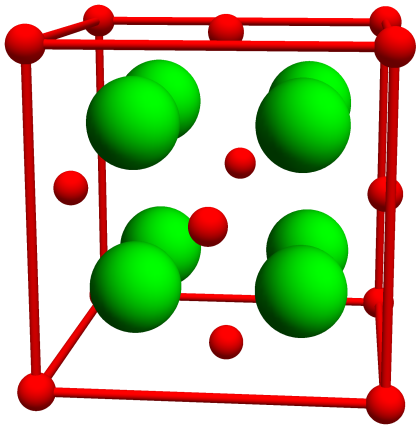
Physics 323, Section 1, Fall Semester 2019
Instructor: Lance Nelson
Exam #2
Nov 6 – Nov 12

The exam questions for this unit will be taken from the following bank of problems. Feel free to use this bank of problems any way you would like. However, once you begin the real test, it will be your work only that counts. The space provided is not an indication of how much space should be used to solve the problem. This exam is **NOT TIMED**.

1. What is meant by the Bravais lattice of a crystal? (One short sentence)

2. What is meant by the primitive unit cell of a crystal (One short sentence)

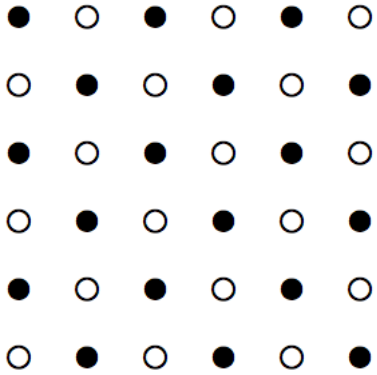
3. Consider the unit cell (repeating unit) shown on the right. The green spheres (bigger) and red spheres (smaller) represent two different kinds of atoms. The green spheres (bigger) are on the body-centered positions and the red spheres (smaller) are on the face-centered positions.
   (a) Give the x,y,z coordinates of each kind of atom shown in this cube.



   (b) How many distinct atoms are there in this crystal?

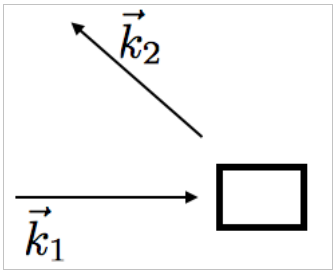
   (c) Is the cube shown a primitive unit cell? (Explain how you know)

4. Consider the two-dimensional crystal shown on the right. The filled circles and open circles represent two different kinds of atoms. (a) Indicate with X's a set of Bravais lattice points (Mark all of them that appear on the figure) (b) Draw a Wigner Seitz cell. (c) Draw a set of basis vectors for this lattice.



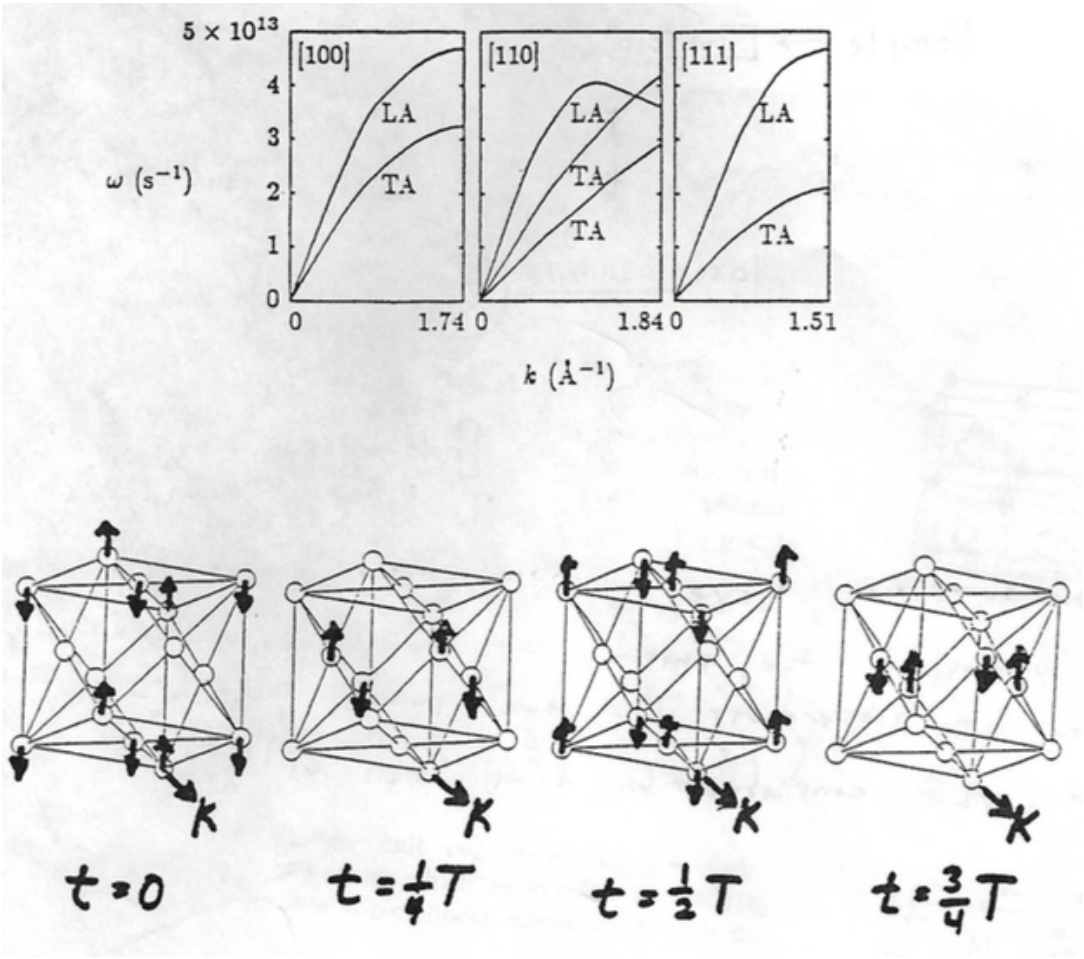
5. What does the d in Bragg's law, $2d\sin\theta = n\lambda$, stand for? (One short sentence. Choose your words wisely!)

6. Consider x-ray diffraction from a crystal. In the figure on the right, $\vec{k}_1$ is the wave vector of the incoming x-ray and $\vec{k}_2$ is the wave vector of one of the outgoing x-rays that produces a Bragg peak. (a) Draw on the figure the plane from which the x rays are reflecting. (b) Draw on the figure the reciprocal lattice vector $\vec{G}$ which corresponds to this peak. Be sure to draw the vector with not only the correct orientation, but also with the correct length.

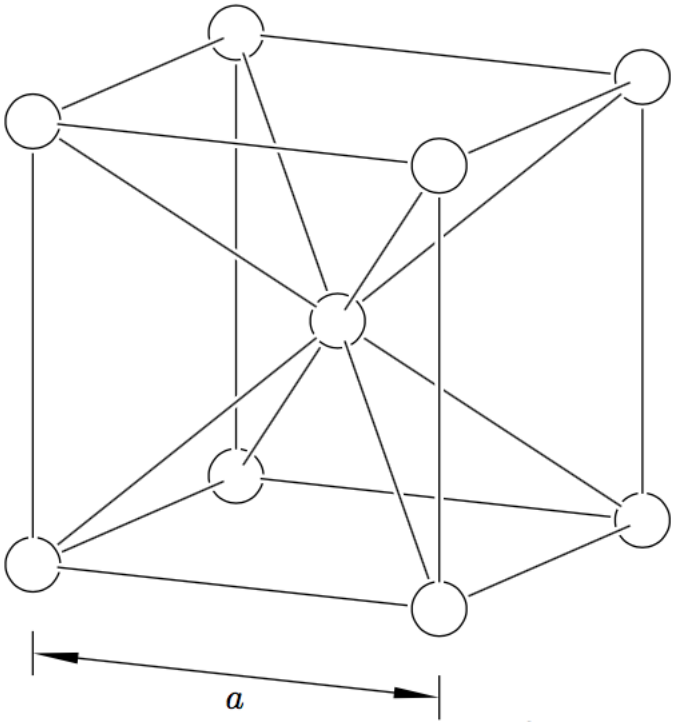


7. The dispersion curves for lattice waves in copper are shown below. Also shown is a lattice wave, or snapshots in time of a lattice wave. The arrows show displacements of the atoms in the unit cell at $t = 0,\ \frac{1}{4}T,\ \frac{1}{2}T,\ \frac{3}{4}T$, where T is the period. The direction of the wave vector $\mathbf{k}$ is also shown on the drawing. Calculate the magnitude of $\mathbf{k}$ for this wave. Indicate with an X the position of this wave on the dispersion curves. If there is more than one possible answer, based on the information you are given here, mark all of them. Copper has an fcc structure with lattice parameter $a = 3.61$ Å.

$|k| =$_____



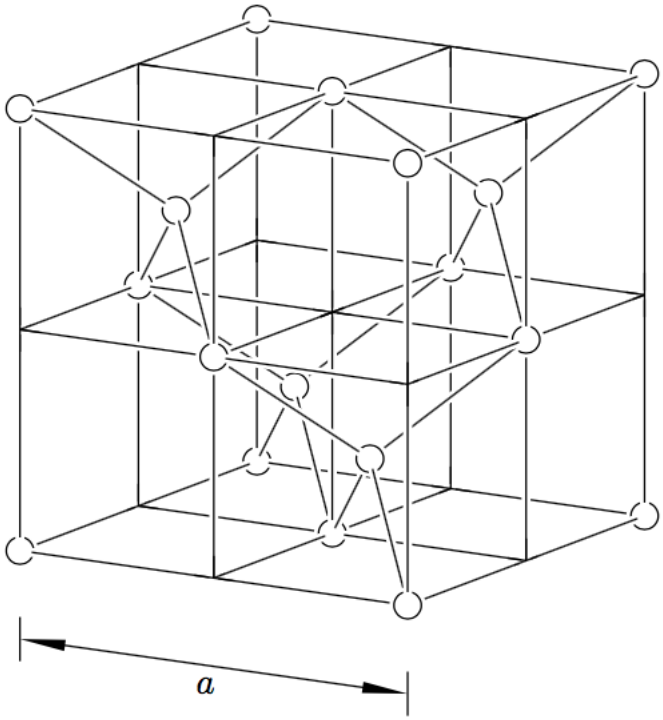
8. The following two questions are related to x-ray diffraction in a crystal of Barium (Ba) which forms a bcc lattice with lattice parameter: $a = 5.02$ Å. (pictured at right) The wavelength of x-rays used is 1.542 Å.



(a) Assemble the structure factor and determine the (hkl) indices for the Bragg peaks that will not appear. Remember to use the conventional unit cell.

(b) Apply Bragg's law in reciprocal space to determine how many Bragg peaks there will be. Find the Bragg angles and (hkl) indices for each peak. Put them in a table for easy viewing.

9. Consider a Germanium (Ge) crystal, which forms in the diamond crystal structure with $a = 5.65$ Å. (pictured at right)



(a) What is the volume of the primitive unit cell. Think carefully about which atoms are equivalent.

(b) What is the density of Ge. (The mass of one germanium atom is: $m = 72.6$ u, where 1 u$= 1.661 \times 10^{-27}$ kg)

(c) What is the distance between nearest neighbor atoms in germanium. Mark these atoms in the picture.

10. Consider a sodium (Na) crystal, which forms a bcc crystal structure. Determine whether the reciprocal lattice vector below is inside or outside the first Brillouin zone. If it is outside, find an equivalent point that is inside the first Brillouin zone.

$$\mathbf{k} = 1.5\hat{i} + 0\hat{j} + 0\hat{k} \tag{1}$$

11. What is the distance between *lattice planes* in the [100] direction of NaCl?

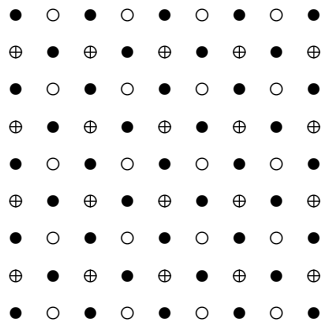
12. What is the distance between *atomic planes* in the [110] direction of NaCl?

13. Consider the following reciprocal lattice vector in Cu: $\vec{k} = 2.3094(\hat{i} + \hat{j} + \hat{k})$. Is this vector inside the first Brillouin zone? If not, find the equivelant point that is inside the first Brillouin zone.

14. Write down the structure factor for zincblende.

15. Find the volume of the primitive unit cell for Lithium.

16. Consider the two-dimensional crystal shown to the right. The three different symbols refer to three different types of atoms.



(a) Are the • atoms in equivalent positions?

(b) Are the ∘ atoms in equivalent positions?

(c) Use x's to indicate the Bravais lattice sites.

(d) Draw the primitive unit cell.

(e) How many • atoms are in a primitive unit cell?

17. The space group of a certain crystal is P $m\bar{3}m$. The lattice is cubic P and the crystal class is $m\bar{3}m$. The space group is symmorphic. A lithium atom is located at $(0, 0, 0)$ and a platinum atom is located at $(1/4, 0, 0)$. Find all of the positions of the lithiums and platinums in the unit cell. Find the chemical formula for the compound.

18. Speaking generally of Bravais lattices, which of the following statements are true ? Mark *all* that apply

(a) The lattice vectors are perpendicular to each other.

(b) The three vectors defining the Bravais lattice are all the same length.

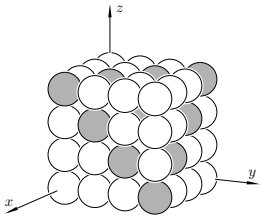
(c) There is one and only one lattice point in each primitive unit cell.

(d) The conventional cell contains 4 lattice points.

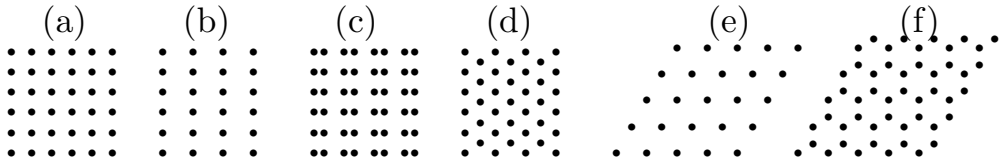
(e) There is a lattice point for every atom in a crystal.

(f) Every lattice point of the Bravais lattice is equivalent to every other point.

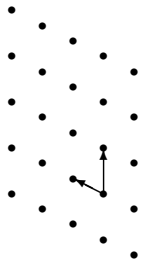
19. What crystal plane(s) is(are) indicated by the shaded atoms in the figure?



20. The figure below shows several lattices with lattice points shown as black dots. Which of the lattices are *Bravais* lattices? Mark *all* that apply. (Technically, lattices are infinite, of course, so we can't really draw a *whole* lattice. Imagine that each of the pictures repeats everywhere in two dimensions.)



21. Consider the lattice shown in the figure to the right. The lattice vectors are $\vec{a}_1 = (-2, 1)$ and $\vec{a}_2 = (0, 3)$. Calculate the largest distance between *adjacent* lattice planes. (These planes are responsible for x-ray diffraction peaks at the smallest Bragg angle.) (a) 3, (b) $\sqrt{5}$, (c) 2, (d) $\sqrt{7}$, (e) 4, (f) $1/\sqrt{7}$, (g) $6/\sqrt{5}$, (h) 1/2, (i) 36/5, (j) $3/\sqrt{5}$



The following three questions are related to the structure of elemental sodium (Na).

22. At ambient temperature and pressure, sodium has the bcc crystal structure. At higher pressures, it transforms to an fcc structure. If its lattice parameter is 4.30 Å in the bcc structure, what is its density (in g/cm^3)?
(a) 0.991, (b) 2.02, (c) 0.496, (d) 0.505, (e) 1.98, (f) 1.41, (g) 1.63, (h) 0.707, (i) 1.01, (j) None of the above.

23. Find the volume of the primitive (bcc) unit cell (in Å^3).
(a) 37.8, (b) 19.8, (c) 9.46, (d) 1.18, (e) 1.51×10^2, (f) 75.7, (g) 3.03×10^2, (h) 8.11, (i) 8.73, (j) None of the above

24. After the phase transition to fcc, the lattice parameter is 4.08 Å. What is the nearest neighbor distance between atoms in this phase?
(a) 2.15, (b) 2.48, (c) 3.04, (d) 7.45, (e) 6.08 (f) 2.04, (g) 2.36, (h) 2.88, (i) 7.07, (j) None of the above.

The following three questions are related to the x-ray diffraction in a crystal of iron (Fe) using x-rays of wavelength 1.542 Å.

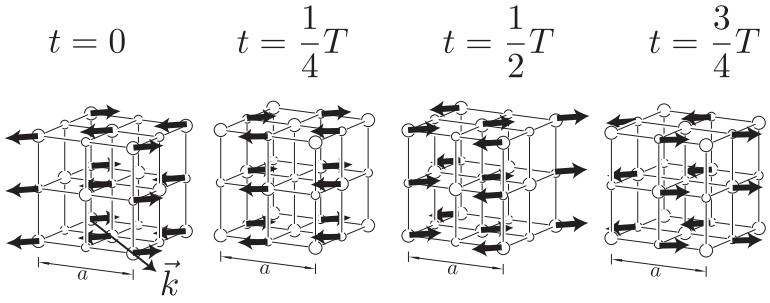
25. Find all of the possible Bragg angles for reflections of the x rays from the (100) planes. How many are there and what are the Bragg angles?

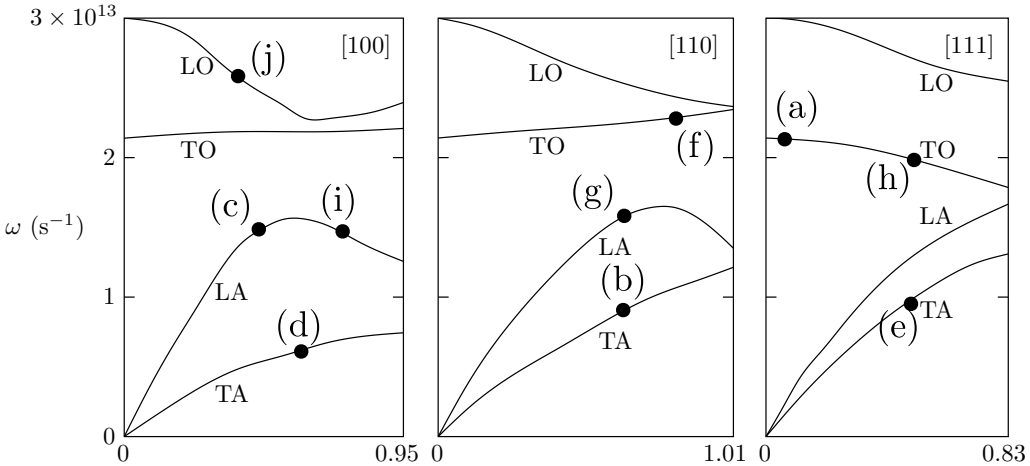
26. Are there any peaks associated with (110) planes? If so how many and what are the associated Bragg angles?

27. Are there any peaks associated with (310) planes? If so, how many and what are the associated Bragg angles?

28. What is the atomic diameter of niobium (Nb)? (Consider the atoms to be spheres that touch each other. The units of the answer choices are Å.) (a) 3.30, (b) 1.91, (c) 2.86, (d) 0.825, (e) 1.65, (f) 2.33, (g) 1.17, (h) 5.72, (i) 4.67, (j) None of the above.

29. In the top figure below, a phonon in a crystal of KBr is depicted. The wave vector lies in the x-y plane and points at an angle halfway between the $\hat{x}$ and $\hat{y}$ directions, as shown. In this problem you are to identify the possible values of $\omega(k)$ and polarization for this phonon, as marked on the dispersion curves shown in the bottom figure. Pick the point or points that are consistent with the depicted phonon. (On the dispersion curves, the labels on the branches indicate the following: L=longitudinal, T=transverse, A=acoustic, O=optical.) Note that the lattice parameter of KBr is on the equation sheet.

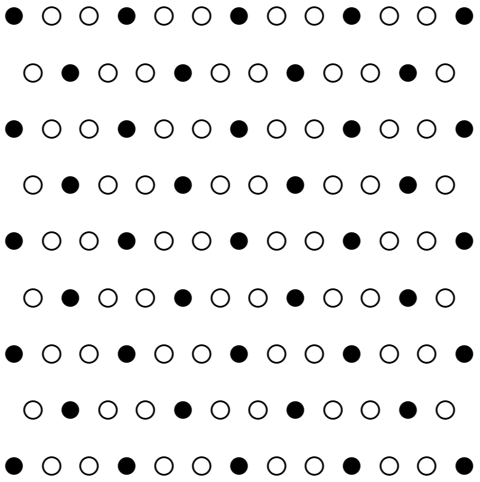




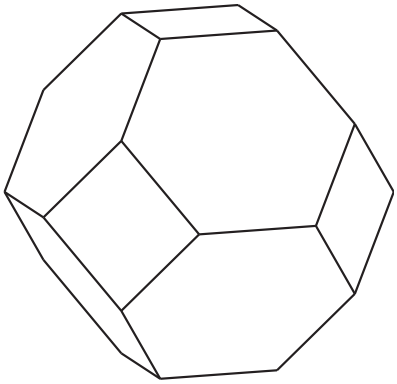
30. What is the Bravais lattice for a crystal of CsCl? (a) simple cubic, (b) face-centered cubic, (c) body-centered cubic, (d) hexagonal close-packed, (e) tetragonal.

28. Draw a primitive unit cell for this crystal.

29. Separately, draw a Wigner-Seitz cell for this crystal, centered on a ∘ atom. Mark the lattice points and show your work for constructing the Wigner-Seitz cell. Label the primitive unit cell and Wigner-Seitz cell so the grader knows which is which.



30. In reciprocal space, this is a picture of what (be specific)? (I.e., what is it called?) Explain why it is important.



31. The figure shows the points of a two-dimensional lattice. The heavy, black circles are the lattice points. What is a set of basis vectors for this lattice?