# *Motofit*

## Fitting Reflectivity from Thin Layers

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## *MOTOFIT*

*Motofit* is a macro that aids the fitting of *specular* X-ray and neutron reflectivity data. It works within the analysis package *IGOR PRO* (Wavemetrics, OR). It was created in version 4 of IGOR, and should work in version 5. Why is it called Motofit? Well Moto is the name of a Parrot!

The specular reflectivity is calculated using the Parratt's recursion formula [1] for stratified thin films, as a function of the perpendicular momentum transfer, $Q_z$.

$$Q_z = \frac{4\pi}{\lambda}\sin\theta \qquad\qquad \textbf{Equation 1}$$

Specular reflectivity is defined as the ratio of reflected intensity over incident intensity, where the angle of reflection ($\theta$) is equal to the angle of incidence.

*Motofit* was created with the aim of allowing a scientist to easily fit her/his reflectivity data. Other reflectivity packages are obviously out there, but sometimes they don't allow you to do what you want.
The advantage with *Motofit*/IGOR is that if the user has a specific requirement for the fit then he/she should be able to code it rather simply. For example, if you want to fit an analytical profile, then you write a *Fitfunc* that will describe your profile. Or perhaps you want to fit with a different resolution function, it would be easy to include that as well.
You can then send your special function to other users. If everyone does that then a wide variety of different capabilities can be built up.

## *Getting started*

Place the Motofit.ipf file wherever you want it. Placing in the IGOR procedures folder will cause it to open whenever IGOR is started. Once the procedure has compiled then a *Reflectivity* heading should appear on the window menus

This menu has three sub-options:
1) Reflectivity Fit Panel
2) Plot Experimental reflectivity
3) Fitting multiple contrasts

### Reflectivity Fit Panel
This option plots a theoretical reflectivity curve.

When you click on this option a dialogue is brought up. This dialogue enables you to select some of the parameters required to produce the theoretical curve.

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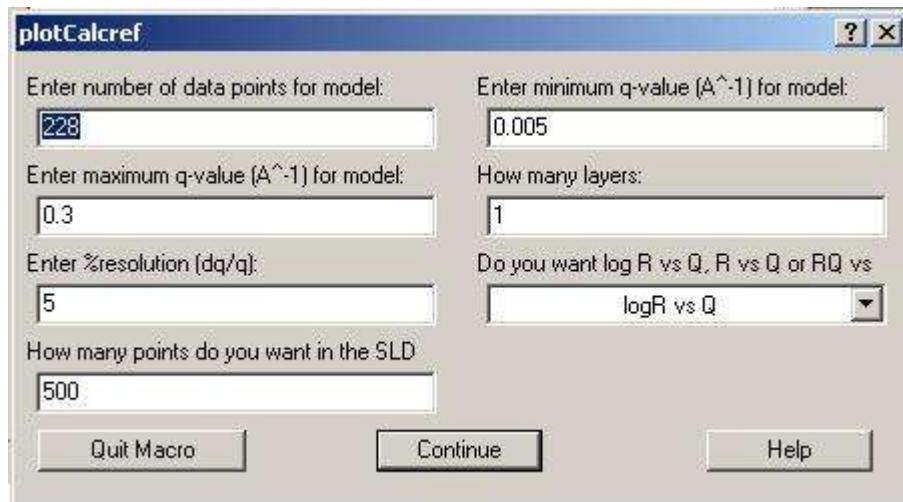[1] L. G. Parratt, *Phys. Rev*, **95**(2), 359-369, 1954

**Figure 1**

Most of the selections are obvious.  You can control the $Q$ range for the plot, as well as the number of points in that plot.  The number of layers refers to the number of layers that lie between the superstrate and the substrate.  DQ/Q relates to the resolution function of your instrument (note use dq/q=0 if you want quicker calculations), if you are unsure set this equal to zero.  You can plot the reflectivity either as log$R$ *vs Q*, *R vs Q* or *RQ⁴ vs Q*.  There are 500 points in the SLD profile graph that is created for your layered system.  When you press continue the Reflectivity Fit Panel and Reflectivity Graph are produced (Figure 2).
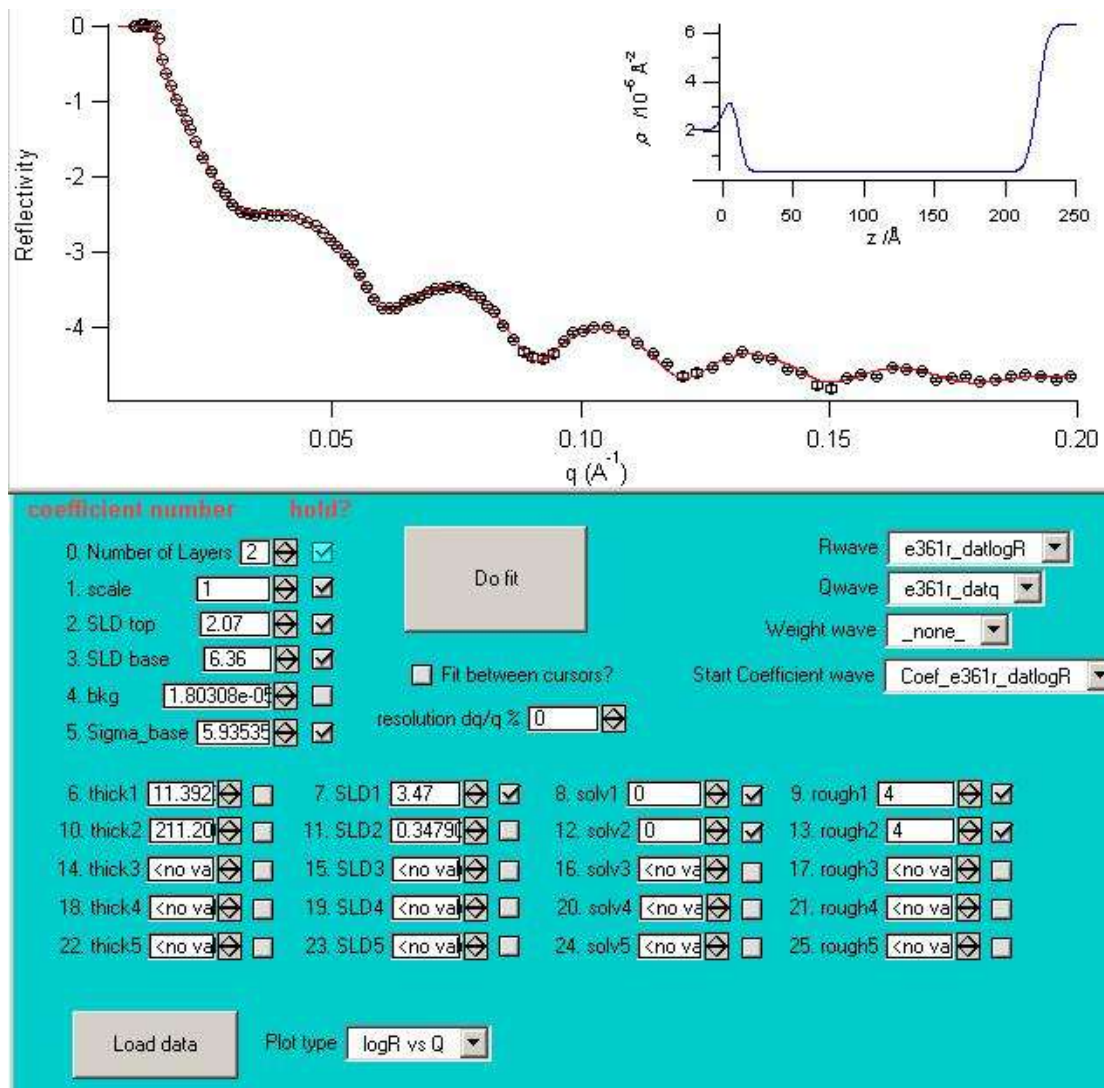
**Figure 2. The motofit panel and the reflectivity plot.**

There are several sections to the panel.

# 1. Load data

This button also loads experimental data. However, the data is normally loaded into a new graph. If you want to plot the experimental data in the same graph as the theoretical data see Plot Experimental reflectivity.

# 2. Rwave/QWave/weight wave/coefficient wave

These popup menus select the experimental data waves that you wish to fit. Make sure you get the *R*-wave and the *Q*-wave the right way around.

You can also perform the fit, with a weight wave. However, at the present time I am not totally sure what the correct weighting procedure is for R vs Q. So I would only fit logR or $RQ^4$ with errors, although it is probably still valid to fit them without errors. (I normally fit log R vs Q without errors).

The default coefficient wave is *coef_Cref*. However, each time you fit a different set of data another coefficient wave is produced (*coef_Rwave*), corresponding to that datasets fit coefficients. You can use these coefficients as a starting point for a new

fit.  (However, if you are fitting the same dataset then beware, the starting coefficients get overwritten).

## 3. Plot type

You can change the plot type by simply using this pop up menu.  The data fitting operates on the sample plot-type.  E.g. if you select $RQ^4$ vs Q, you fit the data as $RQ^4$ vs Q.  The plots update as you change the selection in this box.  However, you may experience difficulties with the fit curve if you fit as R vs Q or logR vs Q, then go to $RQ^4$ vs Q.

## 4. Model Parameters

The model parameters reside in the parameter wave *coef_Cref*.  Note that this parameter wave can be written to file by using *Data→ Save Waves → Save delimited text*.  If you want to use a saved parameter file as a starting point then you should load the file, then copy the wave contents into *coef_Cref*.

0.  Number of Layers: Number of layers: how many layers there are in your model.  Layer 1 is closest to the superstrate, layer *n* is closest to the subphase (refer to Figure 3).
1.  Scale: The scale factor for the reflectivity measurement (should be 1, or close to 1).
2.  SLDtop: Scattering length density of the Superphase (the incident medium for the radiation).  If you are doing an air-solid measurement then this will 0.  If you are doing a solid-liquid measurement, incident through the solid, then this will be the SLD of the solid.
3.  SLDbase: Scattering length density of the subphase.
4.  bkg: This adds in a linear background to the fit.
5.  Sigma_base: The roughness at the top of the subphase (refer to Figure 3)
6.  thick1: thickness of the first layer (in Angstrom).
7.  SLD1: scattering length density of the first layer (
8.  solv1: how much of the subphase (solvent) penetrates into layer 1.  This is expresses as a percentage.
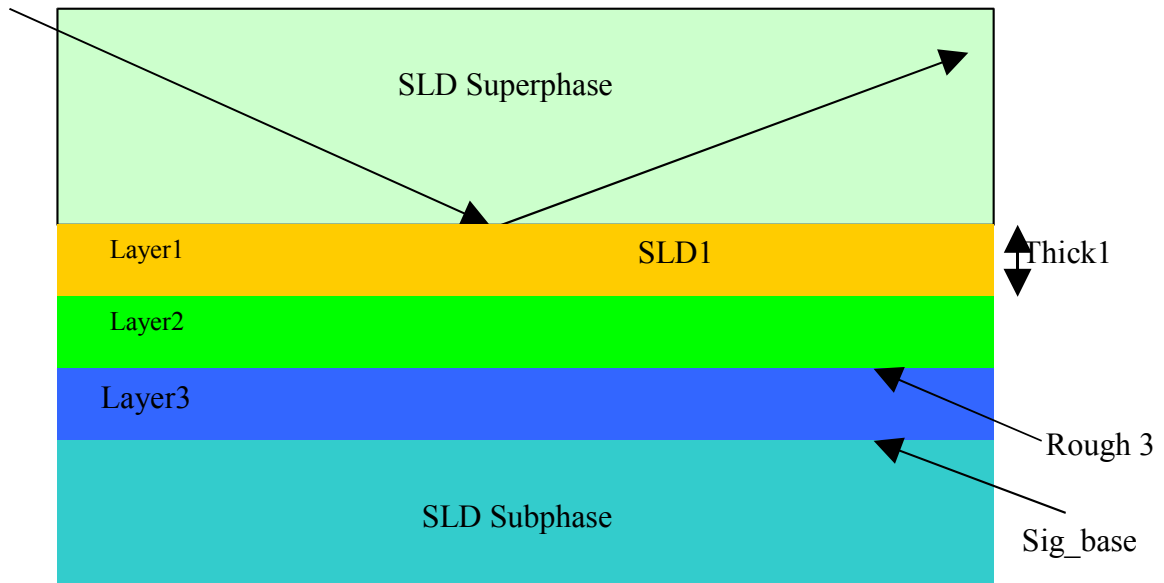9.  rough1: the roughness at the top of the first layer.

**Figure 3. The model**

Parameters *coef_Cref*[10]→ *coef_Cref*[13] represent the second layer, and so on.

All the scattering length densities are expressed as $\rho \times 10^6 \text{Å}^{-2}$.
Roughnesses are implemented in terms of an error function, according to Nevot+Croce[2]

The panel automatically dimensions *coef_Cref* when the number of layers (*n*) are changed. If there are no layers you are fitting a single interface, e.g. air vs $D_2O$, and there are (should be) six parameters.
Otherwise the total length of *coef_Cref* is $4 \times n + 6$.

## 5. Checkboxes
If you want to hold a parameter while fitting then tick the checkbox. If left unchecked then the parameter will vary in the fitting process.

## 6. Resolution
Enter the resolution in terms of a percentage dq/q. This value resides in the wave *resolution*[0]. It is recommended that initial fits be conducted with dq/q=0, as this saves a lot of calculation time.

## 7. Fit between cursors
If you want to limit the region of the dataset that the fit function uses then tick this box. Note that you should have both cursors (A and B) on the *Rwave* you are fitting. To get the cursors press *Ctrl-I*.

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[2] L. Nevot, P. Croce, *Revue de physique appliquee*, **15** (1980), 761

## 8. Do fit

Fits the experimental dataset with the theoretical model, using the parameter wave *coef_Cref*. The fit uses the Levenburg-Marquardt method for minimising the Chi$^2$ value. The *fitfunc* that IGOR uses is called *Motofit*.

The output of the fit are updated graphs. In addition, *coef_Cref* is updated and a new wave *coef_Rwave* is produced, which contains your fit results. The wave *W_sigma* (or the history window) contains the uncertainties in fit parameters. You can obviously print/save those parameter waves.

Note:

1. Negative numbers may appear as fit results, for the thickness and roughness. DON'T PANIC. Internally in *motofit* the absolute value of these numbers are taken, i.e. abs(thickness), or $|thick|$.

2. *Coef_Cref* is always used as the coefficient wave for the fit. If you specify the use of a different coefficient wave using the popup, then the action of selecting the popup makes *Coef_Cref* equal to *Coef_otherwave*

## Reflectivity Graph

This plot shows the theoretical reflectivity curve for the layer model specified in the Reflectivity Fit Panel. Whenever you change a parameter in the panel then the graph will update.

The main part of the graph is the theoretical reflectivity profile, the other part the SLD profile corresponding to your model.

The theoretical reflectivity curve is contained in the waves *ywave_Cref* and *xwave_Cref*.

If you want to save those waves then use:

1) *Data → Save Waves → Save delimited text*
2) Select the waves you want to save
3) Do it

The SLD profile data are contained in the waves *SLD* and *zed*, it is also possible to save these waves.

## Plot Experimental reflectivity

When you bring up this option from the top menu you load in 3 or 4 column reflectivity data.

The data format is tab delimited, with the data columns as:

*Q      R  dR          dQ.*

If you have a graph already open (e.g. you have already opened the reflectivity panel), and this graph is on top, then it asks if you want to append it to that graph, which is quite useful. In other words, you see your experimental data and the theoretical data on the same plot.

If there is no graph already open, then it creates a new graph. You can then open (and append) further reflectivity datasets to this graph.

If you open the experimental data first, then create the theoretical reflectivity curve, you can append the experimental data to the theoretical curve as follows:

1) activate the graph window containing the theoretical curve.
2) From the top menu select *Graph→ Append to Graph*.
3) Select the *ywave* and *xwave* of your experimental data.
4) Select the axes *L=left B=Bottom* (not L=SLDprofile B=z, otherwise the data gets plotted on the SLDprofile).

Note that you can plot experimental data without the theoretical curve if you want to.

## Fitting using the curve fitting dialogue or fitting more than 5 layers

The panel is only able to fit 5 layers.  However, the macro can handle as many layers as you want.
In order to fit 6 or more layers you need to use the curve fitting dialogue.  Here's what you have to do.
1. Bring the parameter table, *coef_Cref,* to the front.
2. Enter the required number of layers in *coef_Cref*[0]. (Wave numbering starts from 0).
3. You will need $4 \times n+6$ parameters in total, so type in:
     Redimension/n=($4 \times n+6$) coef_Cref
   In the command line, where $4 \times n+6$ is a number.  Alternatively you can enter the numbers directly into the table if you want to.  The extra parameters will have the following index numbers: thick(n)=$4 \times n+2$, SLD(n)= $4 \times n+3$, solv(n)= $4 \times n+4$, rough(n)= $4 \times n+5$.
   i.e. the SLD of the $7^{th}$ layer should be in *coef_Cref*[31].
4. You have to have the correct number of parameters for the number of layers entered.
5. Start the curve fitting dialogue, *Analysis→ Curve Fitting*.
6. In the F*unction* tab select *Motofit* as the fitfunc and select the correct *y* and *x* waves.
7. If you want to use the cursor positions to select a particular fit range then press *cursors* on the *data options* tab.
8. in the *coefficients* tab select the *coef_Cref* as the *coefficient wave*.  Select the hold checkbox if you want to hold that parameter.  You **HAVE** to hold the first parameter.
9. If you have more parameters than are required for the number of layers then hold the "extra" parameters.
10. If you want to enter constaints use the *constraints* wave.
11. Press Do-it.  The curve will hopefully fit without a problem

Note that all the *reflectivity panel* does is perform the same procedure as outlined in the 11 steps above.

IGOR can perform a lot more advanced functions than those outlined above.  You should be able to find more options to suit you, if you want them.  (You can get covariance matrices, residual waves, etc).

## Fitting multiple contrasts

Fitting multiple (neutron) contrasts is a cinch in IGOR.  You use the global fit package.  There is a macro that helps you do this.

Simply follow the following steps.
1. Load all the experimental data(preferably in the same graph).
2. Fit the individual datasets/contrasts separately to start off with, with a best guess model. This should give you a better starting point. You should use the same number of layers for each contrast.
3. This procedure should give you coefficient waves, *coef_Rwave*, for each of your datasets.
4. Start up the *Make Global coefficient wave* panel: *Reflectivity→Make Global Coefficients for multiple contrasts*. (see Figure 4).
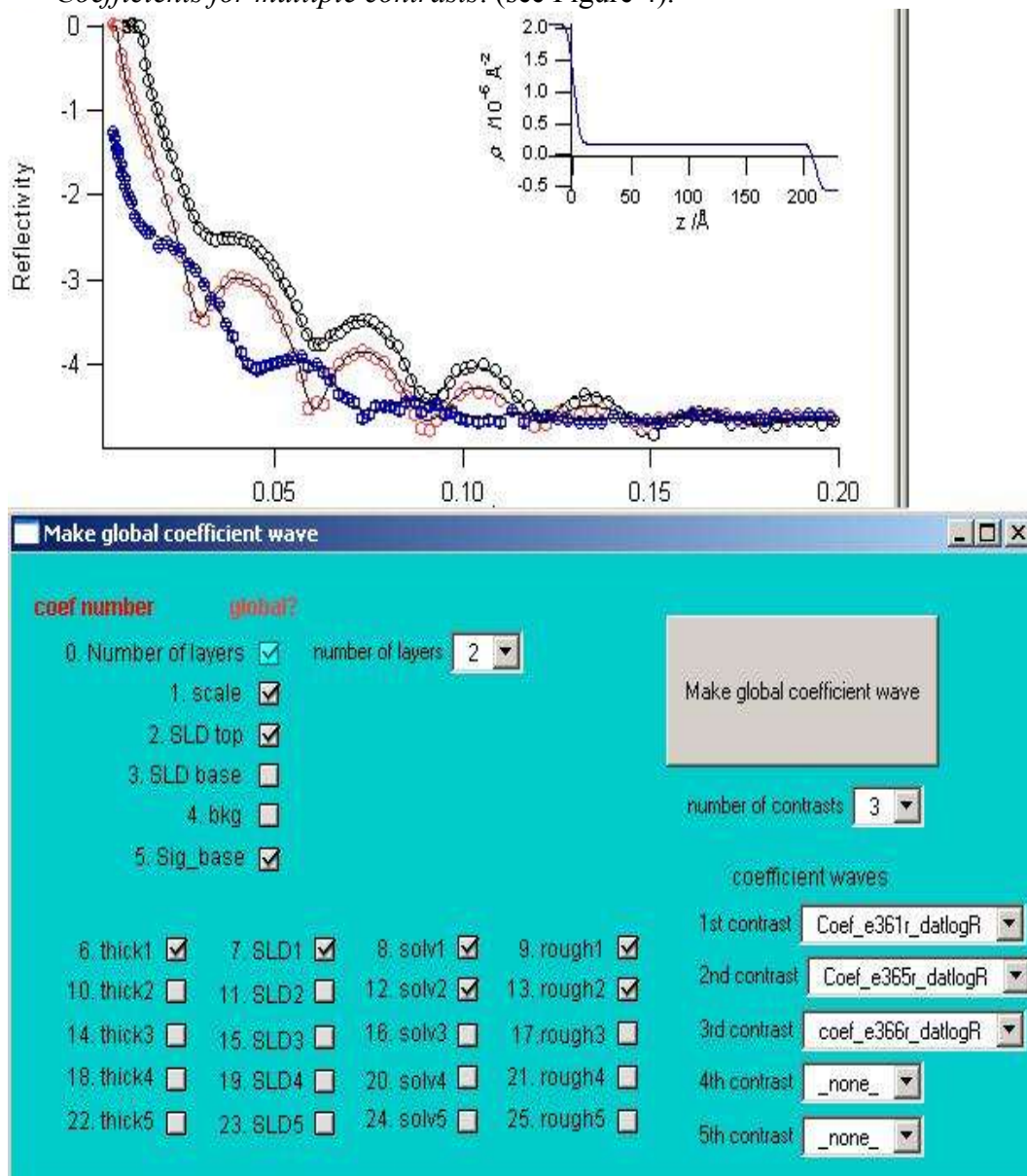


**Figure 4. Setting up a global coefficient wave.**

5. In the example shown in Figure 4 I have 3 datasets/contrasts. I have selected 3 contrasts in the "popup". Since each of the coefficient waves is based on a 2 layer model I have selected 2 layers in the "layer popup".
6. Now select which parameters are the same for each of the contrasts. In Figure 4 parameters *0,1,2,5,6,7,8,9,12* and *13* are equal for all 3 contrasts.

7.  Now click on *Make global coefficient wave*. This concatenates the 3 coefficient waves into 1 wave called *Globalwave*.
8.  Start up the *global analysis package*: *Analysis → Packages → Global Analysis*. (see Figure 5)
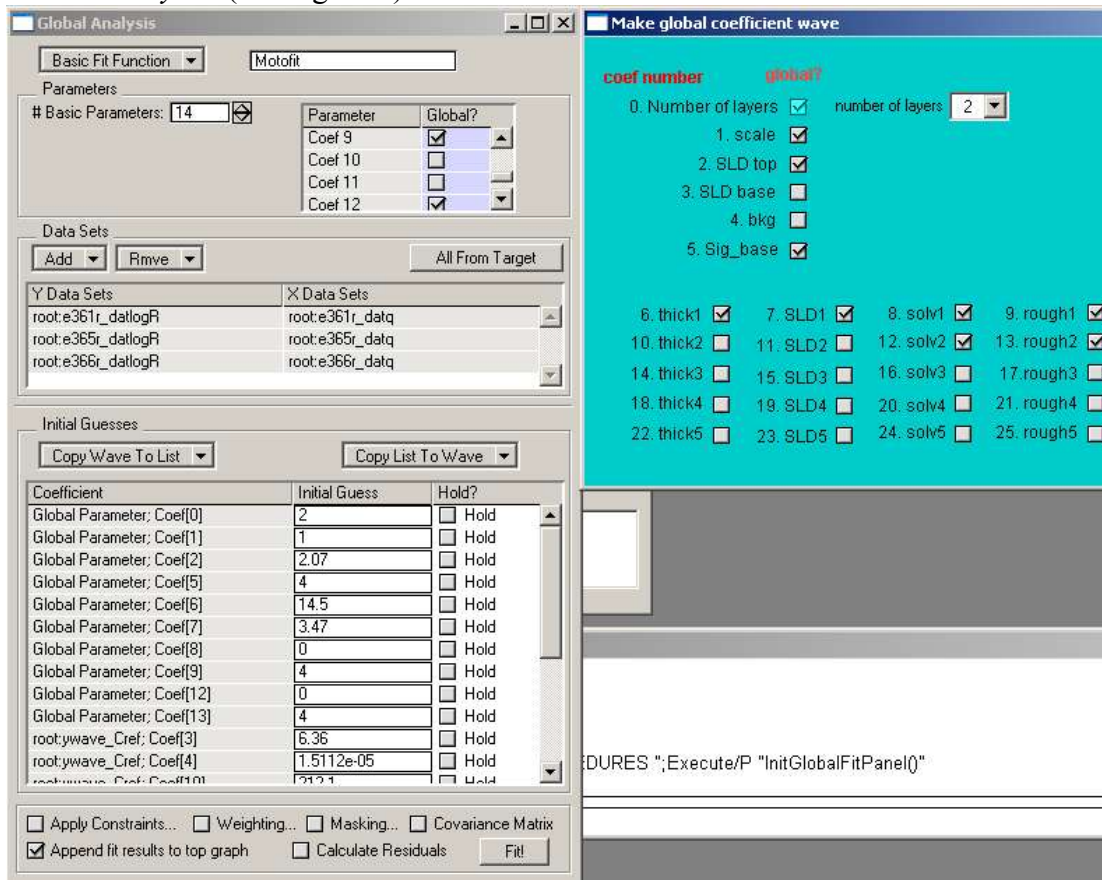


**Figure 5. the global fit dialogue.**

9.  Select *motofit* as the *basic fit function*.
10. Work out how many parameters you need ($4 \times n + 6$), enter that value in *#Basic parameters*. – for two layers the number of parameters is 14 (you can see that from the reflectivity panels).
11. Add the y and x waves corresponding to the 3 contrasts. <u>Make sure they are in the order that you created the *globalwave*.</u> In this example (Figure 4Figure 5) they are in the order *e361r, e365r, e366r*.

12. Check the boxes for the parameters that are global, these should be the same as in the panel (Figure 4Figure 5).
13. To load the initial guesses press C*opy Wave to List;* if you've done everything right then *Globalwave* should appear there.
14. Check the parameters you want to hold (e.g. the superstrate SLD), **you have to hold coef[0], the number of layers**.
15. You can apply constraints, if you want to, by pressing the *constraints* checkbox, e.g. solvent >0%.
16. *Appending the fits to the top graph* plots the fits over your experimental data, which is a good idea.

Note that you don't have to use the panel as described, you can enter all the parameters by hand. It just makes setting up the global wave a *LOT QUICKER!!!*

## Fitting user defined functions.

If you have a specific SLD profile to fit, then this will probably replace *motofit*. In this situation you will have to use the curve-fitting dialogue, as the panel will be useless. You will create a specific parameter wave for your model. You will then send this wave to a user function. This function will then create a specific *coef_Cref* wave which can be read by the kernel that calculates the reflectivity, *Calcreflectivity*. This probably sounds harder than it really is. If you want help then email me and I'll try to help.

## Bugs

Send me details of any bugs and I'll fix them. I have benchmarked the program against other programs and everything seems to be AOK.