Manual for Svensson's Extension to ROD

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1   Introduction

This manual describes utilities suggested by Detlef Smilgies and implemented by Olof Svensson in the "Svensson" extension to the experimental version of the ROD program. The manual is based on the **experimental version 1.2** of ROD. Please give your suggestions or report any bugs in the program (or in this manual) to Olof Svensson. For the latest update of this manual and for accessing Elias Vlieg's ROD manual and other extensions manuals you can consult the ANA-ROD web site at http://www.esrf.fr/computing/scientific/joint_projects/ANA-ROD.

1.1   Grouping of atoms

The ROD package was originally developed by Elias Vlieg for x-ray surface structure analysis for atoms adsorbed on surfaces and has been a very successful package. However, the step of going from atomic structures with 1 to 5 atoms per unit cell to structures of simple organic molecules, like for instance p-quaterphenyl with 24 carbon atoms, is a huge increase in complexity (see Fig.1). However, often the structure of a single molecule is quite well-known from bulk crystallography. Hence it is possible to perform an intermediate step: treating the molecule as a rigid entity assuming the bulk structure. This way, to follow up on the above example, the numbers of degrees of freedom is reduced from 3 x 24 (the Cartesian coordinates of the C atoms) to 6, the three Eulerian angles and the three Cartesian coordinates of the center of rotation of the molecule. If the structure can be refined at this level, one can try a further refinement of atomic positions or groups of atoms (such as one of the benzene rings of the molecule) to determine distortions of the molecule due to the interaction with the substrate surface. In order to achieve this goal we introduce a new feature in ROD, grouping of atoms. Such a group is a rigid cluster of atoms that can be rotated and moved as a whole. Section 2 of this manual describes how to use the grouping of atoms feature.

1.2   Cylinder and ellipsoid models

In some cases, molecular structures may not be known, or molecules have rotational degrees of freedom when they adsorb on the substrate. In this case, the charge distributions have to be statistically averaged to determine the form factor of such objects. We provide some simplified models, the Als-Nielsen's cylinder model for rotating alkane chains and an ellipsoid model that allow to develop a feeling what the scattering from such objects would be. These model form factors are normalized appropriately that they can be combined with the scattering from the substrate, which is always assumed to be a rigid single crystal. Section 3 of this manual describes in more detail these two models.

1.3   Bulk multiplicity, atom overlap and simulation data output

The bulk multiplicity utility can expand a bulk unit cell in the case of having a surface cell that spans several bulk unit cells. Section 4 describes the use of this utility. The atom overlap utility calculates the minimum atomic interdistance in the combined structure (bulk and surface) in order to spot errors in the model structure, this utility is described in section 5. Section 6 finally describes an utility for a new output format where intensities and a simulated error estimate can be output in order to be used as a simulation of experimental data.

2 Grouping of atoms on a surface

The grouping feature is used for designing atoms that will be refined as a rigid group. Only the surface model can contain groups. A group contains the following elements:

- A group name
- A list of atoms, where the co-ordinates for each atom is given in an orthogonal co-ordinate system in Angstroms.
- A co-ordinate fixing the centre of rotation in the group of atoms. This co-ordinate is given in Angstroms and will be mapped to the group co-ordinate in the surface unit cell and be invariant of any applied rotations.
- Six group co-ordinates: Three fractional co-ordinates fixing the rotation centre in the surface unit cell, and three rotation co-ordinates phi, chi, and th defined as:
  - The group is rotated in its orthogonal co-ordinate system.
  - First the group is rotated around its z axis phi degrees,
  - then it is rotated chi degrees around the x axis,
  - and finally it is rotated th degrees around the z axis.
  - The orthogonal atom co-ordinates are then converted to fractional co-ordinates of the surface unit cell.

Example: A plane molecule with seven atoms, six of them arranged in a hexagonal ring and the seventh outside the ring:
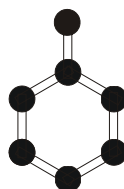
Assume now that we put this molecule in a surface model in ROD. We assign the bottom-most atom to define the centre of the molecule. If we set phi, chi and th to zero, we end up with the following model:
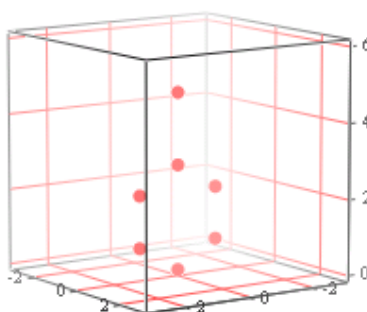
where the molecule is in the x-z plane with the bottom-most atom in origo. Let us now rotate the molecule around its own axis, this we do by changing the angle phi, here we set phi to 15 degrees:
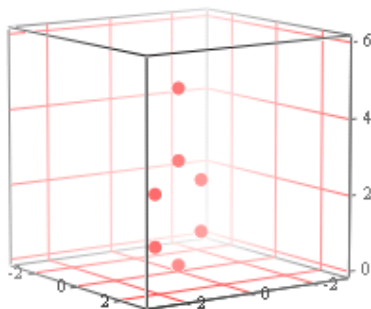
If we go back to phi = 0, but instead set chi to 25 degrees we obtain the following situation:
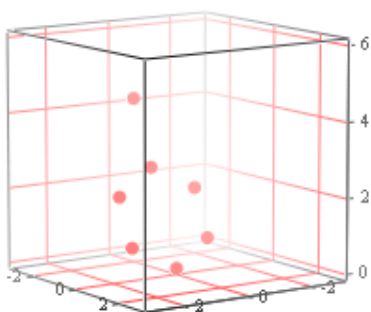
You can see that the molecule has been rotated around its bottom-most atom. It we combine the two rotations we have the following configuration:
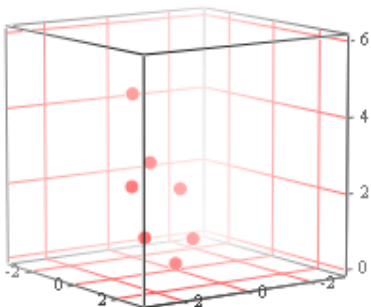
You can see that the molecule has first been rotated along its phi axis, then around chi. If we now set th to 90 degrees we have:

You can see that the molecule has been rotated around the z-axis by 180 degrees.

2.1   Entering groups in ROD

In this section we will show how you can enter the example molecule described above. Groups can be entered either via the ROD.EXT.SVE.SET.GROUP> menu or via the surface structure model input file (.sur). The atomic coordinates of the molecule are:

Atom	x	y	z
C1	0.0	0.0	0.0
C2	1.204	0.0	0.695
C3	-1.204	0.0	0.695
C4	1.204	0.0	2.085
C5	-1.204	0.0	2.085
C6	0.0	0.0	2.780
C7	0.0	0.0	4.690

As you can see we enter the molecule in an orthonormal co-coordinate system where the first atom is in origo and the molecule is in the X-Z plane.

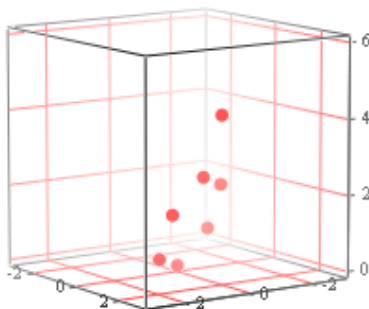## 2.2   The ROD.EXT.SVE.SET.GROUP> menu

The ROD.EXT.SVE.GROUP> menu contains the following functions:

```
ROD.EXT.SVE.SET.GROUP>help
**************************** GROUP MODEL PARAMETERS ****************************
 Name      : Group name
 Xstart    : Start x-position
 XDisplace : Serial number of x-displacement parameter
 Ystart    : Start y-position
 YDisplace : Serial number of y-displacement parameter
 Zstart    : Start z-position
 ZDisplace : Serial number of z-displacement parameter
 Phistart  : Start phi-position
 PHIDispl  : Serial number of phi-displacement par.
 Chistart  : Start chi-position
 CHIDispl  : Serial number of chi-displacement par.
 Thstart   : Start th-position
 THDispl   : Serial number of th-displacement par.
 Origin    : Origin of group atoms
 ADDGroup  : Add a group
 DELGroup  : Delete a group
 NGroups1  : No groups in the first surface cell
```

```
      Element   : Element type of group atom
      XAtom     : X-coordinate of group atom
      YAtom     : Y-coordinate of group atom
      ZAtom     : Z-coordinate of group atom
      B         : Serial # of group atom Debye-Waller par
      ADDAtom   : Add an atom to group
      DELAtom   : Delete an atom from group
      List      : List atoms
      Help      : Display menu
      Return    : Return to main menu
   ROD.EXT.SVE.SET.GROUP>
```

We are assuming that no groups have already been defined:

```
   ROD.EXT.SVE.SET.GROUP>list
   No groups defined.
   ROD.EXT.SVE.SET.GROUP>
```

Now we add one group:

```
   ROD.EXT.SVE.SET.GROUP>addg
   New group added, group no = 1
   ROD.EXT.SVE.SET.GROUP>
```

We have added one group, but it contains nothing so far:

```
   ROD.EXT.SVE.SET.GROUP>list
   # group name    x + d     y + d     z + d   phi + d   chi + d    th + d
    1              0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0
   Origin of atoms:  0.0000   0.0000   0.0000
    # el     x +     y +      z + B
   ROD.EXT.SVE.SET.GROUP>
```

We first give it a name:

```
   ROD.EXT.SVE.SET.GROUP>name
   Group number: 1
   Group name[          ]: Example
   ROD.EXT.SVE.SET.GROUP>
```

Then we add the first atom:

```
   ROD.EXT.SVE.SET.GROUP>adda
   Group number:1
   New atom added in group # 1, atom no = 1
   ROD.EXT.SVE.SET.GROUP>element
   Group number:1
   Atom number: 1
   Element type: C
   ROD.EXT.SVE.SET.GROUP>list
   # group name    x + d     y + d     z + d   phi + d   chi + d    th + d
    1    Example  0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0
   Origin of atoms:  0.0000   0.0000   0.0000
    # el     x +     y +      z + B
    1  C  0.0000  0.0000  0.0000  0
   ROD.EXT.SVE.SET.GROUP>
```

Our group of atoms now contain one atom. We now add the other six atoms, and also set their x and z co-ordinates:

```
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 2 C xatom 1 2 1.204 zatom 1 2 0.695
   New atom added in group # 1, atom no = 2
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 3 C xatom 1 3 -1.204 zatom 1 3 0.695
   New atom added in group # 1, atom no = 3
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 4 C xatom 1 4 1.204 zatom 1 4 2.085
   New atom added in group # 1, atom no = 4
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 5 C xatom 1 5 -1.204 zatom 1 5 2.085
   New atom added in group # 1, atom no = 5
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 6 C zatom 1 6 2.780
   New atom added in group # 1, atom no = 6
   ROD.EXT.SVE.SET.GROUP>adda 1 element 1 7 C zatom 1 7 4.690
   New atom added in group # 1, atom no = 7
   ROD.EXT.SVE.SET.GROUP>list
   # group name    x + d     y + d     z + d   phi + d   chi + d    th + d
    1    Example  0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0  0.0000  0
   Origin of atoms:  0.0000   0.0000   0.0000
    # el     x +     y +      z + B
    1  C  0.0000  0.0000  0.0000  0
    2  C  1.2040  0.0000  0.6950  0
```

```
3  C -1.2040  0.0000  0.6950  0
4  C  1.2040  0.0000  2.0850  0
5  C -1.2040  0.0000  2.0850  0
6  C  0.0000  0.0000  2.7800  0
7  C  0.0000  0.0000  4.6900  0
ROD.EXT.SVE.SET.GROUP>
```

We have now successfully added our atoms to the group.

2.3   The group format in surface model (.sur) files

A group can also be added directly into a surface model (.sur) file. The general format is (the parameters in the bracket are optional):

```
group groupname  [origx origy origz]
startx starty startz phi chi th
Atomtype1    atomx1     atomy1     atomz1    [DebyWaller serial number1]
Atomtype2    atomx2     atomy2     atomz2    [DebyWaller serial number2]
....
AtomtypeN    atomxN     atomyN     atomzN    [DebyWaller serial numberN]
endgroup
```

The example molecule described in the previous section can be input by using the following example.sur file:

```
Example of grouping of atoms
 1.0000 1.0000 1.0000  90.0  90.0  90.0
group Example  0.0000   0.0000   0.0000
0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
 C     0.00000     0.00000     0.00000
 C     1.20400     0.00000     0.69500
 C    -1.20400     0.00000     0.69500
 C     1.20400     0.00000     2.08500
 C    -1.20400     0.00000     2.08500
 C     0.00000     0.00000     2.78000
 C     0.00000     0.00000     4.69000
endgroup
```

3   The cylinder and ellipsoid models

The cylinder and ellipsoid models are simple models to approximate electronic charge distributions of a molecule as a whole, rather than treating it as the overlap of the charge densities of individual atoms. This approach will help to get a first orientation about the system. Furthermore molecules may have rotational degrees of freedom or parts with strong fluctuations. Both models may also be employed to describe such parts of molecules. The cylinder and ellipsoid models are both normalized, so that they will yield the correct number of electrons for the structure factor f(0) at zero scattering vector that equals the total charge per unit cell Z:

$$f(0) = \int \rho(x)\mathbf{dx} = Z$$

This way the cylinder model and the ellipsoid model can be combined in an arbitrary way with detailed atomic models in order to describe molecules, molecular side chains, etc.

A second application, in particular for the ellipsoid model is the description of partially ordered systems. If an atom rather has a position probability distribution than an exact position, the convolution of the atomic electron density with the position probability distribution can often be approximated by an ellipsoid. This may be a more intuitive approach than introducing static anisotropic Debye-Waller-factors, but is essentially equivalent.

In the following both models shall be described in detail.

3.1   The cylinder model

The cylinder model was introduced by Jens Als-Nielsen et al. to describe alkane chains at the air-water-interface. Molecules like fatty acids form ordered molecular layers on a water surface. Often the alkane chains are free to rotate in such phases. The electron density of such a rotating alkane chain is smeared out to a soft cylinder of a height L and a softness parameter a, which has a value of 0.38 Å for alkane chains. The form factor of such a molecule can be written as [1]:

$$f(\mathbf{q}) = \frac{Z}{1 + a^2 Q^2} \frac{\sin(q_z L/2)}{q_z L/2}$$

where Q is the lengths of the scattering vector parallel to the surface:

$$Q^2 = q_x{}^2 + q_y{}^2$$

and qz is its normal component. In the limit of $q \rightarrow 0$ this form factor yields the correct result f(0) = Z. For rod-like molecules other than alkane chains the parameter a can be fitted in the structure determination. However, it is to be recommended that appropriately averaged charge densities should be used to determine a, if the approximate structure of the molecule is known. The parameter value for alkane chains can always be used as a reasonable starting value in the fitting procedure. L can be estimated from the length of the molecule; for an alkane chain in an all-trans configuration this is simply

$$L = (N-1)\,1.265 \text{ Å}$$

where N is the number of carbon atoms in the chain [1].

In the original form the cylinder has hard ends, i.e. the electron density jumps to zero, which is somewhat unphysical. The model can be easily improved, though, by convolution of the cylinder with a Gaussian distribution along the cylinder axis. The result is described by another softness parameter c. The full analytic form of the form factor used in ROD is thus

$$f(\mathbf{q}) = \frac{Z}{1+a^2 Q^2} \frac{\sin(q_z L/2)}{q_z L/2} \exp(-\frac{c^2 q_z^2}{2})$$

In order to determine the form factor fR of an arbitrarily rotated cylinder as described by a rotation matrix R, we note the general property

$$f_{\mathbf{R}}(\mathbf{q}) = f(\mathbf{R}\,\mathbf{q})$$

which will be shown in Section 3.3. So rather than calculating the form factor by Fourier transforming every rotated charge density distribution r(R x), we use the above form factor of an upright cylinder and rotate q. Note that the rotation center was chosen to be the center of the cylinder so that the Fourier transform of the charge density yield real numbers for the form factor.

The full set of parameters describing the cylinder model is hence Z, L, a, c, cC, qC, xC, yC, and zC. cC and qC are the tilt and the azimuth of the tilt, respectively. xC, yC, and zC are the displacements of the center of the cylinder with respect to the surface unit cell in crystal coordinates i.e. relative to the substrate unit cell. Out of the total of 9 parameters Z will be usually known and there will be reasonable guesses for L and a. The remaining parameters will have to be fitted. In some cases it may be helpful to analyse the scattering rods in the spirit of [1,2], in order to get a first idea about the tilt angles.

3.1.1 Entering cylinders in ROD

In this section we will show you how you can enter cylinders in ROD. Cylinders can be entered either via the ROD.EXT.SVE.SET.CYLINDER> menu or via the surface structure model input file (.sur).

The details of how to define the cylinder parameters via the menu or the surface structure model input file have not yet been documented. At the moment only a listing of the menu functions is available. If you want to use this feature of ROD and need more information, please send a message to the author Olof Svensson (svensson@esrf.fr) or to the ANAROD mailing list (anarod@esrf.fr).

3.1.2 The ROD.EXT.SVE.SET.CYLINDER> menu

The ROD.EXT.SVE.SET.CYLINDER> menu contains the following functions:

```
************************ SET CYLINDER MODEL PARAMETERS ************************
Name      : Cylinder name
Xstart    : Start x-position
XDisplace : Serial number of x-displacement parameter
Ystart    : Start y-position
YDisplace : Serial number of y-displacement parameter
Zstart    : Start z-position
ZDisplace : Serial number of z-displacement parameter
Tstart    : Start t-angle
TDispl    : Serial number of t-angle par.
Psistart  : Start psi-angle
PSIDispl  : Serial number of psi-angle par.
ORigin    : Centre of rotation of cylinder
Add       : Add a cylinder
Del       : Delete a cylinder
CHarge    : Total charge of a cylinder
LEngth    : Length of a cylinder
SLength   : Serial no of length
RAdius    : Radius of a cylinder
SRadius   : Serial no of radius
Softness  : Softness of a cylinder
SSoftness : Serial no of softness
Occup     : Occupancy of a cylinder
SOCcup    : Serial no of occupancy
List      : List cylinders
Help      : Display menu
Return    : Return to main menu
ROD.EXT.SVE.SET.CYLINDER>
```

3.1.3   The cylinder format in surface model (.sur) files

A cylinder can also be added directly into a surface model (.sur) file.

3.2   Ellipsoid model

The ellipsoid model describes a soft ellipsoid very much in the spirit of the cylinder model and can be used for a large variety of simple molecular shapes such as spherical, prolate, and oblate. Gaussian charge distributions with standard deviations a, b, and c in the three Cartesian directions are assumed yielding a form factor of

$$f(\mathbf{q}) = Z \exp(- \{a^2 q_x^2 + b^2 q_y^2 + c^2 q_z^2\}/2)$$

The usual normalization f(0) = Z obviously holds, and the structure factor of the rotated object can again be determined by fR(q) = f(R q). Compared to the cylinder model an additional degree of freedom, fE, is introduced, which corresponds to the rotation of the ellipsoid around the z-axis. Hence there is a full number of 10 parameters, the total charge Z, the half axes a, b, c, the Eulerian angles fE, cE, qE and finally the crystal coordinates of the center of the ellipsoid, xE, yE, and zE. In case of rotational symmetry, e.g. a=b, the initial orientation of the ellipsoid can always be chosen, such that fE can be dropped from the fitting model.

3.2.1   Entering ellipsoids in ROD

In this section we will show you how you can enter ellipsoids in ROD. Ellipsoids can be entered either via the ROD.EXT.SVE.SET.ELLIPSOID> menu or via the surface structure model input file (.sur).

 The details of how to define the ellipsoid parameters via the menu or the surface structure model input file have not yet been documented. At the moment only a listing of the menu functions is available. If you want to use this feature of ROD and need more information, please send a message to the author Olof Svensson (svensson@esrf.fr) or to the ANAROD mailing list (anarod@esrf.fr).

3.2.2   The ROD.EXT.SVE.SET.ELLIPSOID> menu

The ROD.EXT.SVE.SET.ELLIPSOID> menu contains the following functions:

```
ROD.EXT.SVE.ELLIPSOID>help
*********************** SET ELLIPSOID MODEL PARAMETERS ***********************
 Name      : Ellipsoid name
 Xstart    : Start x-position
 XDisplace : Serial number of x-displacement parameter
 Ystart    : Start y-position
 YDisplace : Serial number of y-displacement parameter
 Zstart    : Start z-position
 ZDisplace : Serial number of z-displacement parameter
 Phistart  : Start phi-position
 PHIDispl  : Serial number of phi-displacement par.
 Chistart  : Start chi-position
 CHIDispl  : Serial number of chi-displacement par.
 Thstart   : Start th-position
 THDispl   : Serial number of th-displacement par.
 Add       : Add an ellipsoid
 Del       : Delete an ellipsoid
 CHarge    : Total charge of an ellipsoid
 ALength   : Length of a half axis
 ASerial   : Serial number of a half axis
 BLength   : Length of b half axis
 BSerial   : Serial number of b half axis
 CLength   : Length of c half axis
 CSerial   : Serial number of c half axis
 Softness  : Softness of an ellipsoid
 SSoftness : Serial number of softness
 Occupancy : Occupancy of an ellipsoid
 SOCcup    : Serial number of occupancy
 List      : List ellipsoids
 Help      : Display menu
 Return    : Return to main menu
ROD.EXT.SVE.SET.ELLIPSOID>
```

3.2.3 The ellipsoid format in surface model (.sur) files

An ellipsoid can also be added directly into a surface model (.sur) file.

3.3 Form factor of a rotated object

If an object of known form factor f(q) is rotated as described by a rotation matrix R, the form factor of the rotated object is given by

$$f_{\mathbf{R}}(\mathbf{q}) = \int \rho(\mathbf{R}\mathbf{x})\exp(i\mathbf{q}\mathbf{x})\,d\mathbf{x}$$

In order to relate to the known form factor f(q) of the unrotated object, we note the following identity

$$f_{\mathbf{R}}(\mathbf{q}) = \int \rho(\mathbf{R}\mathbf{x})\exp(i\{\mathbf{q}^{1}\mathbf{R}^{-1}\}\{\mathbf{R}\mathbf{x}\})\,d(\mathbf{R}\mathbf{x})$$

where the associated Jacobi determinant of R equals 1. Within the rotated coordinate system Rx we already know the analytical form of the form factor. Since R is orthogonal, we have R-1 = RT and thus {qT R-1}={qT RT} = {R q}T. We arrive at the general property of the Fourier transform:

$$f_{\mathbf{R}}(\mathbf{q}) = f(\mathbf{R}\,\mathbf{q})$$

This results means nothing but the fact that the diffraction pattern rotates along, when the object is rotated.

4 Bulk multiplicity utility

This utility provides the possibility of automatically expanding a bulk unit cell in the case the surface unit cell spans more than one bulk unit cell. The match between the surface unit cell and the bulk unit cell must be integer, i.e. this utility will not work if the surface unit cell covers a fraction of the bulk unit cell. It will not work either if the surface cell is rotated with respect to the bulk unit cell.

As an example, let us assume that the surface unit cell covers 2x3 bulk unit cells (2x3 multiplicity). First load the (simple) bulk unit cell. Here I will use a very simple bulk cell as an example:

```
Test bulk cell for bulk multiplicity example
1.0     1.0     1.0     90      90      90
C       0.0     0.0     0.0
O       0.50    0.50    0.50
```

Then go to the ROD.EXT.SVE> extension menu and choose "bulkmult". The program will ask you for the bulk multiplicity in the h- and k-directions:

```
ROD>ext sve
ROD.EXT.SVE>bulkmult
Bulk multiplicity in h direction[1]:2
Bulk multiplicity in k direction[1]:3
```

The program will calculate the number of atoms in the expanded cell together with the new lattice parameters:

```
Number of atoms in expanded bulk unit cell: 12
New lattice parameters:
2.00000000 3.00000000 1.00000000 90.00000327 90.00000327 90.00000327
Don't forget to save this expanded bulk unit cell in a ".bul" file.
ROD.EXT.SVE>
```

The program is also reminding you to save the expanded bulk cell. The new expanded bulk unit cell looks like this:

```
ROD>list bm t
Lattice parameters:  2.0000 3.0000 1.0000  90.0  90.0  90.0
 C   0.00000000   0.00000000   0.00000000   0 0.00
 C   0.00000000   0.33333334   0.00000000   0 0.00
 C   0.00000000   0.66666669   0.00000000   0 0.00
 C   0.50000000   0.00000000   0.00000000   0 0.00
 C   0.50000000   0.33333334   0.00000000   0 0.00
 C   0.50000000   0.66666669   0.00000000   0 0.00
 O   0.25000000   0.16666667   0.50000000   0 0.00
 O   0.25000000   0.50000000   0.50000000   0 0.00
 O   0.25000000   0.83333331   0.50000000   0 0.00
 O   0.75000000   0.16666667   0.50000000   0 0.00
 O   0.75000000   0.50000000   0.50000000   0 0.00
 O   0.75000000   0.83333331   0.50000000   0 0.00
ROD>
```

5   Atom overlap utility

This utility can spot overlapping atoms by calculating the distances between all atoms in the model and displaying the smallest distance. Since the bulk model and the surface model are separated in ROD, it can be difficult to spot if the two models are overlapping. The program calculates the minimum distance by first calculating the ortho-normal positions of all atoms in a 2x2x2 cell. Thus, overlapped atoms are also spotted if they are on the cell boundaries.

Below is given a small example:

```
ROD>list bm t
Lattice parameters:  1.0000 1.0000 1.0000  90.0  90.0  90.0
Cu   0.00000000   0.00000000   0.00000000   0 0.00
Cu   0.50000000   0.50000000   0.50000000   0 0.00
ROD>list sm t
Lattice parameters:  1.0000 1.0000 1.0000  90.0  90.0  90.0
Cu    1.00000     1.00000     1.00000   0 0.00 0.00
Cu    1.50000     1.50000     1.50000   0 0.00 0.00
ROD>ext sve
ROD.EXT.SVE>overlap
Minimum distance between atoms: 0.866025 [A]
ROD.EXT.SVE>
```

If we now add one atom to the surface model at (0.5,0.5,0.5), it is overlapping with one atom in the bulk model:

```
ROD>list sm t
Lattice parameters:  1.0000 1.0000 1.0000  90.0  90.0  90.0
Cu    1.00000     1.00000     1.00000   0 0.00 0.00
Cu    1.50000     1.50000     1.50000   0 0.00 0.00
Ni    0.50000     0.50000     0.50000   0 0.00 0.00
ROD>ext sve overlap
Warning! Distance = 0.000000 [A] between following atoms:
Cu    0.50000     0.50000     0.50000
Ni    0.50000     0.50000     0.50000
Warning! Distance = 0.000000 [A] between following atoms:
Cu    0.50000     1.50000     0.50000
Ni    0.50000     1.50000     0.50000
Warning! Distance = 0.000000 [A] between following atoms:
Cu    1.50000     0.50000     0.50000
Ni    1.50000     0.50000     0.50000
Warning! Distance = 0.000000 [A] between following atoms:
Cu    1.50000     1.50000     0.50000
Ni    1.50000     1.50000     0.50000
Minimum distance between atoms: 0.000000 [A]
ROD.EXT.SVE>
```

6 Simulation data output

In some cases it is useful to use simulated diffraction intensities as input to ROD. If one uses the SUM option in the ROD.LIST> menu, one gets a list of calculated structure factors and their phase, which cannot be used directly as .dat input to ROD since ROD expects the error estimate instead of the phase. Therefore I wrote a small utility that produces a list of structure factors and the square root of these as an estimate of their error. Here is an example on how to use this utility:

```
ROD>ca ra -1 1 1 -1 1 1 0.2
ROD>list sum t
     h      k      l       f-sum     phase
-1.000 -1.000  0.200    15.66566    35.97
-1.000  0.000  0.200     7.07606   -54.04
-1.000  1.000  0.200    15.66566    35.97
 0.000 -1.000  0.200     7.07606   -54.04
 0.000  1.000  0.200     7.07606   -54.04
 1.000 -1.000  0.200    15.66566    35.97
 1.000  0.000  0.200     7.07606   -54.04
 1.000  1.000  0.200    15.66566    35.97
ROD>ext sve sim
Filename (.dat) (type 't' or <return> for terminal): test
Comments: Test of simulation data
ROD.EXT.SVE>
ROD.EXT>
ROD>read dat test
Test of simulation data
ROD>list dat t
     h      k      l       f-dat      sigma lbr
-1.000 -1.000  0.200    15.66566    3.96000   0
-1.000  0.000  0.200     7.07606    2.66000   0
-1.000  1.000  0.200    15.66566    3.96000   0
 0.000 -1.000  0.200     7.07606    2.66000   0
 0.000  1.000  0.200     7.07606    2.66000   0
 1.000 -1.000  0.200    15.66566    3.96000   0
 1.000  0.000  0.200     7.07606    2.66000   0
 1.000  1.000  0.200    15.66566    3.96000   0
ROD>
```

7 Acknowledgements

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8 References

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[2] Vladimir M. Kaganer, Helmuth Möhwald, and Pulak Dutta: "Structure and phase transitions in Langmuir monolayers", Rev. Mod. Phys. 71, 779-819 (1999).