
```

Note: all entries (also the # from the first one in header line 3) have to be separated by tabs!

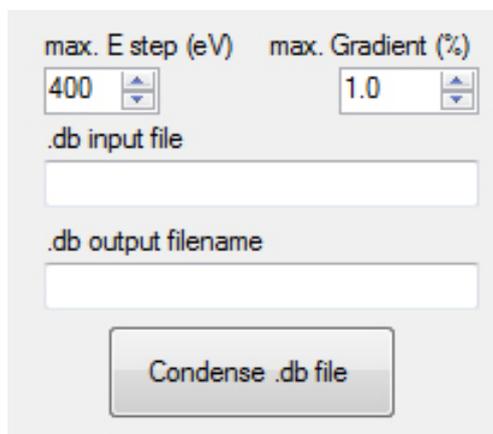
The f1 values can also be replaced by 0 since they are overwritten during the transform...anyway the column must not be omitted!

The Z value and the relativistic correction frel are especially important since they are required for the KK!

Reduce .db file size

The KK transform described in the previous section requires high resolution f1, f2 files. On the other hand, handling of these files slows down ReMagX. The .db condenser tool described here allows reducing the file size by removing points from the file. This is possible because ReMagX interpolates the missing values later.

Just provide an input filename and a result filename and press "**Condense .db file**" and dbEditor will change the stepping according to the parameters:



max. E step (eV)

...maximum width of the stepping in eV.

max. Gradient (%)

...maximal change of delta or beta in % before a step is invoked.

Note: You should always check whether all important features of the curve are preserved! Otherwise reduce the max. gradient.

File Format

The reference files provided with dbEditor were created from the Henke or Chantler tables which are available online (so please cite them properly when using them).

Note all files used with dbEditor have to have the same x-values otherwise dbEditor will produce wrong datasets. The file format, especially the x-range is described in the following:

X stepping:

10 – 2500 in 0.1 eV steps

2510 – 29990 in 10 eV steps

30100 – 400000 in 100 eV steps

Header format:

```
#Cr from Chantler
#Z   A(g/mol)  rho(g/cm3)  frel(e/atom)
# 24  51.996  7.18 -0.0558
# E(eV)  f1    f2
10  4.85608  1.94743
10.1 4.864   1.96177
10.2 4.87192 1.97612
```

The header must contain 4 lines beginning by a #. The information in line 3 has to be separated by tabs and must contain:

Z...the number of electrons in the atom

A...is the atomic mass number

Rho...the density in g/cm³, and

frel...is the relativistic correction for Z

For further information refer to:

S. Brück "Magnetic Resonant Reflectometry on Exchange Bias Systems" (p. 92)
PhD thesis University of Stuttgart 2009

or

Eric M. Gullikson "Section 1.7 ATOMIC SCATTERING FACTORS" (p. 75)
X-ray data booklet, Advanced Light Source