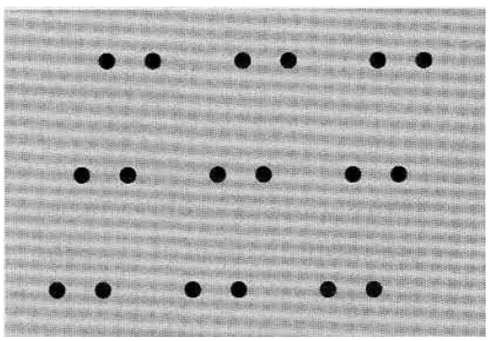
NORTHERN ILLINOIS UNIVERSITY

PHYSICS DEPARTMENT

Physics 580 – Solid State Physics   Fall 2022

<u>Quiz #1 --- Take Home</u>

Problem Set Due: Thurs., Sept. 22, 2022
Read Kittel: Chapter 1 & 2



1. The points in the figure above are identical atoms. Sketch on the figure

   (a) a set of lattice points

   (b) a choice of primitive axes

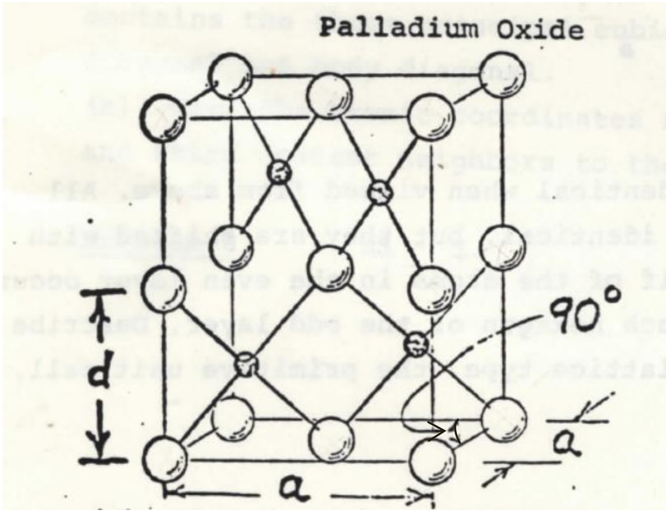
   (c) a primitive cell based on your choice of primitive axes

   (d) the basis of atoms associated with a lattice point

   (e) the Wigner-Seitz primitive cell

   (f) If the 3-dimensional unit cell has a c-axis perpendicular to the plane, and the basal angles in the plane above were 60° and 120°, what would be the lattice type of the crystal. Explain your reasoning (hint, there is a figure in Kittel).

2. ***Tetrahedral angles.*** *Use Vesta to draw a model of the structure of diamond.* The angles between the tetrahedral bonds of diamond are the same as the angles between the body diagonals of a cube as shown in Fig. 14 (6th edition) or Fig. 10 (8th edition). Use elementary vector analysis to find the value of the angle.



3. The figure shows the structure of PdO. The small circles represent palladium atoms and the large circles oxygen atoms. The PdO_4 groups are planar.

   (a) *Use Vesta to draw a model of this structure and the primitive unit cell.*

   (b) What is the lattice type?

   (c) Indicate the primitive unit cell, and give a set of primitive translation vectors for both the lattice shown above and for the primitive unit cell.

   (d) How many atoms are in a primitive unit cell? Give the coordinates of the basis atoms for the lattice shown above and for the primitive unit cell.

   (e) Give the Miller indices for a plane which contains planar PdO_4 groups for the lattice shown above and for the primitive unit cell.

4. Calcium Flourite, CaF_2, has a structure based on the fcc lattice and a basis with Ca at 0 0 0 and F's at $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$ and $\frac{3}{4}\ \frac{3}{4}\ \frac{3}{4}$. *Use Vesta to draw a model of this structure and explain what the symmetry relations are for Fm-3m are.* Draw a projection diagram.

5. Use Vesta to make a model of the unit cell for Po (sc), Fe (bcc), and Cu (fcc) shown in slide 34 of the "Geometry of Crystals" powerpoint slide (the powerpoints are on Blackboard in the "Content" section).

6. On slide 29 of the "Geometry of Crystals" is shows that there can be no face-centered tetragonal lattice. Explain why.

7. On slide 17 of the "Miller Indices": show why the $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ atom of bcc does not lie on the (112) plane. The [112] crystal direction is perpendicular to this plane. Prove this is true for this cubic lattice.

8. What is a family of planes? What are the members of the family of planes for the (112) plane of a cubic crystal?

9. Give the miller indices of all six sides of the simple cubic crystal (note, some of these planes pass through the origin).

10. What is the distance between (100), (200), and (112) planes of a cubic crystal?

11. Kittel: **Problem 4** page 44

4. *Width of diffraction maximum.* We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\boldsymbol{\rho}_m = m\mathbf{a}$, where m is an integer. By analogy with (20), the total scattered radiation amplitude will be proportional to $F = \Sigma \exp[-im\mathbf{a}\cdot\Delta\mathbf{k}]$. The sum over M lattice points is

$$F = \frac{1-\exp[-iM(\mathbf{a}\cdot\Delta\mathbf{k}]}{1-\exp[-i(\mathbf{a}\cdot\Delta\mathbf{k})]} ,$$

by the use of the series

$$\sum_{m=0}^{M-1} x^m = \frac{1-x^M}{1-x} .$$

(a) The scattered intensity is proportional to $|F|^2$. Show that

$$|F|^2 \equiv F^*F = \frac{\sin^2\frac{1}{2}M(\mathbf{a}\cdot\Delta\mathbf{k})}{\sin^2\frac{1}{2}(\mathbf{a}\cdot\Delta\mathbf{k})} .$$

(b) We know that a diffraction maximum appears when $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi h$, where h is an integer. We change $\Delta\mathbf{k}$ slightly and define ϵ in $\mathbf{a}\cdot\Delta\mathbf{k} = 2\pi h + \epsilon$ such that ϵ gives the position of the first zero in $\sin\frac{1}{2}M(\mathbf{a}\cdot\Delta\mathbf{k})$. Show that $\epsilon = 2\pi/M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M. The same result holds true for a three-dimensional crystal.