MLL100: Materials Science and engineering

Practice Problems
Set A: Crystallography and Structure of Solids

NOTES:

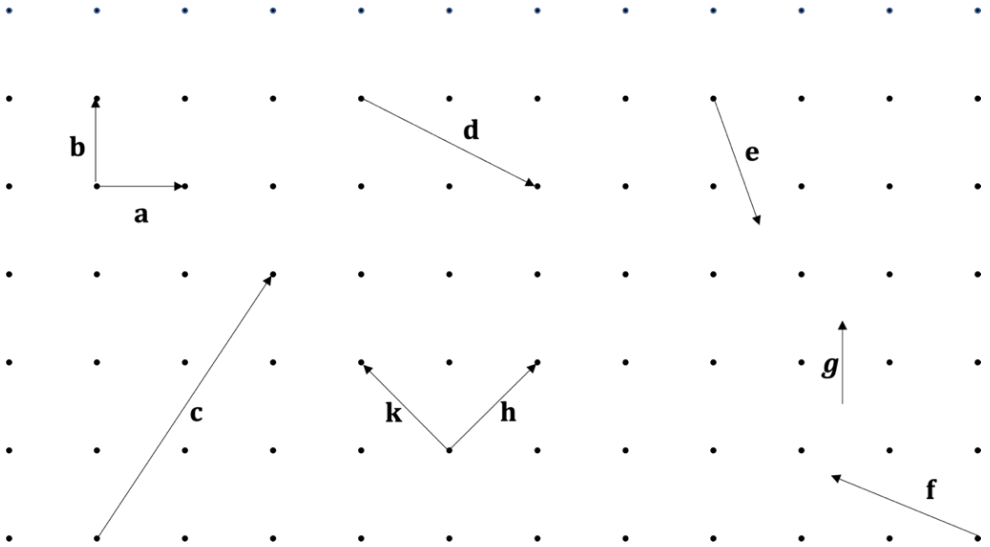
1. These problems are provided to check and improve your understanding of the concepts discussed in lectures. Please look at the lecture notes as well as the corresponding videos when you need relevant information. This will enhance your thinking skill. Use AI only as a final resort if you are stuck.
2. Materials Science and Engineering: A First Course, 5th. Edn. by V. Raghavan is a good source of reading material and further problems.

1 **Lattice translations:** Express all lattice translations in the figure below by choosing

(a) **a** and **b** as the basis vectors

(b) **h** and **k** as the basis vectors.

(c) Which of the two bases (if any) is/are primitive?



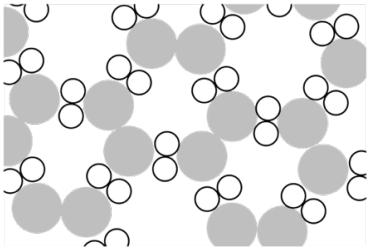
2. Body-centred Hexagonal Lattice? There is no hI lattice in the Bravais list. Give reason for its exclusion. Is it not a lattice? Or is it a lattice which is included as a different Bravais lattice? (Hint: It will help to begin your analysis by drawing a 2×2 four hI unit cells.)

3. Nonconventional Cell: The unit cell (with $a \neq b \neq c; \alpha = \beta = \gamma = 90°$) of a orthorhombic crystal is described below using nonconventional unit cells. What is the Bravais lattice and the motif?

Two atoms of one kind (say element A) per unit cell located at $\frac{1}{2}, 0, 0$; $0, \frac{1}{2}, \frac{1}{2}$ and two of another kind (element B) located at $0, 0, \frac{1}{2}$; $\frac{1}{2}, \frac{1}{2}, 0$.

4. Symmetry planes of a cube: Give the Miller indices of all the nine mirror planes of a cube. You should keep the orientation of the axes fixed, but you will require to choose different origins. Give their family indices of symmetry related mirror planes.

5. The figure below is a reproduction of Figure 1-4 of Vol I of original edition of Feynman's Lectures on Physics.



The accompanying text states

"Figure 1-4 is an invented arrangement for ice, and although it contains many of the correct features of ice it is not the true arrangement. One of the correct features is that there is a part of symmetry that is hexagonal. You can see that if we turn the picture around an axis by 120°, the picture returns to itself.

(a) Find a mistake regarding symmetry in the quoted text.
(b) Find and mark the symmetry axes that you see in the pattern. Do you see any six-fold axes?

R. Prasad, "Errors in The Feynman Lectures on Physics: Symmetry and Crystals" Resonance May 2016, p429-437. (Available on web).
The article will help in understanding many crystallographic concepts related to the course.

6. Proof of Weiss zone law: State and prove Wiess Zone Law.

7. $[\boldsymbol{hkl}]_{\boldsymbol{cubic}} \perp (\boldsymbol{hkl})_{\boldsymbol{cubic}}$: Show that the plane and direction having the same Miller indices in a cubic crystal are orthogonal.

8. Interplanar spacing: Show that the d spacing of (hkl) planes in crystal system with three mutually orthogonal axes (namely cubic, tetragonal and orthorhombic) is given by

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}.$$

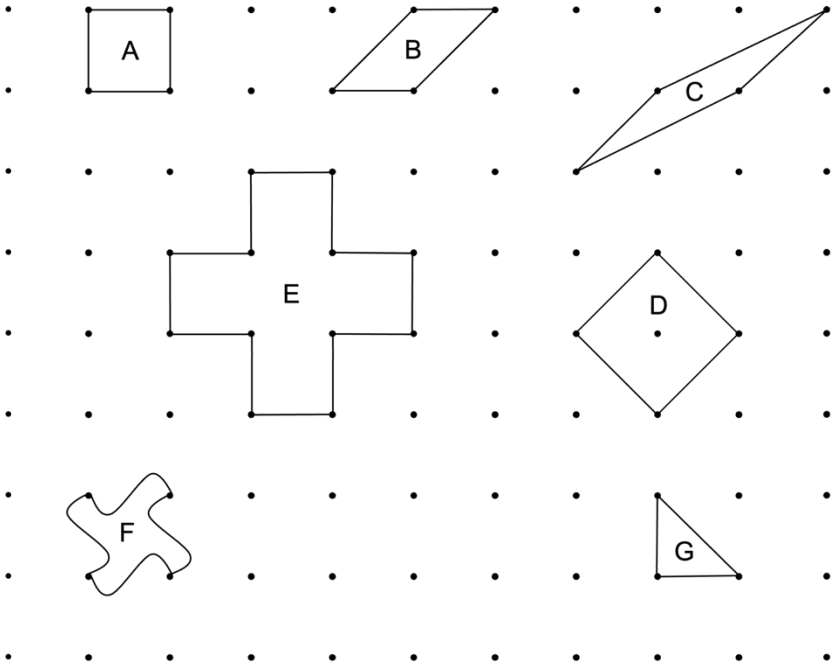
Hence show that for the cubic system

$$d_{hkl}^{cubic} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

9. Plane passing through two lines:

(a)Sketch directions $[111]$ and $[110]$ in a single unit cell.
(b) Hence draw the common plane and find its Miller indices by using a suitable origin in your diagram.
(c) Verify the answer using Weiss zone law.

10. Unit Cells



Determine which of the shapes A to G will qualify as unit cells for the lattice. Among the unit cells which are primitive? Following steps will help you.

(a) On a centimetre graph paper, draw a square lattice with an edge length of squares equal to 1 cm.
(b) Draw a copy of the lattice and the shape A shown on tracing paper. Surround each unit cell with identical unit cells to convince yourself they can fill space without gaps and overlaps.
(c) Repeat exercise (b) for unit cells B, C, D, E, F.
(c) Count the effective number of lattice points belonging to a cell. Hence classify them as primitive or nonprimitive.
(d) Determine the areas of the unit cells and compare them.

11. Line of intersection of two planes:

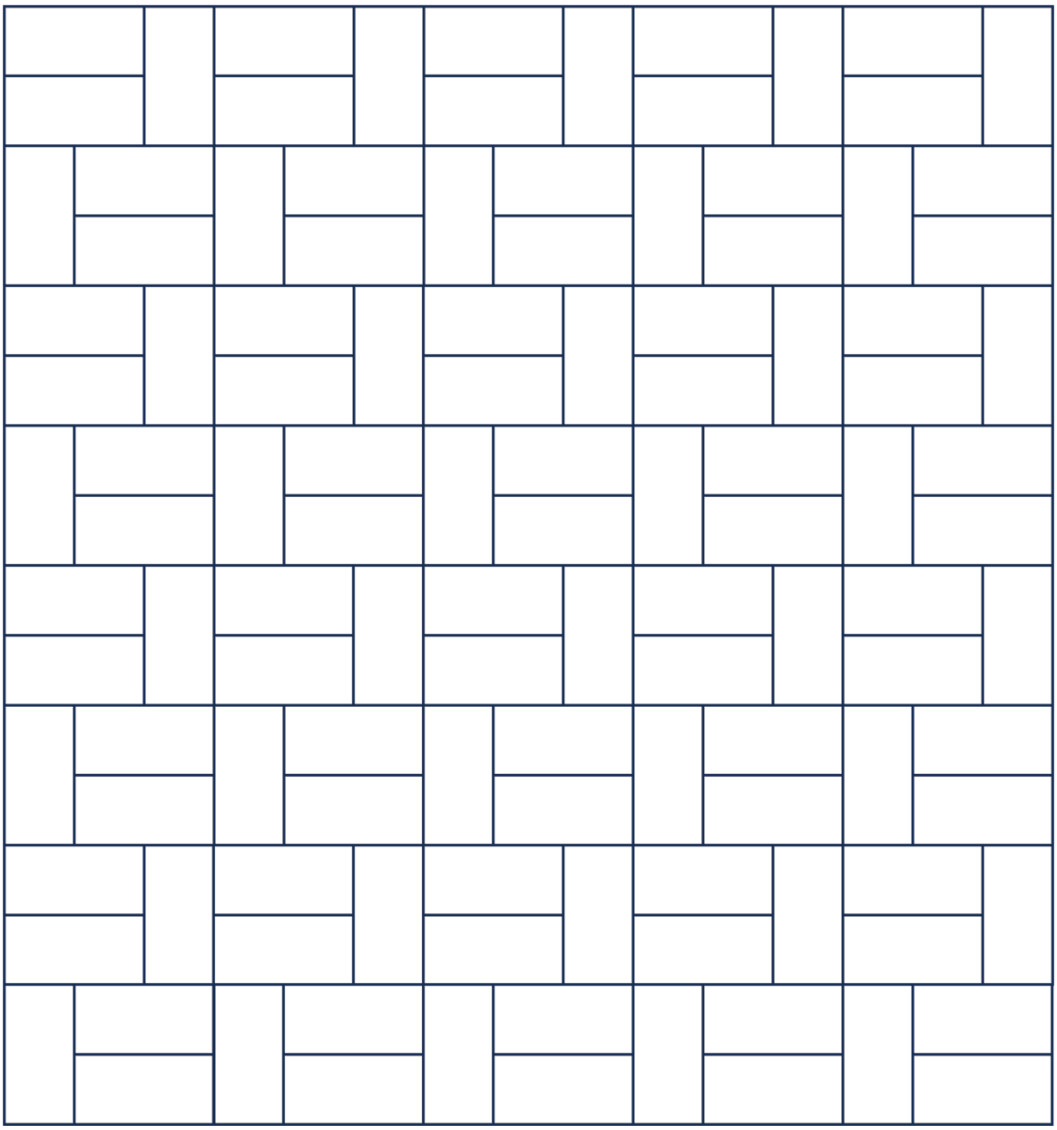
(a) Sketch (111) and $(1\bar{1}1)$ in a given unit cell. You will need to use different origins for the two planes but keep the same orientation of the axes.
(b) Identify the common points on the two plane and hence add the line of intersection of the two planes to your sketch.
(c) Determine geometrically the Miller indices of the line of intersection.
(d) Check your answer by finding the Miller indices of the line of intersection algebraically using the Weiss zone law.

12. **X-ray Diifraction:** The first peak of an FCC crystal occurs at $19.23°$ when CuK_α radiation is used. Determine the lattice parameter.

13. **Highest angle peak in an X-Ray Diffraction:** Find the indices and the Bragg angle 2θ of the highest angle peak in a powder x-ray diffraction pattern from Cr (BCC, $a = 2.88$ Å) using CuK_α radiation ($\lambda = 1.54$ Å) . How the results change if you use MoK_α ($\lambda = 0.71$ Å)instead.

14. **Two-dimensional Periodic Patterns:** Figure below shows a pattern of a tiling by 2:1 rectangular tiles outside the International Guest House as well as the library in IIT Hyderabad. You may like to make a copy of this pattern to do this exercise or use a tracing paper over it.

(a) Mark a point as your reference point. Mark all other points in the pattern which are translationally equivalent to the reference point. This constitutes the lattice of the pattern.
(b) Mark a primitive unit cell. Determine the effective number of lattice points in the cell.
(c) Mark a primitive unit cell of a shape different from the one marked in (b) and determine the effective number of lattice points.
(d) Mark a nonprimitive unit cell. Calculate the effective number of lattice points in the cell.
(e) Calculate the areas of the two primitive unit cells in (b) and (c) and the nonprimitive unit cell of (d). Compare the values obtained.
(f) How many tiles constitute the motif of the pattern.



15. Comparison of Basal planes of graphite and HCP structures: Atomic planes perpendicular to the c-axis in a hexagonal crystal are called basal planes. Although the 2D arrangement of atoms in basal planes of both these structures are 'hexagonal arrangement' in the sense that they have sixfold axes perpendicular to the plane there are important differences.

(a) Sketch the arrangement of atoms in the basal planes of graphite and an ideal hcp crystal. Assume neighbouring atoms in contact.
(b) Indicate the locations of sixfold axes by little filled hexagons.
(c) Mark the conventional 2D unit cells of the two structures using the location of sixfold axes as the lattice points. (These will also form the base of 3D unit cells of the corresponding structures)
(d) Find the coordinates of atoms in the motif for the two structures
(e) Find the two-dimensional packing efficiency of both structures.

16. Size of Voids: Find the size of the largest sphere that can fit in
(a) octahedral void of a CCP crystal.
(b) tetrahedral void of a CCP crystal.

17. Consider a compound of three elements A, B and C with the radii of their atoms $r_A > r_B > r_C$. Atoms A on their own form a CCP crystal. The atoms of B exactly fill all the octahedral voids of A whereas the atoms C fill all the tetrahedral void of A.
(a) What are the ratios r_B/r_A and $.r_C/r_A$?
(b) Determine the chemical formula $A_xB_yC_z$ of the compound.
(c) Determine the overall packing efficiency of the compound.

18. Location of voids: Show the locations and coordinates of centroids of tetrahedral and octahedral voids in CCP and HCP unit cells. Only consider the translationally inequivalent voids.

19. Polymer chain: Calculate the end-to-end distance of an uncoiled chain molecule of polyethylene with a degree of polymerization of 1000. The C-C bond length is 1.54 A.

20. Cross-linking in polymers: Determine the weight of sulphur that is required to fully crosslink 68 kg of polyisoprene.

21. Ionic Crystal: Consider the ionic crystal CaO with $r_{Ca^{2+}} = 0.94\ A$ and $r_{O^{2-}} = 1.32\ A$. Determine the local coordination number. Assuming O^{2-} form a CCP structure determine the Bravais lattice, motif, lattice parameter and density of the crystal.

22. Phase Transformation: During a phase transformation of Fe a BCC crystal changes to FCC crystal. Assuming hard sphere model find the percentage change in volume. This is an important phase transformation in steels which will be discussed in more detail later in the course.

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