

HW2\_2

1. **Nickel (Ni)** has a **FCC** lattice with a cube edge  $a = 3.25 \text{ \AA}$ . In the following, consider a powder sample of **Ni**.
  - a. A beam of electrons of energy **150 eV** falls on the sample. **Calculate** the two smallest Bragg angles at which reflection takes place.
  - b. If, instead of electrons, a beam of neutrons of energy **0.08 eV** falls on the sample, repeat the calculations of part **a** for this case.

2. Work the following problem (#14, from Ch. 1 of the book "**Solid State Physics**" by J.S. Blakemore, 1<sup>st</sup> Edition. W.B. Saunders Co., Philadelphia, 1969).

1.14 Figure 1-58 shows two parallel planes of atoms (with spacing  $d$ ) in a crystal. Each plane consists of lines of atoms in the direction perpendicular to the paper, with a spacing of  $c$  between the lines. X-rays of wavelength  $\lambda$  have an angle of incidence  $\theta$  with respect to the planes. The rays leaving at an angle  $\phi_m$  are those of diffraction order  $m$  for the first plane considered as a plane grating. You are told that these rays are reinforced in phase by components diffracted from lower planes. Show that

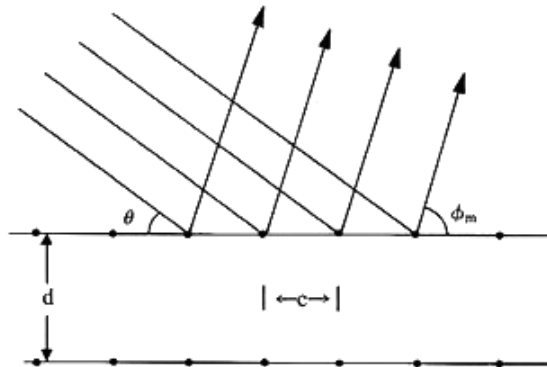
$$m\lambda = c[\cos \phi_m - \cos \theta]$$

and

$$n\lambda = d[\sin \phi_m + \sin \theta]$$

where  $m$  and  $n$  are integers. Show that a crystal plane exists making an angle  $\frac{1}{2}(\phi_m - \theta)$  with the original set of planes, for which the diffracted rays shown in Figure 1-58 are the result of specular reflection satisfying the Bragg condition.

Figure 1-58 Construction for Problem 1.14.



3. The electron density for the 2P state of the hydrogen atom is given by:

$$n(\vec{r}) = \frac{r^2}{64\pi a_0^5} e^{-r/a_0} \sin^2 \theta$$

Where  $r$  and  $\theta$  refer to a spherical coordinate system. Determine the atomic form factor for this state. In your determination, you may assume that the  $z$ -axis is defined by the reciprocal lattice vector.

(4) Simple example of 3-D Fourier transform: A tetragonal lattice has cell dimensions  $a \times a \times c$ , with  $c$  corresponding to  $\bar{a}_3$  according to standard convention (same as problem 1). The periodic potential consists of two Dirac delta functions in each cell:

$$V(\vec{r}) = V_0 \sum_j \left[ \delta(\vec{r} - \vec{r}_1 - \vec{R}_j) - \delta(\vec{r} - \vec{r}_2 - \vec{R}_j) \right],$$

with  $\vec{r}_1 = (0, 0, 0)$  and  $\vec{r}_2 = (1/2, 1/2, 1/\sqrt{3})$ .

[a] What is the general form for the reciprocal lattice vectors,  $\vec{G}$ ?

[b] Find a general form for  $V_G$ , the Fourier coefficients of the potential. Do this by directly computing the Fourier transform.

[c] Show that the  $\vec{G} = (0, 0, 0)$  coefficient is zero. Explain why one can expect this result for this case without calculating the Fourier transform.