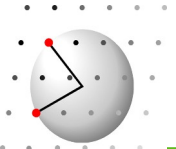


DISCUS Workshop

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:

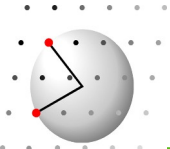
...
User macros in ...
System macros in ...
Start directory ...

suite >

suite > **cd Lectures\03_Diffraction**

suite > **@pdf.mac 10**

Try: different sizes

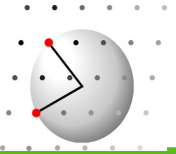


POWDER PDF calculate a powder pair distribution function

Main steps

calculate powder diffraction pattern ==> powder menu

Save as PDF ==> output menu



POWDER calculate a powder diffraction pattern

```
#                               pdf.mac

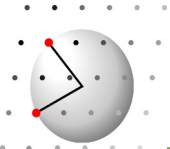
read                            # Switch to read menu
    cell CELL/silicon.cell,$1,$1,$1 # read the unit cell
                                    # expand to $1*$1*$1 cells

#

@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

Main steps

calculate powder diffraction pattern ==> powder menu

Save as PDF ==> output menu

Main influential parameters

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

Relative height of PDF peaks

Q-Range: **set qmax**

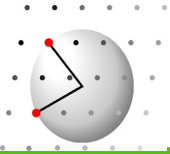
Width of PDF peaks

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



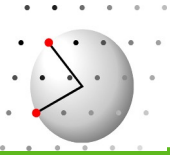
POWDER PDF calculate a powder pair distribution function

powder

powder_pdf.mac

```
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=Lorentzian
set temp,use                         # Use the ADP's
run                                  # Do the actual calculation
exit
```

Modify: radiation
qmax
profile parameters

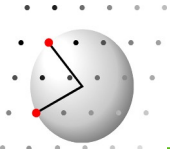


POWDER PDF calculate a powder pair distribution function

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
```



POWDER PDF calculate a powder pair distribution function

Main steps

calculate powder diffraction pattern ==> powder menu

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 **$S(Q=\text{large}) = 1$**

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

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

suite > **@overview.mac 10**

Try: different sizes
variation of all relevant parameters