ORSO Lipid Example 1 - DSPC Bilayer Analysed Using a Standard Layers Model.

Start by making an empty instance of the project definition class:

	= rimentType: 'S rimentName: 'O Geometry: 'a	Orso lipid	example'	(d,rho,ro	ugh) layers'		
Parar	meters:						
p _	Name		Min	Value M	ax Fit?		
1	"Substrate Ro	oughness"	1	3	5 true		
Layeı	rs:						
Name	Thickness	SLD	Roughness	Hydrat	ion Hydrate	with	
0	0	0	0	0	0		
Bulk	In:						
р	Name	Min Val	ue Max	Fit?			
1	"SLD Air"	0 0) 0	false			
Bulk	Out:						
p	Name	Min	Value	Max	Fit?		
1	"SLD D20"	6.2e-06	6.35e-06	6.35e-	06 false		
Scale	efactors:						
p	Name	Min	Value	Max	Fit?		
1	"Scalefactor	1" 0.02	0.23	0.25	false		
Back	grounds:						
(a) I p —	Background Par	rameters: Min	Value	Max	Fit?		
1	"Backs par 1'	' 1e-07	1e-06	1e-05	false		
(b) I	Backgrounds:						

1	"Backgı	cound 1"	"constant"	"Bacl	ks Par 1"	" "	"	п	11 11	п
Resol	lutions	:								
(a) F p —	Resoluti	ions Paramet Name	ers: Min	Value	Max	Fit?				
1	"Resolı	ution par 1"	0.01	0.03	0.05	false				
(b) F p –	Resoluti N a	ions:	Туре		Value 1		Value 2	Value 3	Value 4	Value 5
1	"Resolu	ution 1"	"gaussian"	"Res	olution pa	ar 1"	" "	п п	п п	п п
Data:										
Nan	ne	Data	Data Rang	e :	Simulation	n Range				
"Data	a 1"	"No Data"	" _ "	" [0.0050 ,	0.7000] "			
Const	rasts:									
	р									
"Bulk "Bulk "Scal	a" sground' s in" s out" lefactor	c"								

This is the standard class containing the model definition for any project. We add to it using the class methods, which are fairly self explanatory (although more detailed instructions are pending) -

```
methods(problem)

Methods for class projectClass:
```

addBackground addLayer getAllAllowedNames setBackgroundValue setBulkOut setPar addBacksPar addLayerGroup projectClass setBacksPar setContrast setPar addBulkIn addParam removeBacksPar setBacksParConstr setData setPar removeDatasetBacksParNamesetGeometryremoveParamsetBacksParValuesetLayerValue addBulkOut addParamGroup setPar addContrast addQzshift setPar setSca addData addScalefactor setBackgroundName setBulkIn setParamConstr

Methods of projectClass inherited from handle.

"Model"

In this example, we will use a standard layers model. This defines layers in terms of thickness, SLD, roughness and hydration. These are then grouped into layers and the allocated to contrasts in the normal RasCAI way. For this sample, we have a DSPC bilayer on a Silicon substrate, which will be coated by an oxide layer. Ususally there is a hydration layer between the substrate and the lipid, although this depends on the exact conditions

of the measurement. Start by defining the parameters for the oxide layer. We need a thickness, SLD and hydration. The roughness is assumed to be the bulk substrate roughness.

```
Parameters = {
                                              max fit?
        Name
                          min
                                   val
                        10,
3e-6,
                                              25,
                                                  true
      {'Oxide thick',
                                    20,
                                                          };
                                              4e-6, false };
      {'Oxide SLD',
                                  3.41e-6,
      {'Oxide Hydration' 0,
                                              30,
                                    20,
                                                    true
                                                          }};
```

```
Add these parameters to the project class, and group them into a layer to demonstrate how this is done:
    problem.addParamGroup(Parameters)
 ans =
    experimentType: 'Standard Layers with (d,rho,rough) layers'
    experimentName: 'Orso lipid example'
        Geometry: 'air/substrate'
    Parameters: ------
   р
             Name
                         Min
                               Value
                                        Max
                                             Fit?
       "Substrate Roughness" 1 3 5 true "Oxide thick" 10 20 25 true
    1
       "Oxide thick"
"Oxide SLD"
"Oxide Hydration"
    2
                        3e-06 3.41e-06 4e-06 false
    3
                        0 20
                                        30
                                              true
         Thickness SLD
                       Roughness Hydration Hydrate with
   Name
            0 0
                           0
                             0
               Min
                     Value Max
        Name
                                 Fit?
   р
       "SLD Air" 0 0 0
    1
                                false
    Bulk Out: -----
                 Min
                        Value
                                        Fit?
   р
    1
       "SLD D20" 6.2e-06 6.35e-06 6.35e-06 false
   Scalefactors: ------
                   Min Value
          Name
                                 Max
                                      Fit?
      "Scalefactor 1" 0.02 0.23 0.25 false
    Backgrounds: -----
    (a) Background Parameters:
                   Min
                                       Fit?
         Name
                          Value
                                 Max
```

```
"Backs par 1" 1e-07 1e-06 1e-05 false
   1
   (b) Backgrounds:
          Name
                                            Value 2 Value 3 Value 4
  р
                       Type
       "Background 1" "constant"
                              "Backs Par 1"
                                               11 11
                                                        11 11
                                                                11 11
  Resolutions: -----
   (a) Resolutions Parameters:
           Name Min Value Max
                                            Fit?
      "Resolution par 1" 0.01 0.03 0.05
                                            false
   (b) Resolutions:
          Name
                       Type
                                   Value 1
                                                Value 2
                                                          Value 3 Value 4
                                                                            Value 5
  р
                                "Resolution par 1"
      "Resolution 1" "gaussian"
    Name
             Data
                      Data Range
                                  Simulation Range
   "Data 1" "No Data"
                        " - "
                                "[ 0.0050 , 0.7000 ]"
   "name"
   "Data"
   "Background"
   "Bulk in"
   "Bulk out"
   "Scalefactor"
   "Resolution"
   "Model"
   % Now make the oxide layer
   Oxide =
               {'Oxide Layer',...
                                          % Name of the layer
               'Oxide thick',...
                                         % Layer thickness
               'Oxide SLD',...
                                          % Layer SLD
               'Substrate Roughness',...
                                          % Layer roughness
               'Oxide Hydration',...
                                         % Oxide hydration (precent)
               'bulk out' };
                                          % Which bulk phase is hydrating the layer
   % Add this to the project...
   problem.addLayer(Oxide)
ans =
   experimentType: 'Standard Layers with (d,rho,rough) layers'
   experimentName: 'Orso lipid example'
       Geometry: 'air/substrate'
```

	Name		M:	in 	Value	Max	Fit?				
	"Substrate Roug "Oxide thick" "Oxide SLD" "Oxide Hydratic		3e-	1 10 -06 0	3 20 3.41e-06 20	25 4e-06	true true false true				
yer	Name				SLD		Roughr				
			1 .1'	1 "						 	
lk	"Oxide Layer"									нуагат	:10n"
		in V			Fit?						
	"SLD Air" (
lk	Out:				Max					 	
	"SLD D20" 6	.2e-06	6.35	5e-06	6.35e-06	false					
,	efactors:										
ате	eractors									 	
ale					Max					 	
	Name	Mi - 0.	n v	Value	Max 0.25	Fit? false					
ckg	Name	Mi " 0.	n 7	/alue 	Max 0.25	Fit? false					
ckg	Name "Scalefactor 1" rounds:	Mi " 0. meters:	02 (0	/alue 	Max 0.25	Fit?					
ckg) E	Name "Scalefactor 1" rounds: Background Param	Mi " 0. meters: Min 1e-0	02 (0	Value 0.23	Max 0.25	Fit? false Fit? false					
ckg	Name "Scalefactor 1" grounds: Background Param Name "Backs par 1" Backgrounds:	Mi " 0. meters: Min ———————————————————————————————————	n va va Type	7alue 0.23 alue e-06	Max 0.25 Max 1e-05	Fit? false Fit? false	e 2 \			 	
ckg) E	Name "Scalefactor 1" grounds: Background Param Name "Backs par 1" Backgrounds: Name	mi 0. " 0. meters: Min 1e-0	n va	7alue	Max 0.25 Max 1e-05 Value 1	Fit? false Fit? false	e 2 \	Value 3	Value	 Value	
ckg) E) E	Name "Scalefactor 1" grounds: Background Param Name "Backs par 1" Backgrounds: Name "Backgrounds:	Mi " 0. meters: Min 1e-0	n va	7alue	Max 0.25 Max 1e-05 Value 1	Fit? false Fit? false	e 2 \	Value 3	Value	 Value	
ckg) E) E	Name "Scalefactor 1" Trounds: Background Parame "Backs par 1" Backgrounds: Name "Background 1" Background 1" Background 1"	Min	n v 02 0 1 V 7 16 Type nstant	Value 0.23 alue e-06	Max 0.25 Max 1e-05 Value 1	Fit? false Fit? false Fit? Fit? Fit?	e 2 \	Value 3	Value	 Value	

Data: -----

Name	Data	Data Range	Simulation Range
"Data 1"	"No Data"	п _ п	"[0.0050 , 0.7000]"
Constrasts:			
p			
"name"			
"Data" "Background] "		
"Bulk in"	•		
"Bulk out"			
"Scalefacto	or"		

Now we'll build the layers for the lipid, The bilayer is symmetrical, so we can have mostly the same values for the inner and outer tails and heads. We have to be a bit careful with roughness' however, since we want to have a slightly different roughness for the head/water interface and the head/alkyl interface, and for layer model in this geometry the roughness for each layer refers to the next interface. So we'll make separate layers for inner and outer lipids, but all sharing the same parameters, and just differeing in the roughness order.

Define the parameters we will need:

"Resolution"
"Model"

```
% Bilayer parameters:
bilParams = {
                                                                          };
        { 'Bilayer head thick',
                                 5,
                                             10,
                                                          15,
                                                                  true
        {'Bilayer head sld',
                                 1e-6,
                                             1.47e-6,
                                                          1.6e-6, true
                                                                           };
        { 'Bilayer heads hydr',
                                 20,
                                                          40,
                                                                           };
                                             30,
                                                                  true
        { 'Bilayer Heads rough'
                                 5,
                                             7,
                                                          15,
                                                                  true
                                                                           };
        {'Bilayer tails thick', 10,
                                             15,
                                                          20,
                                                                  true
                                                                          };
        {'Bilayer tails SLD',
                                 -5e07,
                                             -4e-7,
                                                          -1e-7,
                                                                  false
                                                                          };
                                                          20,
        {'Bilayer tails hydr', 0,
                                                                          };
                                             10,
                                                                  true
        { 'Bilayer tails rough', 5,
                                             9,
                                                          15,
                                                                  true
                                                                           };
};
% We want the water layer to be matched in SLD to the bulk water phase. So
% we give it an SLD of 0, and a hydration of 100%, and make these
% non-fittable
watParams = {
        {'Water thick',
                                                          15,
                                                                           };
                               5,
                                             1,
                                                                  true
        {'Water SLD',
                                0,
                                             0,
                                                          0,
                                                                  false
                                                                           };
}
```