MCSL'S EXTENSIONS FOR ROD

Marie-Claire SAINT-LAGER,
laboratoire de Cristallographie-CNRS, 25 avenue des Martyrs
BP 166 38042 Grenoble cedex FRANCE
mail : 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 of lecture 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 recognizes the format and also
  - read the files with arbitrary position & number of the columns

BUT the third line of comments must

- begin by **#el** and contain the column names with exactly the good 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 by **#el** is absent, ⇨ ROD uses the standard way ⇨ or the way corresponding to the activated extensions
XS cxl nxl 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	
czl nzl 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 NTELTAZS is set to FALSE (0)
The position of the atom **I** along the Z axis is given by (standard way) :
Z(I)= ZS(I) + cx1(I)*displ(nz1(I))+ cx2(I)*displ(nz2(I)) + cx2(I)*displ(nz2(I))

➔ **format 2:**

#el	*(as in format 1)*
XS cxl nxl cx2 nx2	*(as in format 1)*
YS cyl nyl 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 averaged Z value of the atoms in the previous plan (NP-1)
DZS = 0 for NP=1

czl nzl 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) + cx1(I)*displ(nz1 (I))+ cx2(I)*displ(nz2(I)) + cx2(I)*displ(nz2(I)),
<Z(NP-1)> is the averaged Z value of atoms on plane NP-1 :

The averaged <Z(NP)> value is calculated as followed :

NP=1
- ⇨ <Z(NP=1)>= <DSZ(NP=1)>
- ⇨ <DSZ(NP=1)>= averaged value of DZS of all the atoms on the plane NP=1

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

……

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

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

In any case, ROD list 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 which allow change the setting 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 in 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>

- ***O**pen* => open the file where the selected fit parameters and the Chisq and R-value will be written after the fit
- ***Lf**it* : list all the fit parameters
- ***S**ave, **Sr**ange and **Sa**ll* : to select the fit parameters to be saved
- ***D**elete, **Dr**ange :* to remove parameters of saving
- ***W**rite* : to write the selected parameters names at the beginning of the columns, useful after any change
- ***C**lose* : to close the output file
- ***Li**st* : to list the name of the file and the selected parameters

II) SET

- Not yet available

III) LOOP

ROD.EXT.MCSL.LOOP>

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

Warning! : You have to pass trough the fit menu first, (where the fit parameters are defined) before coming to this menu

- The loops are included in each others: L1⊃ L2⊃ L3⊃ L4⊃ L5⊃ L6
- The selected parameters for the loops and the loosed ones are automatically saved in the "output" file (which has to be open 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 going out this menu, all the loop parameters are forgotten.**

This option gives access to the menu :

- ***L1**oop* to define loop1 parameters
- ***L2**oop* to define loop2 parameters
- ***...***
- ***L6**oop* to define loop6 parameters
- ***F**it* to go to the fit menu (with all the usual options)
  ***The key "R**un" =>* **run the automatic fit**
  (the total number of fit and the running one is screened)
- ***Li**st* to list the parameters of all the loops

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

- ***Lf**it* List all the available fit parameters
- ***P**ar* choose the fit parameter to vary in the loop i
- ***I**nit* choose the initial value
- ***E**nd* choose the final value
- ***S**tep* increment of the loop
- ***Li**st* list the parameters of the loop

ANNEXE 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 plane 2 and 3 are occupied by Ni and Pd (interdiffusion)
For each atom : occuptot= occ(oc1) – occ(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 value for the displacement parameters and the corresponding Z
(with disp 11, 12 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	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	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	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	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	0.0.00	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 extension is activated**

ANNEXE 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
```

ANNEXE C : example of automatic fit

Example of macro for automatic fit:

```
E M A Y ret ret                              /*activate Mcsl's extension */
R b ni110 r d dep r f depformat2 r p depformat2   /* read bulk, data, fit and parameters files */
F ret                                        /* go through the fit menu */
E M O O  fitpar  "comments"  ret             /* open the output file fitpar.tab */
LO                                           /* 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                                   /* rest the unused loops */
L4 P 0 ret
L5 P 0 ret
L6 P 0 ret
F R ret ret                                  /* go to 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