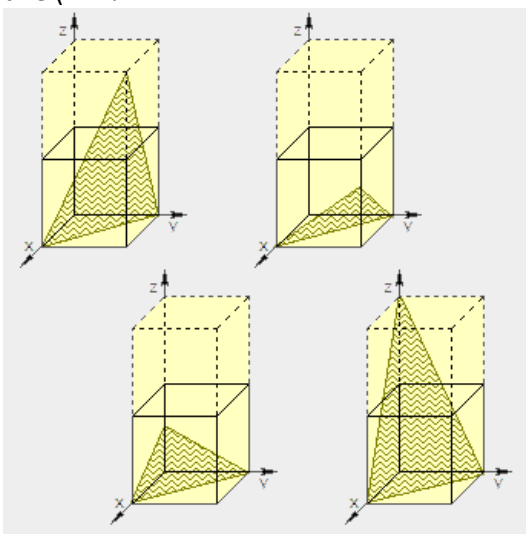
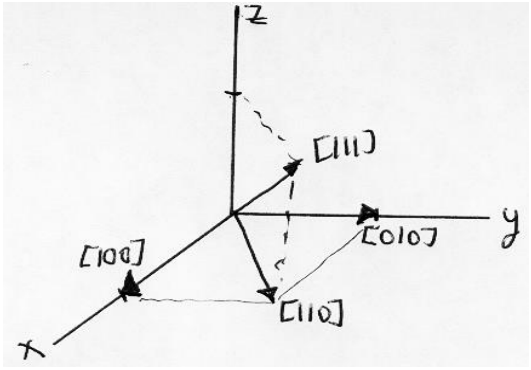
Problems on Crystal Planes and Miller Indices given by William Hallowes Miller

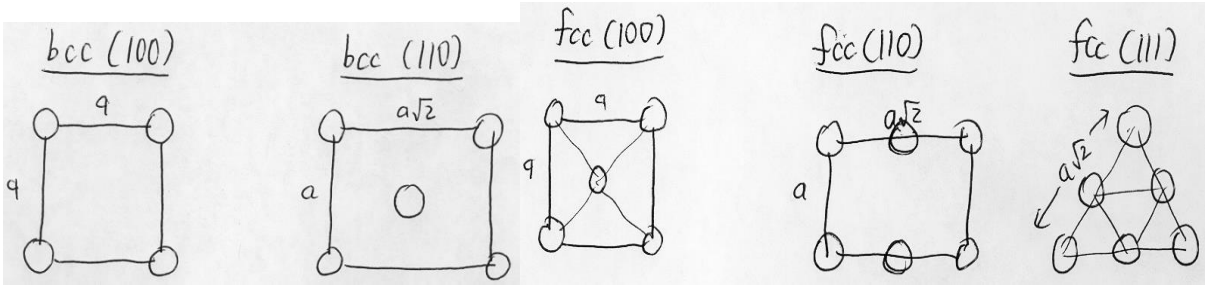
1. Which one is showing the plane (221?



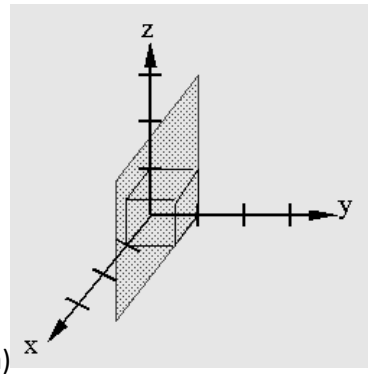
2. On a simple cubic lattice of spacing = 1, draw the [100], [010], [110], and [111] directions.

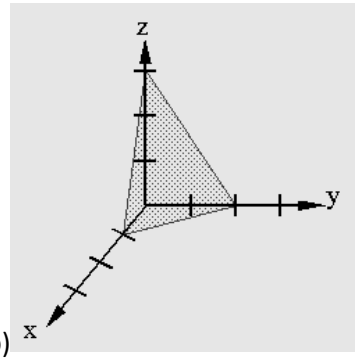


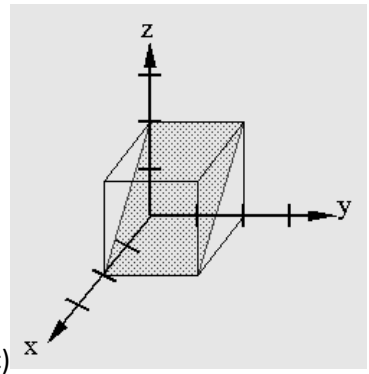
3. Draw the (100) and (110) planes of a body centered cubic (bcc) lattice to *THE CORRECT scale (Give dimensions)*. You can assume that the length of the cell is 1. Repeat part (b) for a face centered cubic (fcc) crystal lattice for the (100), (110), and (111) planes. FCC crystals have atoms at each corner and atoms at the center of each face.



4. Determine the Miller indices (hkl) of the shaded planes below. Show your work on each step to determine the plane (IE. Intercept, reciprocals, reduction, etc …)

a) 

b) 

(c) 

Answer: a) (010), b) (632), (c) (101)

5. For the intercepts x, y, and, z with values of 3,1, and 2 respectively, find the Miller indices.
Answer: (263)

6. Compute the Miller Indices for a plane intersecting at x= ¼ , y=1, and x=1/2,
Answer: (4,1,2)

7. Graph the plane and determine the axis intersects of a surface with the Miller Index (013).

8. Explain the meaning of {100} and it's importance.
Answer: {100} is a short way of referring to 6 different planes. These indices all refer to the same lattice as viewed from different points of reference defined by the axis. 1. (100) 2. (010) 3. (001) 4. (-100) 5. (0-10) 6. (00-1)

9. A certain crystal has lattice parameters of 4.24, 10 and 3.66 Å on X, Y, Z axes respectively. Determine the Miller indices of a plane having intercepts of 2.12, 10 and 1.83 Å on the X, Y and Z axes.

Solution: Lattice parameters are = 4.24, 10 and 3.66 Å
The intercepts of the given plane = 2.12, 10 and 1.83 Å
i.e. The intercepts are, 0.5, 1 and 0.5.
Step 1: The Intercepts are 1/2, 1 and 1/2.
Step 2: The reciprocals are 2, 1 and 2.
Step 3: The least common denominator is 2.
Step 4: Multiplying the lcd by each reciprocal we get, 4, 2 and 4.
Step 5: By writing them in parenthesis we get (4 2 4)

Therefore the Miller indices of the given plane is (4 2 4) or (2 1 2).

10. Calculate the miller indices for the plane with intercepts 2a, - 3b and 4c the along the crystallographic axes.

Solution: The intercepts are 2, - 3 and 4

Step 1: The intercepts are 2, -3 and 4 along the 3 axes

Step 2: The reciprocals are

Step 3: The least common denominator is 12.

Multiplying each reciprocal by lcd, we get 6 -4 and 3

Step 4: Hence the Miller indices for the plane is $(6\ \bar{4}\ 3)$

11. The lattice constant for a unit cell of aluminum is 4.031Å Calculate the interplanar space of (2 1 1) plane.

Answer: d = 1.6456 Å

12. Find the perpendicular distance between the two planes indicated by the Miller indices (1 2 1) and (2 1 2) in a unit cell of a cubic lattice with a lattice constant parameter 'a'. Ans: d-d1-d2 = 0.0749 a

13. What is the distance between the adjacent Miller planes if the first order reflection from X-rays of wavelength 2.29 A occurs at 27o 8' ?

Solution : n = 2d sin n = 1, = 2.29 , = 27o 8' d = 0.5 * 1 * 2.29 * 10 -8 / sin (27o 8') = 2.51

14.(a) Consider the two following planes that cut the crystallographic axes as indicated. Plane 1 cuts the axes at a / 3, b / 2 and c /4 and plane 2 cuts the axes at a / 2, b /3 and . What are the Miller indices of these planes ?

(b) Draw the planes for which the Miller indices are (112), (200), (120) and (221)

15. What are the unit cells for the NaCl and the CsCl structures ? How many atoms are there in these unit cells ?

16. The edge length of the Ag FCC structure is 408.6 pm An X-ray beam produces a strong interference (intense reflection) from the 111 planes at 2 = 38.2 o . What is the X- ray wavelength ?

17. The X - rays of wavelength 154.2 pm produce reflections from the 200 planes and the 111 plane of Cu which has FCC structure and density of 8.935 g /cm^3. At what angles will the diffracted intensity be maximum?

18. The molecular weight of NaCl is 58.448 and its density 2.165 g / cm^3. What is the edge length of a cube that contains one mole of NaCl ? How many sodium and chloride ions lie along this edge if the distance between the nearest neighbour ions is 2.819 ? Calculate the Avogadro number using the information given above.

19. From the face of a FCC lattice of NaCl, the Bragg diffraction from X-rays of 0.0586 nm wavelength occurs at an angle of 5° 58'. What is the distance separating these planes and what is the smallest distance between Na+ and Cl - and Cl - and Cl - ? Study the NaCl structure closely for a clear picture of the problem.

20. The lattice parameter of the FCC silver unit cell is 408.6 pm. An X-ray beam produces a strong reflection from the 111 plane at angle 2 = 38.2° . What is the wavelength of the X-ray ?

21. X-rays with = 154.2 pm produce reflections from the 110 and 200 planes of FCC Cu of density 8.935 g / cm3. At what angles will these reflections appear?

22. X- rays of wavelength = 179 pm produce a reflection at 2 = 47.2o from the 110 planes of BCC lattice. Calculate the edgelength of the unit cell.

23. If a = b = c = 8 Å, find d-spacings for planes with Miller indices (1 2 3) Calculate the d-spacings for the same planes in a crystal with unit cell a = b = 7 Å, c = 9 Å. Calculate the d-spacings for the same planes in a crystal with unit cell a = 7 Å, b = 8 Å, c = 9 Å. (1 Å = 1 x 10^{-10}m)

24. X-rays with wavelength 1.54 Å are "reflected" from the (1 1 0) planes of a cubic crystal with unit cell a = 6 Å. Calculate the Bragg angle, θ, for all orders of reflection, n

25. X-rays of wavelength λ=1.5Å are reflected from the (2 2 2) planes of a cubic crystal with unit cell a = 5Å. Calculate the Bragg angle, θ, for n=1.

26. The cubic crystal in the previous question is replaced with a tetragonal crystal, unit cell a = 4.5Å, c = 6Å. Calculate the Bragg angle, θ for the 222 reflection.

27. An orthorhombic crystal is now studied. What is the Bragg angle for the 222 reflection if a = 3Å, b= 3.5Å and c = 8Å

28. At 278 K, iron (Fe) is found to show bcc structure with a lattice parameter of 0.2866 nm. Obtain the density of iron from this information.
Answer: 7.88 ×10^6 g/m^3 :

29. The atomic weight per 1 mol of copper (Cu) with face-centered cubic (fcc) structure and the density at 298 K are 63.54 g and 8:89 106 g=m3, respectively. Estimate the nearest-neighbor distance of Cu atoms.
Answer: 0.2560 nm

Sample Questions:

1. Write down the d-spacing formula for orthogonal crystals.
2. How does this simplify for tetragonal and cubic symmetry?
3. What is the minimum value of a (in an optical grating) for first order diffraction to be observed?
4. What happens when a << λ? What happens when a >> λ?
5. What are the wavelength requirements for diffraction by a crystal lattice?
6. State Bragg's Law and explain the terms.
7. Explain why, in practice, n is set to 1 in the Bragg equation.