DANSE/Reflectometry User Instructions

Starting the Program:

To start the program, click on the "KSrefl" icon.

Fitting in 5 Easy Steps:

1. Load the data
2. Set up the model
3. Adjust fit parameters
4. Adjust fit options
5. Start the fit

Loading the Data:

To load data, click on the "File" menu, select "Data", and click on your data file in the window that appears. The other options such as "Load," "Save," "Save As", etc. are not implemented at this time.

Setting Up the Model:

A model consists of the following:

- A semi-infinite flat layer on the left
- A semi-infinite flat layer on the right
- Any number of layers in between
- A "roughness" value at each interface between layers. The roughness value is used to smooth the transition between layers.

Adding and Removing Layers:

To add a layer, select the "Layer" menu and select which type of layer you want. Each type of layer uses a different function for its profile, and has a different set of fit parameters. The layer types are as follows:

(note: All values of "z" mentioned in these formulas are counting from the beginning of the layer, not from the beginning of the profile.)

- *Flat Layer:* A layer with the same SLD at all points. Fit parameters are "depth", the depth of the layer, and "value"; the value of the SLD.
- *B-Spline Layer:* A B-spline layer is a cubic parametric B-spline with a user-specified number of control points. If there are N control points, there are (2N-1) fit parameters: "depth", the depth of the layer, "z_1" to "z_N-2" representing the z coordinates of the control points as a fraction of the total depth of the layer (z_0 is always zero and z_N-1 is always 1, so they are not fit parameters) and "rho_0" to "rho_N-1" representing the rho coordinates of the control points. (The control points are numbered from 0 to N-1, and control point i has coordinates (z_i, rho_i)). A B-spline layer with N control points can be "refined" into a spline with a nearly identical profile but 2N+1 control points by using the "Refine B-spline layer" option. Use of the B-spline layer is not recommended unless you do

not know the general shape of the profile, because use of the B-spline layer can produce profiles which fit the data very well but are still wildly inaccurate (this can happen because the mapping from SLD profiles to reflectivity profiles is not one-to-one)

- *Cosine Layer:* A cosine layer uses the formula $A + B\cos(2\pi((z/C)+D))$, where the fit parameters are "depth", the depth of the layer, "offset", the value of A in the above formula, "amplitude", the value of B, "wavelength", the value of C, and "phase", the value of D.
- *Power Law Layer:* A power law layer uses the formula $A((1+Bz)^C)$, where the fit parameters are "depth", the depth of the layer, "multiplier", the value of A in the above formula, "lin_coeff", the value of B, and "power", the value of C.
- *Tethered Polymer Layer:* A tethered polymer layer uses the formula described in Kent et al[1]. The aforementioned formula gives the volume fraction of the polymer, which must then be converted to an SLD. The fit parameters are "length of flat part," which is the length of the flat section before the drop-off point, "SLD of polymer" and "SLD of solvent," which are self-explanatory, and "phi_0", "L_0", and "y", which are the parameters to the formula in Kent et al.

To remove a layer select "Remove layer" from the Layer menu and enter the number of the layer you want t remove. The layers are numbered starting from zero, and the layer number for each layer is displayed right below the layer name.

To change the order of the layers, select "Move layer". At the prompt, enter the number of the layer you would like to move, and then the position you would like to move it to. "0" means move it to the beginning, "1" means move it so there is one layer between it and the beginning, etc.

Roughness:

The roughness is used to smooth the interfaces between layers. Each interface between layers has an associated roughness. Hence, if there are N user-specified layers (in addition to the two semi-infinite layers), there are N+1 roughnesses. Note that each layer has both a "Left Rough" (the roughness on its left interface) and a "Right Rough" (the roughness on its right interface). For any N, the Right Rough of layer N is always equal to the Left Rough of layer N+1, so changing one will automatically change the other.

The smoothing uses an error function where sigma is equal to the roughness. Hence, two adjacent flat layers with a roughness of zero (indicating no smoothing) will look like a step function, while if there is a positive roughness it will look like an error function.

It is important to note that the smoothing only passes through one layer. Hence, if the depth of a layer is very small relative to the roughnesses at its interfaces, discontinuous behavior can result.

Changing Fit Parameters:

There are three types of things that can be fit parameters: the fit parameters for each layer, the roughnesses at the interfaces, and the left and right values. Each fit parameter has four attributes: its current value, its minimum value ("low"), its maximum value ("high"), and a flag indicating whether or not it can vary ("varying"). "Varying" should be set equal to 0 if the parameter is fixed, and to 1 if it can vary. The minimum, maximum, and varying values are not used to calculate the profile, but are used by the fitting algorithm so it knows which parameters can vary and what range they can vary between. Note that if "varying" is zero, then the low and high values are ignored.

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1 Kent et al. *Tethered chains in theta solvent conditions: An experimental study involving Langmuir diblock copolymer monolayers.* J. Chem. Phys, vol. 108, no. 13, p. 5637.

Adjusting Fit Options:

There are several options you can use from the Options menu in order to adjust your fit.

- *Step Size:* The step size represents the width of each "slab" of the profile. Since the value of the profile is calculated at the boundary of each slab, using a smaller step size will result in more accurate results, but will cause the fit to take much longer.
- *Constant dA:* This option allows you to use a variable step size. Instead of using a constant width of each slab, it selects the widths so that the area of the "slab box" (i.e., the width of the slab multiplied by the difference in rho from that slab to the next) is approximately constant. This allows for a smaller step size in steeper areas of the profile, thus giving more accuracy only in the areas where it is really needed. This option allows you to select the value of the area to use. Note that in general, when using this option, in order to increase the number of slabs by a factor of N you have to decrease the dA by a factor of N^2.
- *Fit Range:* This option allows you to select which of the data points will be used for fitting. You must enter three values: "From", "To", and "Step." The "From" and "To" values allow you to select the smallest and highest values of Q to fit. The "Step" option allows you to select how far apart the data points to be fitted are. Internally, the region between the "From" and "To" values are divided up into many regions of length "Step", and one data point is selected from each of the regions that have a data point. Hence, an extremely low value of Step will cause every data point in the range to be fitted, while a higher value of Step will only fit some of the data points. This allows you to restrict the fit to a specific range (if, for example, you know that some of the data points near the beginning and end are inaccurate) and to fit fewer data points over the same range (again gaining speed at the cost of accuracy).
- *Background:* This option adds a fixed amount to all points on the reflectivity profile when calculating it. It is used to model the background noise in the measurement.
- *Show R/Ro:* This option toggles between the normal log(R) plot of the reflectivity and a plot of the "R/Ro", which is a plot of the calculated reflectivity divided by the Fresnel reflectivity. This option affects the display only and does not affect the fit in any way.

Fitting the Data:

To start the fit, go to the "Action" menu and select "Fit".

Fitting Tips:

- If the fit is going very slowly, start off with a higher step size or dA. If it is still too slow, use the Fit Range option to fit fewer data points as described above. After the fit is complete, switch to a lower step size or dA and go back to fitting all the data points if you need higher accuracy.
- Make sure you have a sufficient range on all your fit parameters. If the true value of a fit parameter is outside its range, the fitting algorithm clearly won't be able to find it.
- The parameter space may have many local minima. Since the fitting algorithm uses gradient descent, it is liable to get stuck on a local minimum that is very far away from the true values. If the fit stops and you are still far away from a good fit, try changing one of the parameters and starting the fit again. It is also common for a fit parameter to get stuck at either end of its range, so if there is a fit parameter at the end of the range then try changing it.

Finding the Error:

After you finish fitting, you can try to find the error in your fit parameters by going to "Action," then selecting "Covariance". This works by generating synthetic data sets by perturbing each data point randomly based on its variance, and then refitting the model to each synthetic data set. To view the results, click on the "Covariance" tab on the bottom half of the UI. The first three columns give the name, value, and standard error of each fit parameter. The matrix to the right of that is the correlation matrix between the fit parameters. (A value of 1 means that the parameters are perfectly correlated, a value of -1 means that they are perfectly anticorrelated, and a value of zero means they are not correlated at all.)

Important: The reported errors are only the errors in the fit parameters caused by random errors in the measurement of the data. Other sources of error, such as being on the wrong local minimum or having a bias in the data, cannot be detected by the resampling method.

Known Issues:

- You will receive the error "incorrect number of params for setpars" if you try to start the fit after you have double-clicked on a cell in the table to modify its value, but before you have typed in a new value.
- The "refine" option on the B-spline layer changes the profile slightly. Ideally, the refinement should increase the number of control points without changing the profile
- The values of the fit parameters in the model will change slightly after selecting the covariance option. However, the original values will still be preserved in the table containing the covariance values.