

041122 Quiz 8 XRD

- a) The structure factor, F^2 , for the NaCl unit cell is a good demonstration of the concept of phase information. For this unit cell, phase information is manifested in the choice of Na or Cl as the [000] atom. Show that F (amplitude) contains phase information while F^2 (intensity) does not contain phase information.
- b) What type of information is contained in both F^2 and F compared to the information only in F ?
- c) Describe 4 levels of the structural hierarchy observed in semi-crystalline polymers.
- d) Give 3 reasons why the Bragg diffraction peaks in polymers might be broad compared to a metal crystal.
- e) For sizes between 1 nm (10 Å) and 50 nm (500 Å) what structural level of the hierarchy gives rise to small-angle scattering (diffraction below $6^\circ 2\theta$)?

ANSWERS: 041122 Quiz 8 XRD

a) For Na at $[0,0,0]$

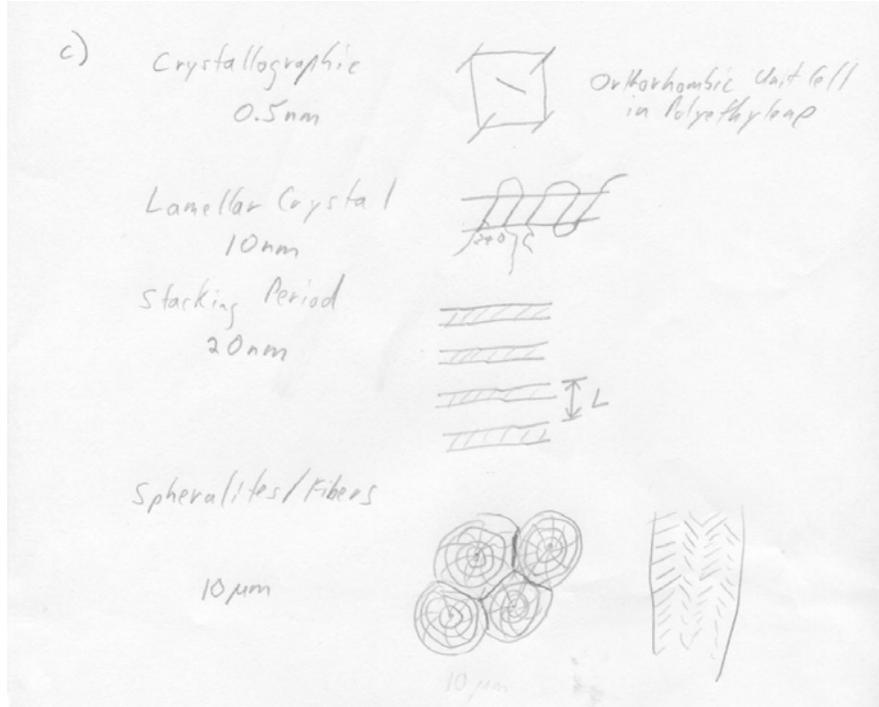
$$F = (f_{Na} + f_{Cl} e^{-\pi(h+k+l)}) (1 + e^{-\pi(h+k)} + e^{-\pi(k+l)} + e^{-\pi(h+l)})$$
 For Cl at $[0,0,0]$

$$F = (f_{Cl} + f_{Na} e^{-\pi(h+k+l)}) (1 + e^{-\pi(h+k)} + e^{-\pi(k+l)} + e^{-\pi(h+l)})$$
 if $h+k+l$ is odd & unmixed
 For Na @ $[0,0,0]$

$$F = 4(f_{Na} - f_{Cl}) \quad F^2 = 16(f_{Na}^2 + f_{Cl}^2 - 2f_{Cl}f_{Na})$$
 For Cl @ $[0,0,0]$

$$F = 4(f_{Cl} - f_{Na}) \quad F^2 = 16(f_{Cl}^2 + f_{Na}^2 - 2f_{Cl}f_{Na})$$
 so F is different while F^2 is the same

b) Both F and F^2 contain information concerning the FCC structure and the relative arrangement of Cl and Na. Only F contains information concerning the exact spatial placement of atoms such as which atom is at the $[000]$ position.



- d)
- 1) Nano-scale crystals give rise to broad peaks following the Scherrer equation
 - 2) Disorder of the first kind, similar to Debye-Waller Thermal broadening

- 3) Disorder of the second kind, loss of some extremely long range order, similar to the effects of residual stress in metal crystals.
- e) The stacking of lamellar crystalline sheets gives rise to a prominent peak in the small angle regime, see figure below:

