Friedrich-Alexander-Universität
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DISCUS Workshop
Pair Distribution Function PDF

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Calculating a powder PDF

Open in Windows Explorer: Lectures\
03_Diffraction\

Start DISCUS_SUITE

You should see:

...
User macros in ...
System macros in ...
Start directory ...

suite >

suite > **cd Lectures\03_Diffraction**

suite > **@pdf.mac 10**

Try: different sizes

POWDER PDF calculate a powder pair distribution function

Main steps

calculate powder diffraction pattern ==> powder menu

Save as PDF ==> output menu

pdf.mac

```
#                                    
read                                  # Switch to read menu
  cell CELL/silicon.cell,$1,$1,$1      # read the unit cell
                                      #    expand to $1*$1*$1 cells
#
@powder_pdf.mac                       # Calculate powder pattern
#
output                                # Switch to output menu
  outf  PDF/silicon.grcalc            # Define output file name
  value PDF                           # Select Powder PDF as output value
  form  pdf,r,0.01,100.0,0.01         # Write output as powder PDF data
  run                                 # Perform the actual output
exit                                  # Go back to main DISCUS menu
#
```

Modify to accept different structures

POWDER PDF calculate a powder pair distribution function

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Main influential parameters

Radiation: **xray**; **neutron**; **electron**

Relative height of PDF peaks

Q-Range: **set qmax**

Width of PDF peaks

Profile: **set profile, pseudo**; **set profile, off**

Height of PDF peaks as function of distance r

Atomic displacement parameters: **b[atom_type]**

Width of PDF peaks

POWDER PDF calculate a powder pair distribution function

powder_pdf.mac

```
powder
  xray                                  # Select X-rays
  set qmin,0.5500                       # Starting value for Q
  set qmax,25.0000                      # Final value for Q
  set profile, off                      # Switch convolution off
#  set profile, pseudo                  # Use Pseudovoigt
#  set profile, uvw, 0.000, 0.000, 0.001 # Cagliotti u,v,w values
#  set profile, eta, 0.500              # Mixing parameter 1=Lorenzian
  set temp,use                          # Use the ADP's
  run                                   # Do the actual calculation
exit
```

Modify: radiation
qmax
profile parameters

POWDER PDF calculate a powder pair distribution function

pdf.mac

```
read                                    # Switch to read menu
  cell CELL/$1.cell,$2,$2,$2            # read the unit cell
                                        # expand to $2*$2*$2 cells
#
do LOOP=1, n[2]
  b[LOOP] = $3
enddo
#
@powder_pdf.mac                          # Switch to powder menu
```

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Save as PDF ==> output menu

Save as **normalized intensity S(Q)** ==> output menu

Save as **reduced normalized intensity F(Q)** ==> output menu

Intensity ==> **S(Q)**: Division by $\langle f \rangle^2$; normalization **S(Q=large)** = 1

S(Q) ==> **F(Q)**: **F(Q)** = Q* [**S(Q)** – 1]

$$G(r) = \frac{2}{\pi} \int_{Q_{min}}^{Q_{max}} \boldsymbol{F(Q)}\, dQ$$

suite > **@overview.mac 10**

Try: different sizes
variation of all relevant parameters