tutorial session III

Pair Distribution Function
PDF

```
pdf
#
     set bound, periodic,3D
     set density,  auto
     set corrquad, 0.0
     set corrlin,  0.0
     set srat,     0.7, 3.0
     set qbroad,   0.0
     set qdamp,    0.0
     set qmax,     25.000
     set rad,      xray
     set range,    32.08,0.02
     set therm,    gauss
#
     set weig,     1.0
     set finite,    periodic
#
     show
     calc
     save pdf,calculated.pdf
exit
```

Enter PDF menu

distances are calculated with 3D periodic boundary conditions
number density is calculated automatically
thermal peak width correction, square part
thermal peak width correction, linear part
sharpen peaks at r < 3.0 Å by factor of 0.7
instrumental resolution
instrumental resolution
Maximum Q value that was used in experiment
calculate PDF for X-ray /neutrons
calculate up to 32.08 Å in steps of 0.02 Å
calculate peak width from thermal parameters

optional wheighting scheme
$4 \pi \rho_0$ r line is calculated for periodic==infinite structure

show settings
calculate the PDF
store result in file „calculated.pdf“

Make sure you have started discus_suite

Change to directory Lectures/03_Pair_Distribution_Function

run macro **pdf.mac**

suite> @pdf.mac

This macro will take you in steps through the main PDF parameters

```
pdf
#
     set bound, periodic,3D
     set density,  auto
     set corrquad, 0.0
     set corrlin,  0.0
     set qbroad,   0.0
     set srat,     0.7, 3.0
     set qdamp,    0.0
     set qmax,     25.000
     set rad,      xray
     set range,    32.08,0.02
     set therm,    gauss
#
     set weig,     1.0
     set finite,periodic
#
     show
     calc
     save pdf,calculated.pdf
exit
```

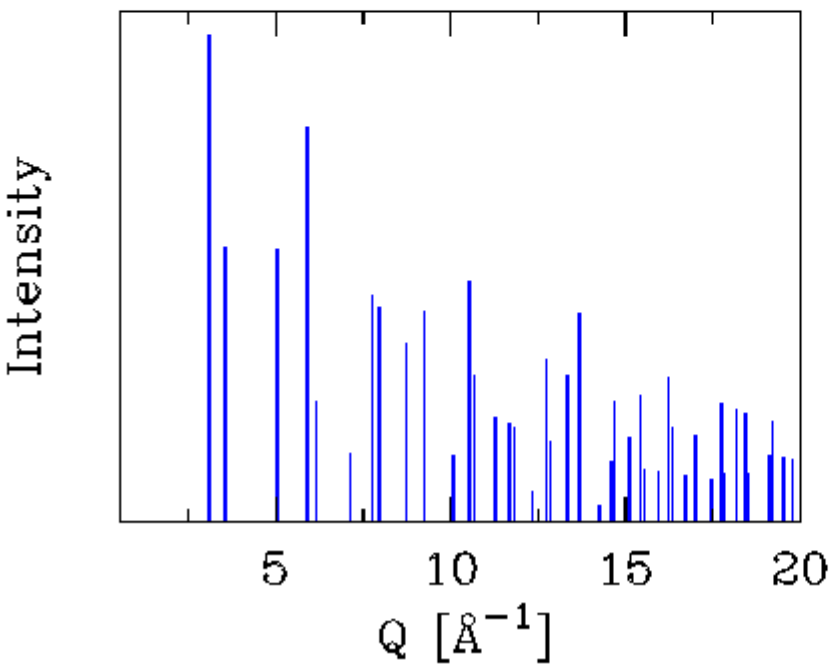
Enter PDF menu

distances are calculated with 3D periodic boundary conditions
number density is calculated automatically
thermal peak width correction, square part
thermal peak width correction, linear part
sharpen peaks at r < 3.0 Å by factor of 0.70
instrumental resolution
instrumental resolution
Maximum Q value that was used in experiment
calculate PDF for X-ray /neutrons
calculate up to 32.08 Å in steps of 0.02 Å
calculate peak width from thermal parameters

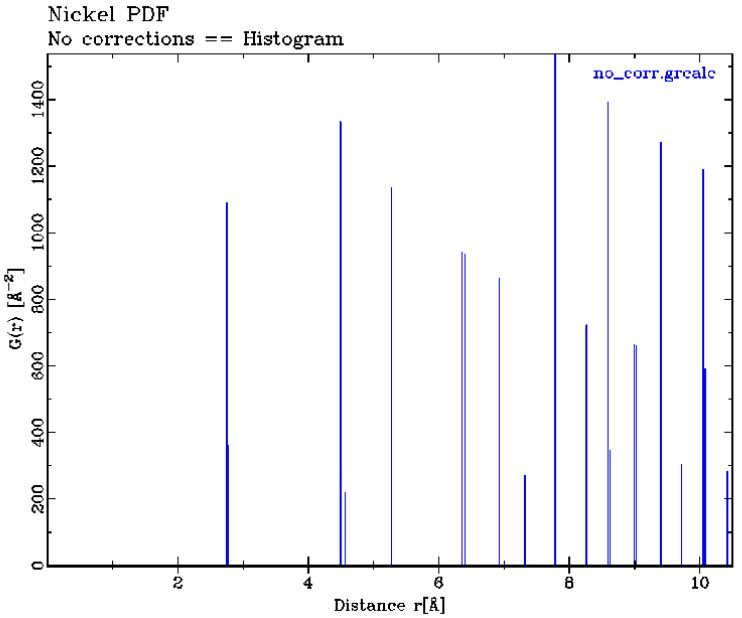
optional wheighting scheme
$4 \pi \rho_0$ r line is calculated for periodic==infinite structure

show settings
calculate the PDF
store result in file „calculated.pdf“

An ideal powder diffraction pattern

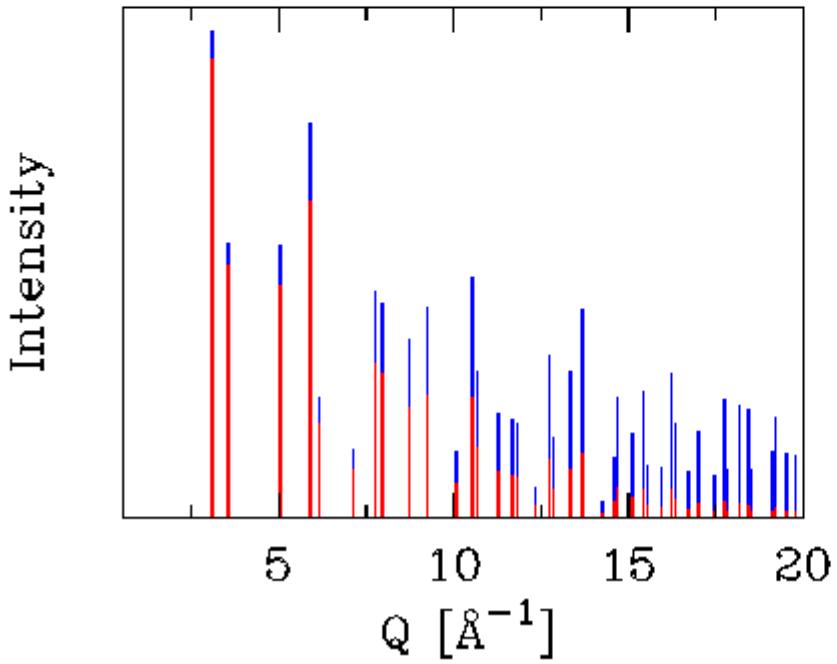


An ideal histogram

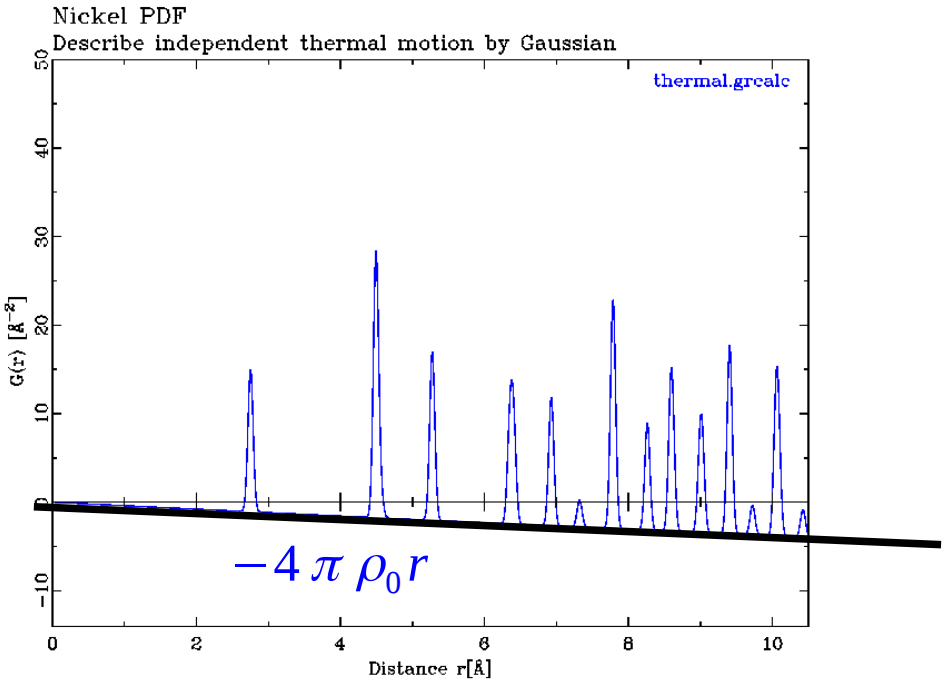


An ideal powder diffraction pattern

With thermal motion



PDF with thermal motion

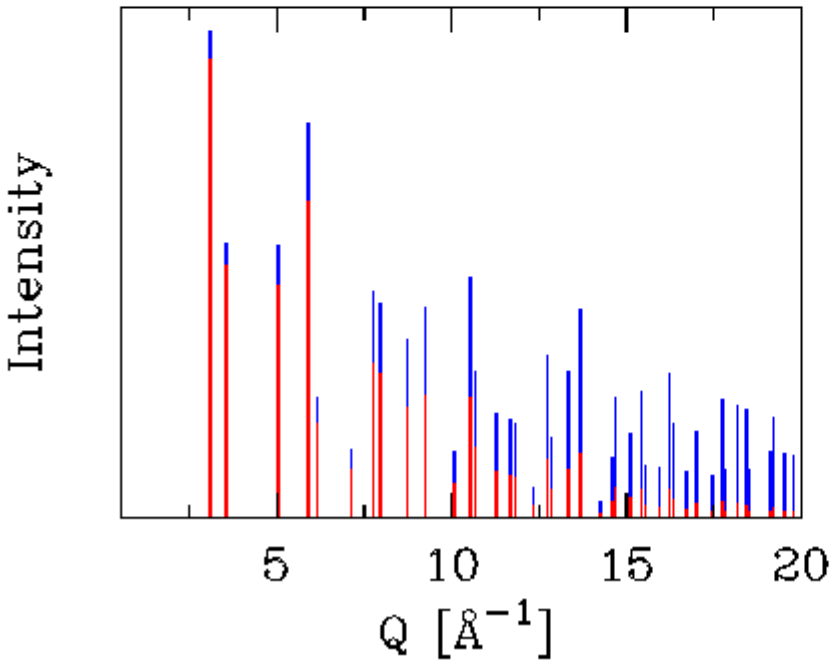


Subtract ‚background' line

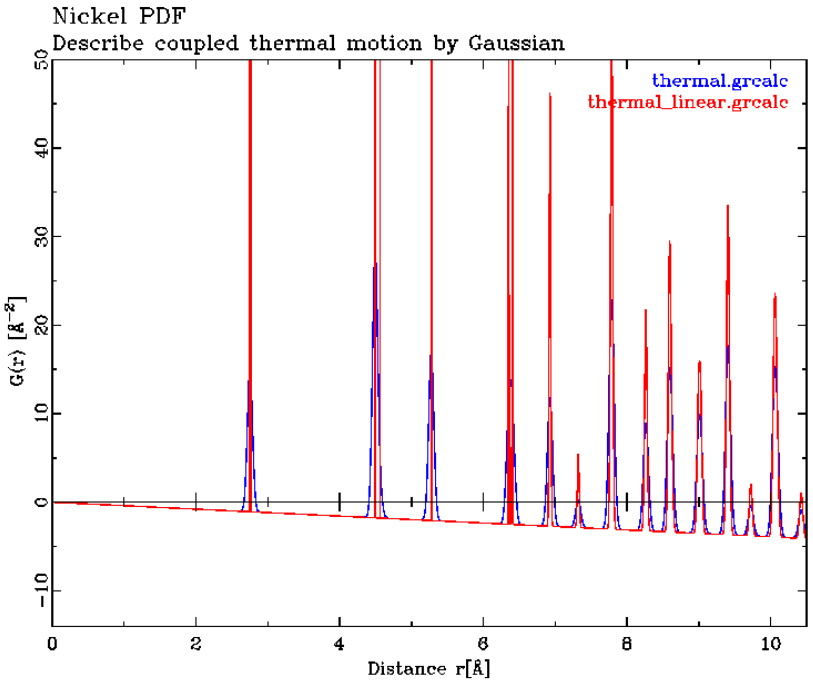
Maxima widened by Gaussian distribution

An ideal powder diffraction pattern

With thermal motion

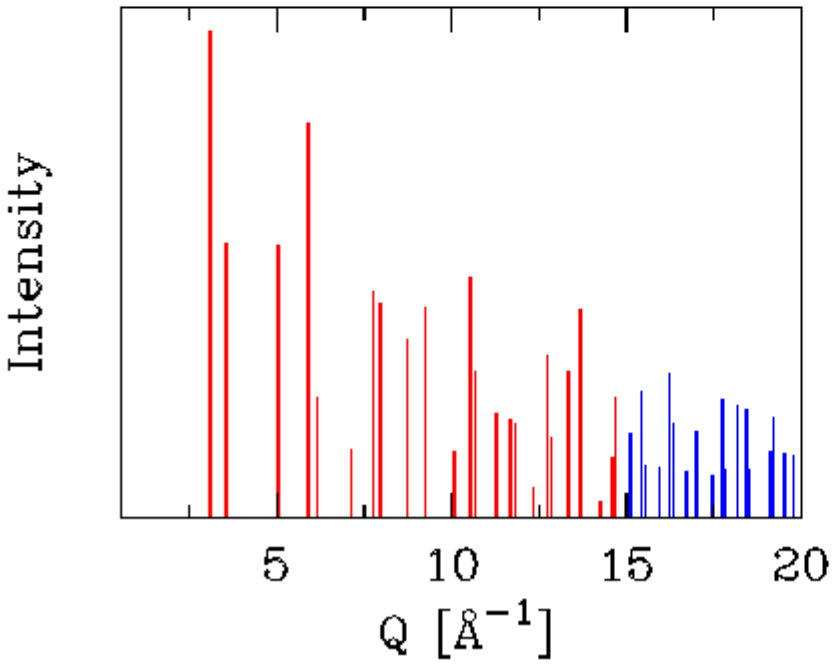


PDF with CORRLIN

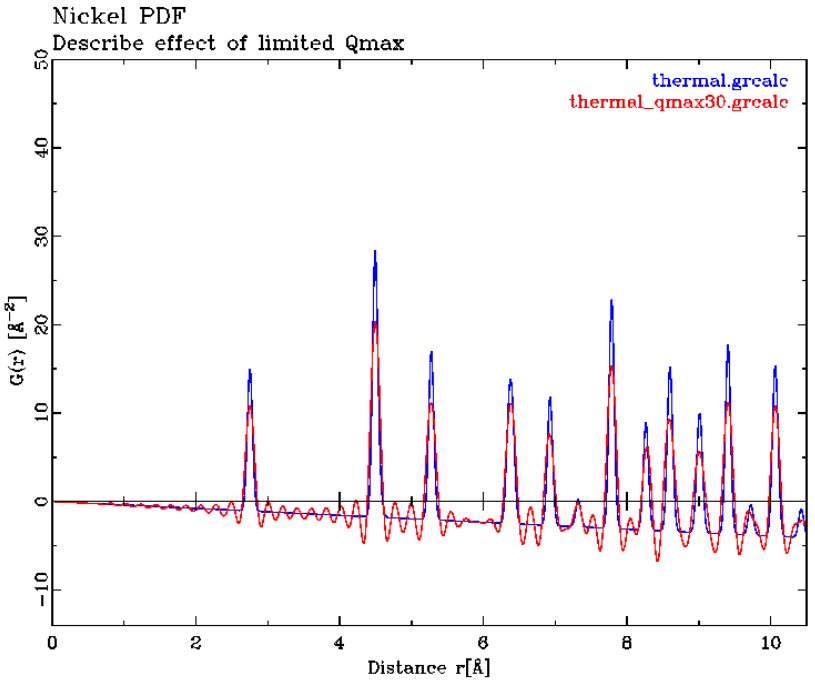


Maxima at short distances are narrower

An ideal powder diffraction pattern
With limited Q max

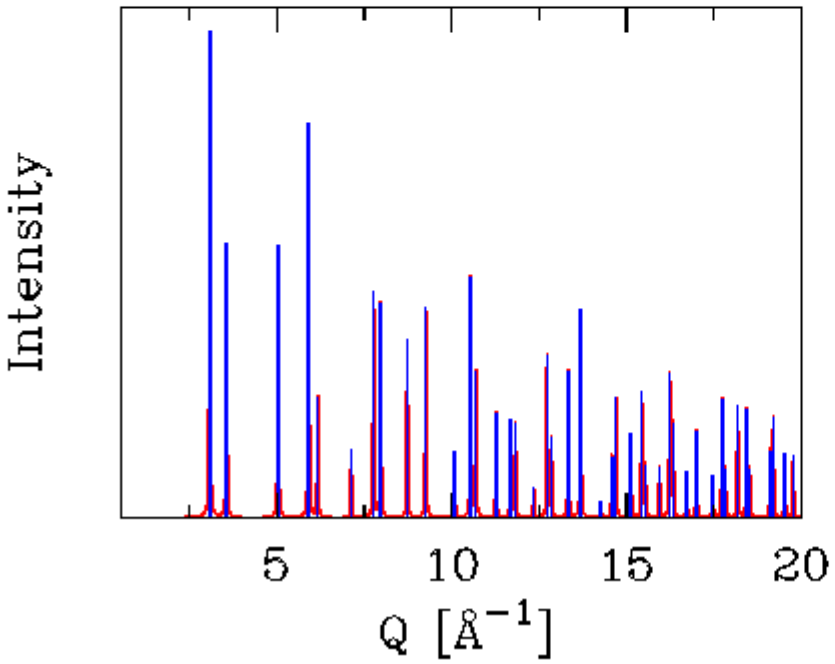


PDF with Qmax ripples

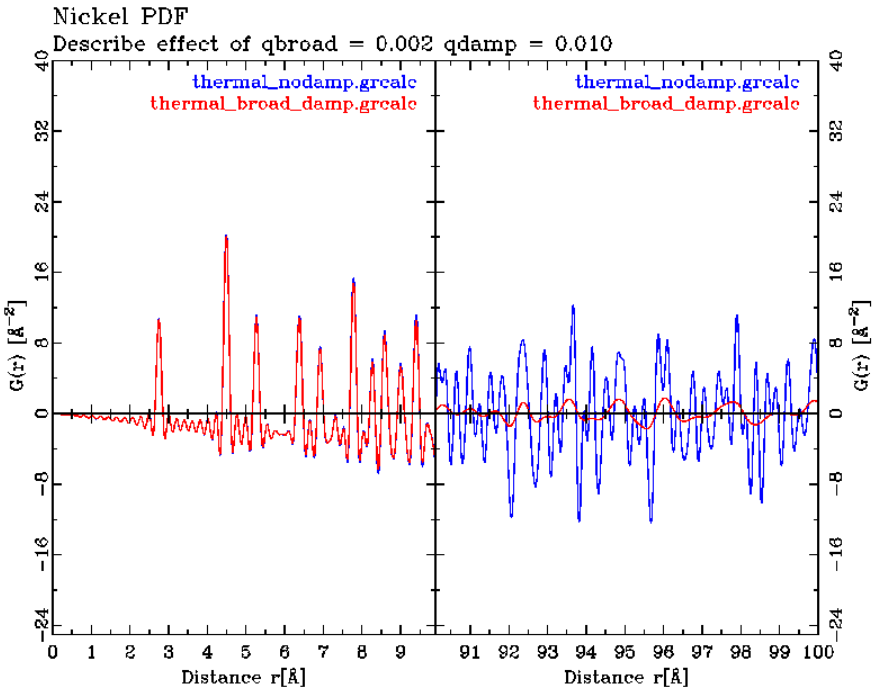


Maxima convoluted by Qmax effect (convoluted by sinc-function)

An ideal powder diffraction pattern
With limited angular resolution



PDF dampened / broadened
Towards larger distance r



Maxima broadened and dampened by broad Bragg reflections

Make sure you have started discus_suite

Change to directory Lectures/03_Pair_Distribution_Function

run macro **pdf.mac**

suite> @pdf.mac

This macro will take you in steps through the main PDF parameters

Edit macro **pdf_1.mac** to calculate just one PDF.

Modify individual parameters to get a feeling on the effect

suite> @pdf_1

Compare the effects that the different parameter values have on the PDF

Create a macro that:

simulates a crystal of N * N * N unit cells
calulates the pdf with
set boundary, crystal
set finite, sphere, <diameter>
set range, 1.5*diameter, 0.02

Try to establish a good diameter.
For a good diameter the pdf should:
Oszillate arund G(r)=0 for r < diameter
Be zero for r > diameter

in kuplot run macro kpdf_generic.mac :

kuplot > @kpdf_generic <your_file_name_base>