Week 3 - Diffraction
Comprehension Check

Total points = 25 (scaled by a factor of 1/10 in the system)

Question 1 (10 points)

The conventional fcc lattice has four atoms located at (0,0,0), (1/2,1/2,0), (1/2,0,1/2), and (0,1/2,1/2).

(a) Find the structure factor assuming that all atoms are alike. Remember that the structure factor is given by

$$S(h,k,l) = \sum_j f_j \exp[-i2\pi(hx_j + ky_j + lz_j)]$$

$$S = f\left(1 + \exp^{-i\pi(h+k)} + \exp^{-i\pi(h+l)} + \exp^{-i\pi(k+l)}\right)$$

(b) Which of the following rules describe the allowed x-ray reflections for an fcc structure where all atoms are alike:

- Sum of indices, $h + k + l$, must be even	✗
- Indices h, k, l, must be all even	✗
- Indices h, k, l, must be either all even or all odd	✓
- Indices h, k, l, must be all odd	✗

Question 2 (5 points)

Consider a crystal where the distance between a certain set of planes is 0.1 nm. If we use x-ray radiation with 0.1 nm wavelength to diffract off these plane, what should the angle θ be to satisfy the Bragg condition?

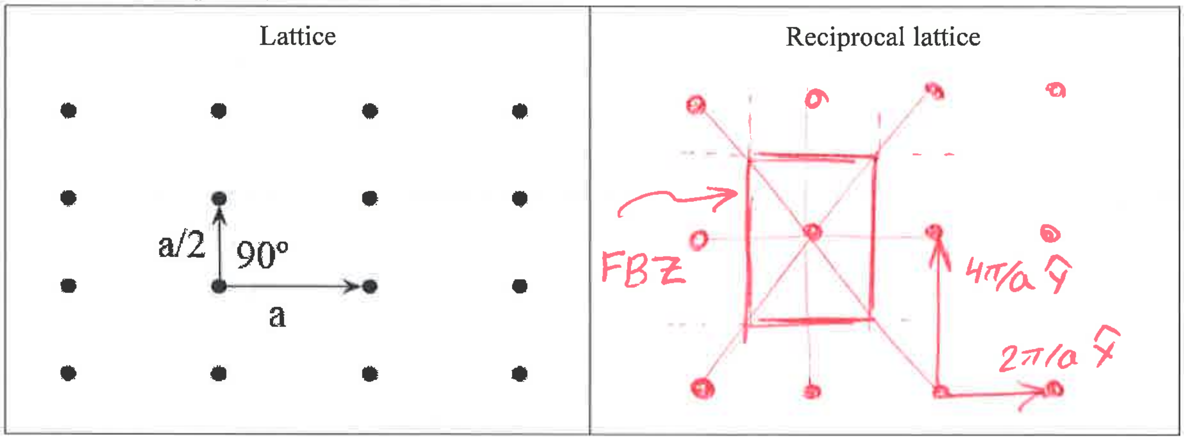
$$2d\sin\theta = n\lambda \qquad n = 1$$

$$2(0.1)\sin\theta = 0.1$$

$$\sin\theta = 1/2$$

$$\theta = 30^\circ$$

Question 3 (10 points)



For the rectangular lattice shown above:

(a) Find the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$

(b) Sketch the reciprocal lattice space

(c) Construct a primitive reciprocal lattice cell using the Wigner Seitz method.

(remember that $\mathbf{a}_i\mathbf{b}_j = \delta_{ij}$)

$$a_1 b_1 = 2\pi \qquad a_2 b_1 = 0$$

$$\Rightarrow b_1 = \frac{2\pi}{a}\hat{x}$$

$$a_1 b_2 = 0 \qquad a_2 b_2 = 2\pi$$

$$\Rightarrow b_2 = \frac{2\pi}{a/2}\hat{y} = \frac{4\pi}{a}\hat{y}$$