





Materials Science

Lecture 7







Dr. Ali HARKOUS

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Chap3: Crystalline Structure — Perfection

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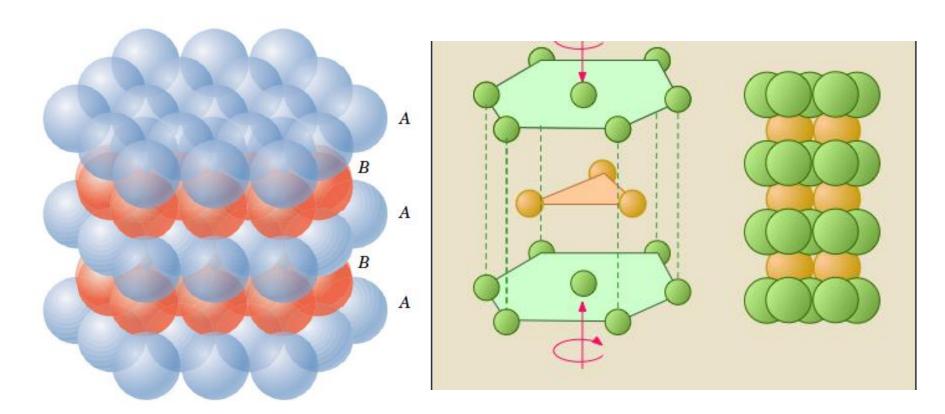


You may remember from the discussion on metallic crystal structures that both face-centered cubic and hexagonal close-packed crystal structures have atomic packing factors of 0.74, which is the most efficient packing of equal-size spheres or atoms.





- For HCP, the centers of the third layer (the second A) are aligned directly above the original A positions. This stacking sequence, ABABAB..., is repeated over and over.
- These close-packed planes for HCP are (0001)-type planes.

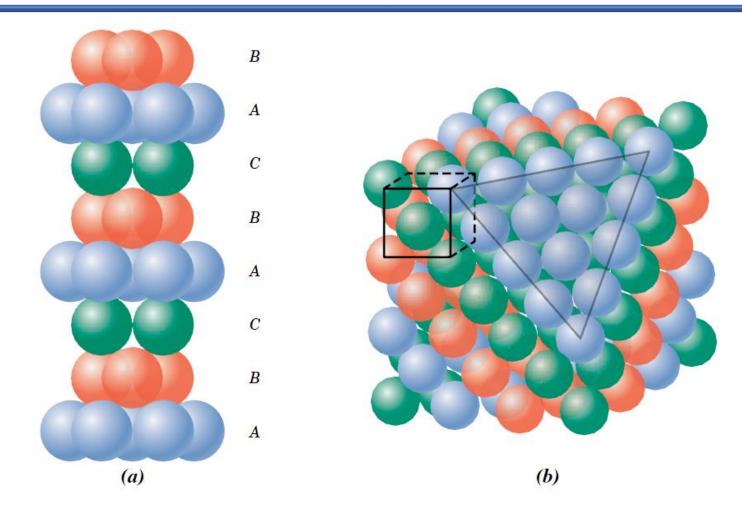


Close-packed plane stacking sequence for the hexagonal close-packed structure.



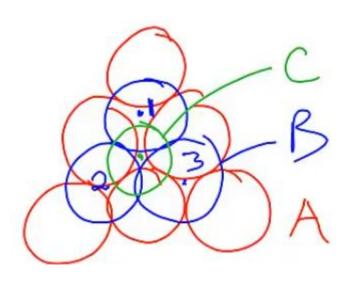
- For the face-centered crystal structure FCC, the centers of the third plane are situated over the C sites of the first plane (Figure).
- This yields an ABCABCABC . . . stacking sequence; that is, the atomic alignment repeats every third plane.
- It is more difficult to correlate the stacking of close-packed planes to the FCC unit cell. However, this relationship is demonstrated in the **next Figure**. These planes are of the (111) type.

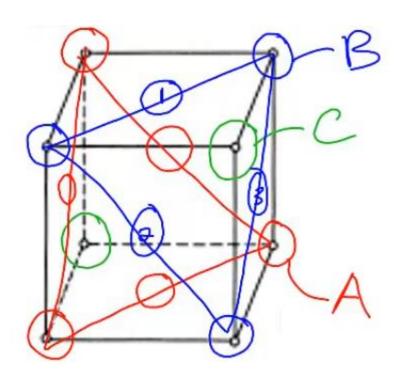




(a) Close-packed stacking sequence for the face-centered cubic structure.
(b) A corner has been removed to show the relation between the stacking of close-packed planes of atoms and the FCC crystal structure; the heavy triangle outlines a (111) plane.







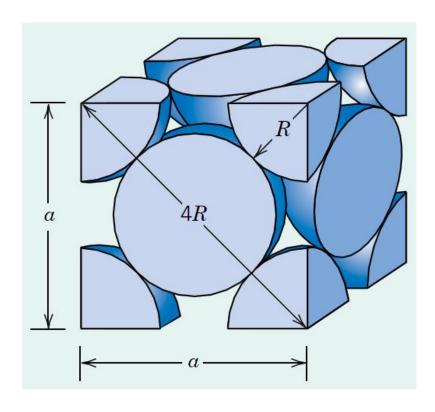
Close-packed stacking sequence for the face-centered cubic structure FCC.



Chap 3 Exercises

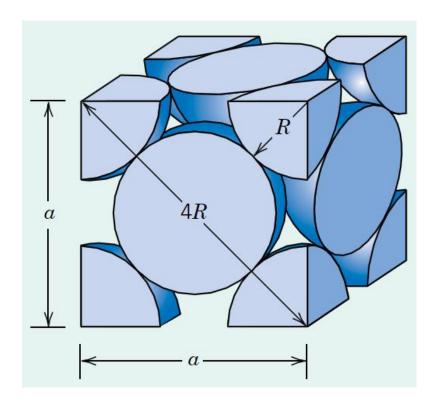


Calculate the volume of an FCC unit cell in terms of the atomic radius *R*.



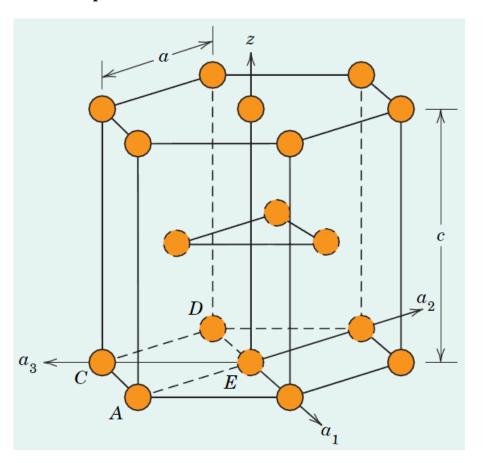


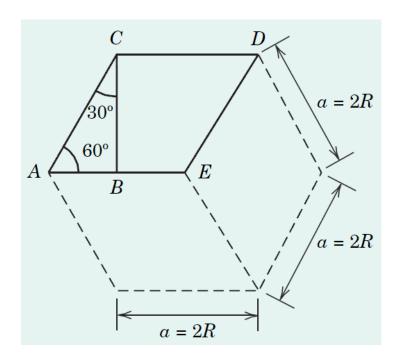
Using volumes, Show that the atomic packing factor for the FCC crystal structure is 0.74.





- (a) Calculate the volume of an HCP unit cell in terms of its a and c lattice parameters.
- (b) Now provide an expression for this volume in terms of the atomic radius, R, and the c lattice parameter.







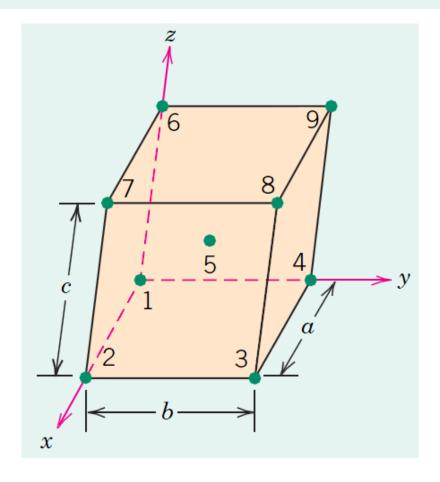
Theoretical Density Computation for Copper

Copper has an atomic radius of 0.128 nm, an FCC crystal structure, and an atomic weight of 63.5 g/mol. Compute its theoretical density, and compare the answer with its measured density.



Specification of Point Coordinate Indices

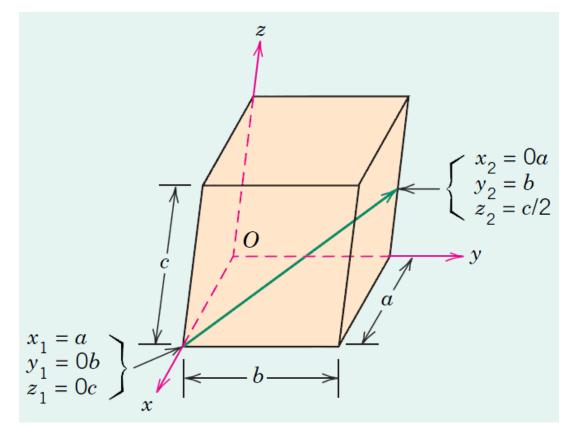
Specify coordinate indices for all numbered points of the unit cell in the illustration on the next page.





Determination of Directional Indices

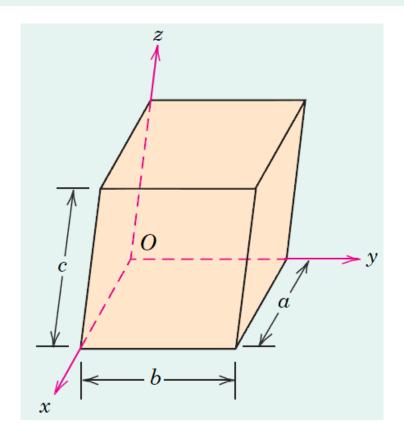
Determine the indices for the direction shown in the accompanying figure.





Construction of a Specified Crystallographic Direction

Within the following unit cell draw a $[1\overline{1}0]$ direction with its tail located at the origin of the coordinate system, point O.





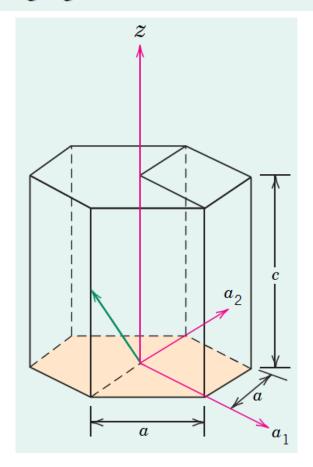
Conversion and Construction of Directional Indices for a Hexagonal Unit Cell

- (a) Convert the [111] direction into the four-index system for hexagonal crystals.
- **(b)** Draw this direction within a ruled-net coordinate system (per Figure 3.10).
- (c) Now draw the [111] direction within a hexagonal unit cell that utilizes a three-axis (a_1, a_2, z) coordinate scheme.



Determination of Directional Indices for a Hexagonal Unit Cell

Determine the indices (four-index system) for the direction shown in the accompanying figure.





Determination of Planar (Miller) Indices

Determine the Miller indices for the plane shown in the accompanying sketch (a).

