

## RMCPow PRACTICAL

### Modelling the thermal diffuse scattering of AgBr

Files needed are found in the same zip file as this instruction. Copy or extract the files into a suitable directory and follow the instructions below. The different programs used can be accessed with the shell program called **WinNFLP**, available at [ftp://ftp.studsvik.uu.se/Pub/WinNFLP/Win\\_NT/](ftp://ftp.studsvik.uu.se/Pub/WinNFLP/Win_NT/). To run, click on the WinNFLP icon, a browser window will then appear. Select your working directory by clicking on a file in that directory (any will do). Now you can access the programs you want to run from the menus **Useful** or **RMC**. If you do not have the WinNFLP program it is still possible to run the RMCPow simulations since all necessary input files are provided here.

The general approach of the practical is as follows:

- The long-range and local order of crystalline AgBr will be modelled by a simultaneous fit to the thermal diffuse and Bragg scattering.
- Correlation of atomic displacements of atoms with small separation will be studied and compared to the long-range limit results.

**The times given in this practical, for running RMCPow is real time and NOT CPU time. The times may have to be increased on a slow computer. The output you get will probably not be identical to the output in this example. The plotting and programs used in this practical can also be done with in principle any standard plotting program, such as Origin or SigmaPlot, since most data is easily imported as ASCII files.**

1. The model is based on the neutron scattering data obtained on the Studsvik Liquid and Amorphous Diffractometer SLAD. This is in the file `agbr_slad.fq`. Plot it with the program FqPlot.

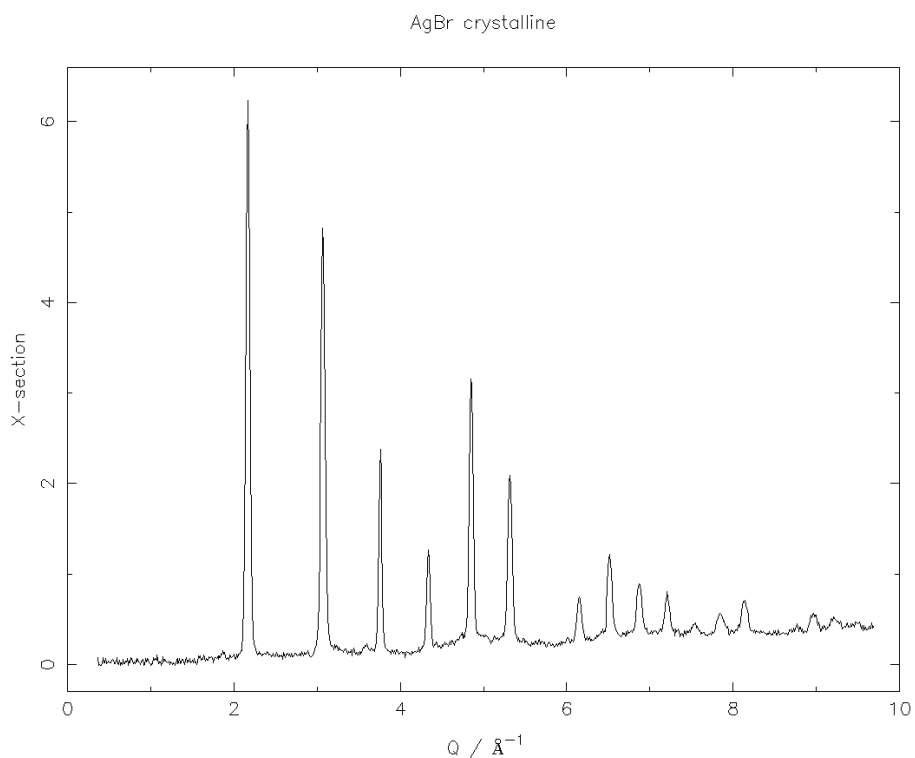
Useful → User programs → FqPlot.exe

When the FqPlot program starts type:

```
Filename [.fq] > agbr_slad.fq  
agbr_slad.fq  
Format? G(ENIE)/T(EXT)/D(ATA) > d  
Graphics device/type (? to see list, default/W9):<RETURN>
```

Now you should have a plot on the screen. To plot with other limits select the FqPlot text input window and type

```
Change limits? [T/F] > t  
Data limits are           :   .370   9.690   -.012   6.231  
Current plotting limits are :   .000  12.000   -.324   6.543  
New limits > 0 10 -.1 6.3
```



To exit type

```
Change limits? [T/F] > f  
Hardcopy output? [T/F] > f  
Type <RETURN> to close graphics window # 1 <RETURN>
```

If you want a hardcopy output (e.g. a GIF file) type

```

Hardcopy output? [T/F] > t
Graphics device/type (? to see list, default/W9):name/gif
Output to name

```

where name will be the GIF filename.

**2.** AgBr is an example of a system with the NaCl fcc lattice type with lattice parameter 5.78 Å at ambient temperature. We start with a lattice of multiple unit cells with atoms placed on equilibrium positions. To create the atomic configuration we use the Crystal program. As input we give the name of an input file, agbr\_rmcpow.atom, containing relevant parameters. These include the space group number, lattice parameters, the number of unit cell copies along each edge etc. Use an editor (like Notepad) to look at the input file.

```

.false.          ! do not apply to an existing cfg
225 1            ! fm_3m spg, setting 1
5.7814 5.7814 5.7814 90.0 90.0 90.0 ! a1,a2,a3,g1,g2,g3
 1 5 5 5        ! isym,n1,n2,n3
n               ! no displacements
 2             ! No. of atom types
 1             ! No. of sites
4a 0.0 0.0 0.0 ! site,x,y,z
 1             ! No. of sites
4b 0.5 0.5 0.5 ! site,x,y,z
.true.         ! RMC coordinates

```

To create the configuration run the program: **Useful → CFG programs → Crystal.exe** and give **agbr\_rmcpow.atom** as input file and **agbr\_rmcpow.cfg** as output file. Have a look at the new configuration file if desired. Note that there are 1000 atoms (500 Ag and 500 Br) in the configuration.

Next we need the control input file, agbr\_rmcpow.dat:

```

AgBr crystalline
 0 0              ! ncoll,ncycles
200 0 15 15      ! iprint,iplot,timelim,timesav
5.7814 5.7814 5.7814 90.0 90.0 90.0 !
a1,a2,a3,g1,g2,g3
0 0 0 0 0 0      ! lattice parameter flags
 6 5 5 5        ! isym,n1,n2,n3
2 0             ! ntypes,ntypesm
 0.1 0.1        ! delta
0 0.0           ! nswap,swapfrac
0 0.0           ! nref,reffrac
      3.2 2.2
      3.2       ! rcut
0             ! ncoord
0             ! nasc
0             ! nval
0             ! naval

```

```

1 0 0 ! nexpn,nexpx,nsingle
5.0 0.2 ! rwdt,swdt
0 1 ! ijob,iexist
agbr_slad.fq
0.3 11.0 ! Qmin,Qmax
0 ! nexcl
2 0.01 ! isign,sigman
1 0 ! nbpol,nbfix
0.0 1 ! alpha0,flag
1.0 1 ! beta,flag
1.115 1.0 ! wave,qwmax
1.3817 -0.8919 0.4607 0.0 0.0 ! U,V,W,IG,eta
0 0 0 0 0 ! resolution flags
0 ! wextn
1 ! Ag noccn
ag 1.0 ! symbol,coccn
1 ! Br noccn
br 1.0 ! symbol,coccn

```

A full description of the control file is given in the RMCPOW manual. Here we just make a few comments on some parameters:

- In addition to varying the model scattering we are also refining an overall scale factor and constant background (the flags for fitting beta and alpha0 are set to 1). This is generally useful because experimental data inevitably contains such errors. These parameters should however be close to 1 and 0 resp. if data is properly normalised.
- timelim and timesav are both set to 20 minutes, i.e. the program will run for that period and only save at the end. Later we will change these parameters.

Now start the simulation:

### RMC → RMC programs → RMCPOW.exe

A browser window will appear. Select **agbr\_rmcpow.dat** as input file, the initial calculation will take one or two minutes. After the initial results are saved copy agbr\_rmcpow.cfg and agbr\_rmcpow.out to e.g. agbr\_rmcpowA.\* for comparison with later results. Run the program for some 6000 generated moves or about 20 minutes as set up in the control file. On the screen you see how  $\chi^2$  decrease as the fitted  $F(Q)$  approach the experimental  $F(Q)$ . You should obtain a  $\chi^2 \sim 250$ .

**3.** While running have a look at the initial output with the RMCPlot program: **Useful → Plot programs → RMCPlot.exe** and give agbr\_rmcpowA.out as the file to plot. Note that there is no diffuse scattering since all atoms are initially at their equilibrium positions. Correspondingly the Bragg peaks are also too intense at large Q. We can also check the configuration by calculating the partial pair distribution functions, g(r): **Useful → Analyze Cfg programs → GrSq.exe** and type

```

Parameter file [.par] > <RETURN>
r spacing, rmax > .1 100
Q min, Q spacing, Qmax > 0 0 0

```

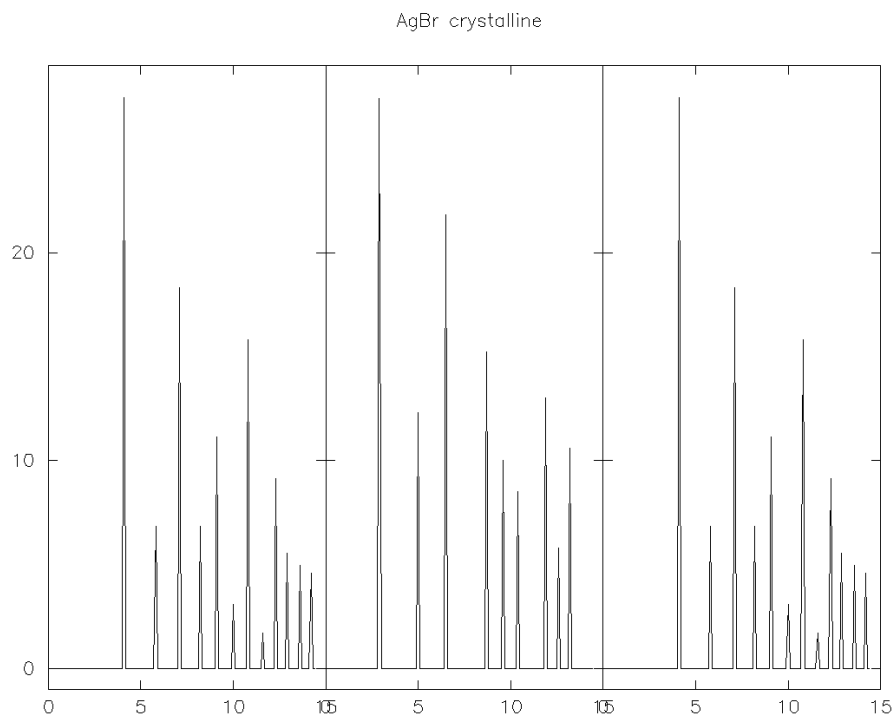
```

No. of configs          > 1
Totals                  [T,F] > f

Configuration file [.cfg] > agbr_rmcpowA
Output file           [.grs] > agbr_rmcpowA

```

The resulting plot is shown below. The three panels show the Ag-Ag, Ag-Br and Br-Br partials resp. If your result is significantly different something is wrong and you should go back and check your input files.



**4.** Back to the simulation, if necessary exit the RMCPOW program using **File → Exit** and save the results. Before continuing edit the control file to make the new run last for an hour or more. Also copy `agbr_rmcpow.cfg` and `agbr_rmcpow.out` to e.g. `agbr_rmcpowB.*`. Restart the simulation and meanwhile examine `agbr_rmcpowB.out` with RMCPlot. You should now see a significant diffuse contribution that is approaching the average experimental level although the details are not yet fitted. This means that we so far have obtained a configuration with almost correct mean square displacements (msd) of atoms but without correlated displacements. We can quantify this further by calculating the pair distribution function,  $g(r)$ . First use the GrSq program and compare to the fully ordered initial configuration. Since there is now considerable overlap of various shells we will use another program, GrDir, to resolve the peaks in the (100) direction. This program differs from GrSq in the sense that pairs are only counted if their joining vectors are located inside a tube along the specified direction. We can also take account of the average cubic structure by applying the appropriate symmetry operators so that all the equivalent {100} directions are considered. Start **Useful → Cfg programs → GrDir.exe** and type

```

Parameter file (or <CR> for manual) [.par] >
r spacing, rmax > .1 100
Q min, Q spacing, Qmax > 0 0 0
No. of configs > 1
Totals [T/F] > f

Tube, layer or spherical [T/L/S] > t
Symmetrize [T/F] > t
Space group and setting > 225 1
Reading symmetry data from c:\msdev\NFLProg\ ...
No. of unit cells > 5 5 5
Tube direction (UC units) > 1 0 0
Tube diameter (Angstroms) > 1
Configuration file [.cfg] > agbr_rmcpowB
Output file [.grs] > agbr_rmcpowB_100

```

We now want to investigate the peak widths of various shells. This can be done with the RMCFit program, run **Useful → Plot programs → RMCFit.exe** and type

```

Input file (0 to quit) > agbr_rmcpowb_100.grs
Format? G(ENIE)/T(EXT)/D(ATA)/R(MC) > r
Parameter output filename [.dat] > agbr_rmcpow100b_100
r, g(r)
Block 1 consists of 3 columns
Select column (0 for skip) > 1
Graphics device/type (? to see list, default /W9):
<RETURN>
Change limits? [T/F] > f
Fit a linear background [T/F] > f
Constant to be subtracted > 0

```

This will set up a graphical interface to fit Gaussians to the Ag-Ag partials. Do the fits as instructed in the PGPLOT Graphics Window and when finished go on to fit the data also in the 2<sup>nd</sup> and 3<sup>rd</sup> columns, for Ag-Br and Br-Br partials reps. Fitted parameters are saved to agbr\_rmcpowb\_100.dat. Inspection of this file should reveal that peak widths are mostly independent of pair separation.

Even in the case of correlated NN displacements the widths of far neighbour peaks are essentially determined by the convolution of two (more or less) independent Gaussian distributions, i.e. the peak width should approach the sum of the msd's of the two atom types considered. We can check this with the Disp3D program. This program will translate all atoms into a single unit cell and apply appropriate rotation and reflection symmetry operations within the cell to make up a histogram of displacements around the equilibrium positions. The histogram is then fitted with a 3-dimensional Gaussian distribution from which the msd can be calculated. An input file for this program is also supplied, agbr\_rmcpow.par:

```

agbr_rmcpow
225 1          ! ispg, isetting
6 5 5 5       ! isym, n1, n2, n3
t             ! Gaussian
t             ! Interactive
f             ! histogram

```

```

agbr_rmcpow
  1 1                      ! type,cbeta
  1.0 30                  ! rmax,nbin
  4a 0.0 0.0 0.0         ! Wsite,x,y,z
t                          ! another
  2 1                      ! type,cbeta
  1.0 30                  ! rmax,nbin
  4b 0.5 0.5 0.5         ! Wsite,,x,y,z
f                          ! another

```

Edit this file so that agbr\_rmcpow is replaced by e.g. agbr\_rmcpowB and save as agbr\_rmcpowB.par. Run **Useful → Analyze Cfg programs → Disp3D.exe** and just type t to repeat iterations until each type converges (probably some 4-5 times), then type f to go on with the next type. Output is written to a file agbr\_rmcpow.dis. Look at this file and locate " Average (fitted and total) msd and position". The first number following this line is the fitted msd. As discussed above we expect to find that e.g.  $\sqrt{[\text{msd}(\text{Ag})+\text{msd}(\text{Br})]}$  is similar to our Ag-Br far neighbour results with RMCFit.

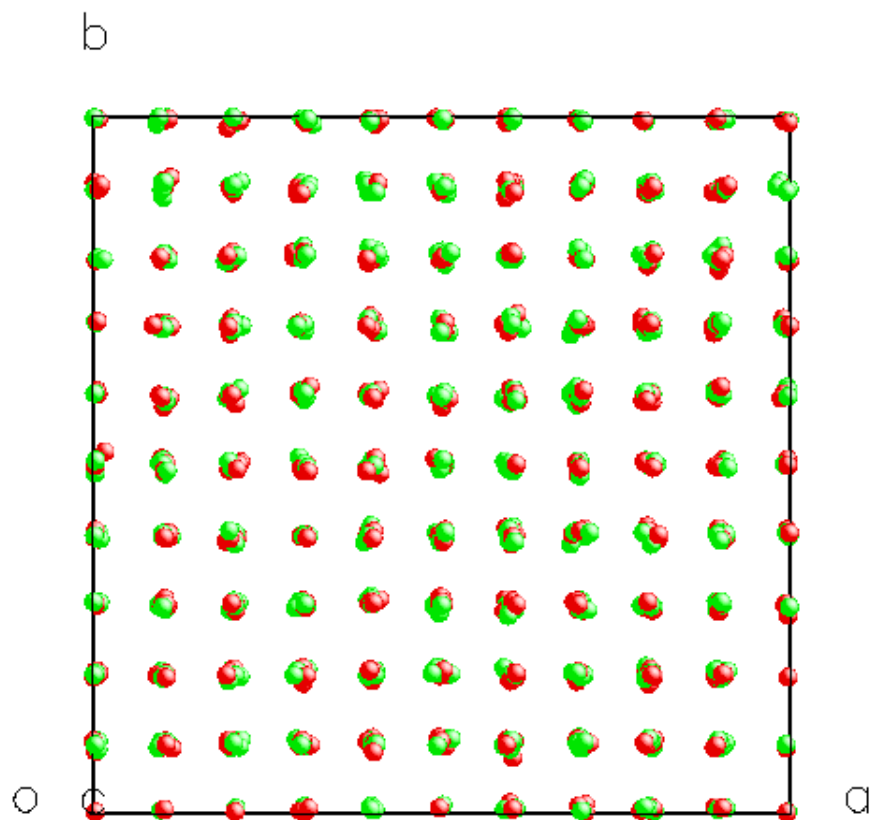
6. By now you should probably be finished with the final simulation. Use the various programs described above to investigate whether there are now actually some local correlations! You can also study  $g(r)$  in other directions, e.g. {110}. The size of the configuration used here is really at the lower limit for the purposes of our study. As a further exercise it is suggested to repeat the simulations for various smaller or larger configurations. One can also compare with the results obtained with the MCGR and RMCA programs for the same data (practical can be found on the NFL homepage).

7. Finally, we can view the atomic configurations using the ConfPlot program: **Useful → Plot programs → ConfPlot.exe** and at the ConfPlot prompt type

```

> open agbr_rmcpow.cfg
Reading file: agbr_rmcpow.cfg
Configuration contains 1000 atoms of 2 types.
> dir 1 0 0
> view 0 0 0 1000
> back 1
> box 0 1
> pl
Configuration: agbr_rmcpow.cfg
PLEASE WAIT...
Type: 1

```



See the ConfPlot manual for more information or use the online Help command. It is especially recommended to try out the contour plot option for the atom density reduced to a single unit cell, see the **unitcell** and **cplot** commands.