

MCSL'S EXTENSIONS FOR ROD

Marie-Claire SAINT-LAGER
 Laboratoire de Cristallographie-CNRS
 25 avenue des Martyrs, BP 166
 F-38042 Grenoble cedex FRANCE
 email: stlager@polycnrs-gre.fr

Changes induced when the MCSL's extension is activated:

A- In the general menus:

I) Read menu:

- Possibility of adding an occupation serial number for the bulk atoms in the bulk file (useful for substrate alloy) (*as for Robach extension*)
- Possibility of adding a second serial number for the occupation in the fit file (useful for alloy and/or for interdiffusion: the total occupancy $occtot = occ(nocc1) - occ(nocc2)$). (*as for Robach's extension*)
- Two formats for reading exist depending on the mode of calculation of the atomic position in the Z direction
- A new way of reading .fit files:
 - the program can recognize the format and also
 - reads the files with arbitrary position & number of the columns

BUT the third line of comments must

- begin with **#el** and contain the column names with exactly the correct spelling
- the number of columns as well as their sequence are arbitrary

→ format1:

#el this indicates to ROD that it has to recognize the columns itself.
 If the line starting with **#el** is absent,
 ⇒ ROD uses the standard way
 ⇒ or the way corresponding to the activated extensions

XS cx1 nx1 cx2 nx2 => for the X direction (*no change compared to the standard form*)
 $X = XS + cx1*displ(nx1) + cx2*displ(nx2)$,
 XS is the reference value,
 nx1 & nx2 are serial number of displacement fit parameters,
 cx1 & cx2 are fixed coefficients

YS cyl nyl cy2 ny2 => for the Y direction (*idem*)

ZS => ZS gives the reference position of the atom

cz1 nz1 cz2 nz2 cz3 nz3 => coefficient and displacement parameters in the Z direction,
3 fit parameters are possible

dwl dw2 => serial number of Debye Waller fit parameters

ocl oc2 => serial number of occupancy fit parameters
 the total occupancy = $occ(oc1) - occ(oc2)$

For this format the flag NDELTAZS is set to FALSE (0)

The position of the atom **I** along the Z axis is given by (standard way):

$$Z(I) = ZS(I) + cz1(I)*displ(nz1(I)) + cz2(I)*displ(nz2(I)) + cz3(I)*displ(nz3(I))$$

→ **format 2:**

#el (as in format 1)
XS cx1 nx1 cx2 nx2 (as in format 1)
YS cy1 ny1 cy2 ny2 (as in format 1)

NP => gives the serial number of the plane where the atom is localized,
 additional column compared to format 1
 => indicates to ROD that the .fit file is written in the 2d format
 => NP = 1 for the plane just above the substrate

DZS => DZS gives the reference distance of the atom relative to the
 average Z value of the atoms in the previous plan (NP-1)
 DZS = 0 for NP = 1

cz1 nz1 cz2 nz2 cz3 nz3 (as in format 1)

dwl dw2 (as in format 1)

ocl oc2 (as in format 1)

For this format the flag NDELTAZS is set to TRUE (1)

The position Z(I) of the atom **I on the plane NP** is given by:

Z(I) = <Z(NP-1)> + DZS(I) + cz1(I)*displ(nz1(I)) + cz2(I)*displ(nz2(I)) + cz3(I)*displ(nz3(I)),
<Z(NP-1)> is the average Z value of atoms on plane NP-1:

The average <Z(NP)> value is calculated as follows:

NP=1
 ⇨ <Z(NP=1)> = <DZS(NP=1)>
 ⇨ <DZS(NP=1)> = average value of DZS of all the atoms on the plane NP=1
 NP=2
 ⇨ <Z(NP=2)> = <Z(NP=1)> + <DZS(NP=2)>,
 ⇨ <DZS(NP=2)> = average value of DZS of all the atoms on the plane NP=2

 NP=J
 ⇨ <Z(NP=J)> = <Z(NP=J-1)> + <DZS(NP=J)>,
 ⇨ <DZS(NP=J)> = average value of DZS of all the atoms on the plane NP=J

If NSURF2 > 0, the values are independently calculated for the two domains.

In any case, ROD lists on the screen the name of the columns, NDELTAZ and the number of planes (NP max).

II) Set plot menu:

A new option is added in ROD.SET.PLOT>: "FB"

It activates a new submenu that allows to change the settings of the "FB", "FT" and "FD" plots
(plot of the theoretical and experimental structure factors)

- color of two 1/2 circles can be chosen (fth & fdata ⇔ "FB")
- idem for the color of the circles for Fth ("FT") and Fdata ("FD")
- color of their contour
- fix the Xmin, Xmax, Ymin and Ymax of the axes
- automatic X and Y scales
- the scale of the X and Y axis: cte/Angström or rlu
(Warning! If the scales are anisotropic, this gives ellipses. This problem remains to be solved.)

III Fit menu:

After a fitting session, the R_factor is also written on the screen.

If an outfile has been opened (cf: ROD.EXT.MCSL> menu) the values of the selected fit parameters are written to it as well as the R_factor and chisqr values.

If no outfile is opened, the flag "no outfile" is written at the end of the listing on the screen.

B- The ROD.EXT.MCSL> menu:

gives access to:

I) outfile = save fit parameters menu

ROD.EXT.MCSL.SAVE>

- **Open**: open the file where the selected fit parameters and the Chisq and R-value will be written after the fit
- **Lfit**: list all the fit parameters
- **Save, Strange and Sall**: select the fit parameters to be saved
- **Delete, Drange**: remove parameters from saving
- **Write**: write the names of the selected parameters at the beginning of the columns, useful after any change
- **Close**: close the output file
- **List**: list the name of the file and the selected parameters

II) SET

Not yet available.

III) LOOP

ROD.EXT.MCSL.LOOP>

Allows to do automatically a series of fits by varying several fit parameters (1 to 6)

Warning! You have to pass through the fit menu first (where the fit parameters are defined) before going to this menu

- The loops are included in each others: L1⊃ L2⊃ L3⊃ L4⊃ L5⊃ L6
- The values of the selected fit parameters for the loops as well as the R_factor and chisqr values are automatically saved in the “output” file (which has to be opened before running the fit), with their name at the beginning of the run
- Most of the listing on the screen has been removed to accelerate the program
- It does not work for fitting in the “COOLDOWN” mode
- **When leaving this menu, all the loop parameters are forgotten.**

This option gives access to the menu:

- **L1oop** define loop1 parameters
- **L2oop** define loop2 parameters
- ...
- **L6oop** define loop6 parameters
- **Run** **run the automatic fit**
(the total number of fits and the one being run are displayed)
- **List** list the parameters of all the loops

If one the **Lioop** is chosen (i=1, 2, ..6), this gives access to the menu ROD.EXT.MCSL.LOOP.SET>:

- **Lfit** list all the available fit parameters
- **Par** choose the fit parameter to vary in the loop i
- **Init** choose the initial value
- **End** choose the final value
- **Step** increment of the loop
- **List** list the parameters of the loop

ANNEX A: .fit file for the same surface film: 1) in the format 2

```

Ni(110) 1x2
2.491 7.046 2.491 90 90 90
#el  XS  YS  cy1  ny1  Np  DZS  cz1  nz1  cz2  nz2  oc1  oc2
Ni  0.00 0.00 0.0  0  1  0.000 1.0  4  0.00 0  1  0
Ni  0.00 0.50 0.0  0  1  0.000 1.0  4  0.00 0  1  0
Ni  0.50 0.25 0.0  0  2  0.500 1.0  5  -1.0 11  2  0
Ni  0.50 0.75 0.0  0  2  0.500 1.0  5  1.00 11  2  0
Ni  0.00 0.00 1.0  1  3  0.500 1.0  6  0.00 0  3  0
Ni  0.00 0.50 -1.0  1  3  0.500 1.0  6  0.00 0  3  0
Pd  0.50 0.25 0.0  0  2  0.500 1.0  5  -1.0 11  8  2
Pd  0.50 0.75 0.0  0  2  0.500 1.0  5  1.00 11  8  2
Pd  0.00 0.00 1.0  1  3  0.500 1.0  6  0.00 0  8  3
Pd  0.00 0.50 -1.0  1  3  0.500 1.0  6  0.00 0  8  3
Pd  0.50 0.25 0.0  0  4  0.550 1.0  7  1.00 12  4  0
Pd  0.50 0.75 0.0  0  4  0.550 1.0  7  -1.0 12  4  0
Pd  0.00 0.00 -1.0  2  5  0.550 1.0  8  0.00 0  5  0
Pd  0.00 0.50 1.0  2  5  0.550 1.0  8  0.00 0  5  0
Pd  0.50 0.25 0.0  0  6  0.550 1.0  9  -1.0 13  6  0
Pd  0.50 0.75 0.0  0  6  0.550 1.0  9  1.00 13  6  0
Pd  0.00 0.00 1.0  3  7  0.550 1.0  10 0.00 0  7  0
Pd  0.00 0.50 -1.0  3  7  0.550 1.0  10 0.00 0  7  0

```

In this surface film the planes 2 and 3 are occupied by Ni and Pd (interdiffusion)
For each atom: $\text{occup}_{\text{tot}} = \text{occ}(\text{oc1}) - \text{occ}(\text{oc2})$

With occupancy 8 = 1

occupancy 2 = 0.66

occupancy 3 = 0.33

⇒ Composition of plane 2 = Ni : 66% Pd : 34%

⇒ Composition of plane 3 = Ni : 33% Pd : 67%

Example of values for the displacement parameters and the corresponding Z
(with $\text{disp } 11, 12 \text{ and } 13 = 0$)

```

NP = 1 displace 4 0.0000 => Z = 0
NP = 2 displace 5 0.0120 => Z = 0.512
NP = 3 displace 6 0.0280 => Z = 1.04
NP = 4 displace 7 0.0000 => Z = 1.59
NP = 5 displace 8 0.0000 => Z = 2.14
NP = 6 displace 9 0.0000 => Z = 2.69
NP = 7 displace 10 -0.0100 => Z = 3.23

```

2) in the format 1

```

Ni(110) 1x2
2.491 7.046 2.491 90 90 90
#el  XS  YS  cy1  ny1  ZS  cz1  nz1  cz2  nz2  oc1  oc2
Ni  0.0 0.00 0.00 0  0.00 1.0  4  0.0 0  1  0
Ni  0.0 0.50 0.00 0  0.00 1.0  4  0.0 0  1  0
Ni  0.5 0.25 0.00 0  0.50 1.0  5  -1. 11  2  0
Ni  0.5 0.75 0.00 0  0.50 1.0  5  1.0 11  2  0
Ni  0.0 0.00 1.00 1  1.00 1.0  6  0.0 0  3  0
Ni  0.0 0.50 -1.0  1  1.00 1.0  6  0.0 0  3  0
Pd  0.5 0.25 0.00 0  0.50 1.0  5  -1. 11  8  2
Pd  0.5 0.75 0.00 0  0.50 1.0  5  1.0 11  8  2
Pd  0.0 0.00 1.00 1  1.00 1.0  6  0.0 0  8  3
Pd  0.0 0.50 -1.0  1  1.00 1.0  6  0.0 0  8  3
Pd  0.5 0.25 0.00 0  1.55 1.0  7  1.0 12  4  0
Pd  0.5 0.75 0.00 0  1.55 1.0  7  -1. 12  4  0
Pd  0.0 0.00 -1.0  2  2.10 1.0  8  0.0 0  5  0
Pd  0.0 0.50 1.00 2  2.10 1.0  8  0.0 0  5  0
Pd  0.5 0.25 0.00 0  2.65 1.0  9  -1. 13  6  0
Pd  0.5 0.75 0.00 0  2.65 1.0  9  1.0 13  6  0
Pd  0.0 0.00 1.00 3  3.20 1.0 10 0.0 0  7  0
Pd  0.0 0.50 -1.0  3  3.20 1.0 10 0.0 0  7  0

```

Occupancies work as in format 2

To obtain the same coordinates along the Z axis as in format 2, the value of the displacement parameters becomes:

```
displace 4 0.0000
displace 5 0.0120
displace 6 0.040
displace 7 0.0400
displace 8 0.0400
displace 9 0.0400
displace 10 0.0300
```

(the changes for one interplane distance must be propagated on all the above planes)

3) in the standard form

```
Ni(110) 1x2
2.491 7.046 2.491 90 90 90
Ni 0 0 0 0 0 0.000 0.0 0 0 0 0.00 1.0 4 0. 0 0 0 1 0
Ni 0 0 0 0 0 0.500 0.0 0 0 0 0.00 1.0 4 0. 0 0 0 1 0
Ni 0.5 0 0 0 0 0.250 0.0 0 0 0 0.50 1.0 5 -1. 11 0 0 2 0
Ni 0.5 0 0 0 0 0.750 0.0 0 0 0 0.50 1.0 5 1. 11 0 0 2 0
Ni 0 0 0 0 0 0.000 1.0 1 0 0 1.00 1.0 6 0. 0 0 0 3 0
Ni 0 0 0 0 0 0.500 -1.0 1 0 0 1.00 1.0 6 0 0 0 0 3 0
Pd 0.5 0 0 0 0 0.250 0.0 0 0 0 0.50 1.0 5 -1. 11 0 0 8 2
Pd 0.5 0 0 0 0 0.750 0.0 0 0 0 0.50 1.0 5 1. 11 0 0 8 2
Pd 0 0 0 0 0 0.000 1.0 1 0 0 1.00 1.0 6 0 0 0 0 8 3
Pd 0 0 0 0 0 0.500 -1.0 1 0 0 1.00 1.0 6 0 0 0 0 8 3
Pd 0.5 0 0 0 0 0.250 0.0 0 0 0 1.55 1.0 7 1. 12 0 0 4 0
Pd 0.5 0 0 0 0 0.750 0.0 0 0 0 1.55 1.0 7 -1. 12 0 0 4 0
Pd 0 0 0 0 0 0.000 -1.0 2 0 0 2.10 1.0 8 0 0 0 0 5 0
Pd 0 0 0 0 0 0.500 1.0 2 0 0 2.10 1.0 8 0. 0 0 0 5 0
Pd 0.5 0 0 0 0 0.250 0.0 0 0 0 2.65 1.0 9 -1. 13 0 0 6 0
Pd 0.5 0 0 0 0 0.750 0.0 0 0 0 2.65 1.0 9 1. 13 0 0 6 0
Pd 0 0 0 0 0 0.000 1.0 3 0 0 3.20 1.0 10 0. 0 0 0 7 0
Pd 0 0 0 0 0 0.500 -1.0 3 0 0 3.20 1.0 10 0. 0 0 0 7 0
```

- Z is calculated in the same way as in format 1

- Occupancies work as in format 1 and 2 **if Mcsl's or Robach's extensions are activated**

ANNEX B: example of macro using set.plot.fb> menu

```
E M A Y ret ret
set plo fb CFT green CFD yellow
xa ya
xu 7.046 yu 7.046 xmi -1
ret ret ret
```

ANNEX C: example of automatic fit

Example of macro for automatic fit:

```

E M A Y ret ret          /*activate Mcsl's extension */
R b n i l 1 0 r d dep r f depformat2 r p depformat2 /* read bulk, data, fit and parameters files */
E M O O fitpar "comments" ret /* open the output file fitpar.tab */
L O                      /* go into the loop menu
L1 P 20 I 0.5 E 0.8 S 0.1 ret /* set loop1 parameters */
L2 P 21 I 0.2 E 0.5 S 0.1 ret /* set loop2 parameters */
L3 P 0 ret              /* disable the unused loops */
L4 P 0 ret
L5 P 0 ret
L6 P 0 ret
R ret ret              /* do automatic fit and return to the root */

```

⇒ Fitpar.tab generated by the automatic fit session:

```

comments
Occupancy 2  Occupancy 3  chisqr  R-factor
0.5000 0.2000  0.16395  0.01252
0.5000 0.3000  0.24356  0.01190
0.5000 0.4000  0.37367  0.01216
0.5000 0.5000  0.55222  0.01422
0.6000 0.2000  0.02512  0.00620
0.6000 0.3000  0.03351  0.00458
0.6000 0.4000  0.09494  0.00559
0.6000 0.5000  0.20788  0.00843
0.7000 0.2000  0.09177  0.00643
0.7000 0.3000  0.02482  0.00359
0.7000 0.4000  0.01305  0.00420
0.7000 0.5000  0.05553  0.00708
0.8000 0.2000  0.37884  0.01202
0.8000 0.3000  0.23385  0.01043
0.8000 0.4000  0.14563  0.01081
0.8000 0.5000  0.11368  0.01203

```