

Homework X. BCBP 6870. Fall 2008

due Nov 24

(1)

If you scratch a row of evenly spaced regular lines into a glass slide, each scratch will scatter all wavelengths of light in all directions. If there are enough lines and they are all separated by exactly the same distance d , then you get what is called "diffraction grating" and you see a rainbow of colors. If you have a single white light source shining on the glass slide at an angle $\theta=90.0^\circ$ at infinite distance, and the spacing between the lines is $2\ \mu\text{m}$, at what angle(s) do you see green light ($\lambda=550\ \text{nm}$)? At what angle(s) do you see red light ($\lambda=700\ \text{nm}$)?

Draw me a picture to illustrate the diffraction of red light.

(2)

You have a crystal of butane, C_4H_4 , the dimension of the cubic unit cell are $10 \times 10 \times 10 \text{ \AA}$. The coordinates (X,Y,Z) of the carbon atoms are as follows:

C1 (1.000, 8.000, 3.000)

C2 (2.000, 7.500, 3.500)

C3 (3.000, 7.000, 3.000)

C4 (4.000, 6.500, 3.500)

Find the phase of the reflection F with Miller indices $hkl = 1\ 2\ 0$ using the Fourier transform. Show your work. Convert \AA coordinates (X,Y,Z) to fractional coordinates (x,y,z). Graph the 4 scattering vectors, summed. Assume the scattering factor $f=6.00$ for each carbon atom. Here is the Fourier transform:

$$F(h\ k\ l) = \sum_r f(r) e^{2\pi i(hx+ky+lz)}$$

$F(1\ 2\ 0) =$ _____ (amplitude), _____ (phase in degrees)

(3)

What is the upper limit coordinate error in Å of a protein crystal structure if the resolution is $d=2.5\text{Å}$ and the R-factor is $R=0.25$? (You may use the Luzzati plot, or you can assume the phase error = $2\pi R/2.3$)