Structural metallic materials

2. Structure and organisation of solid

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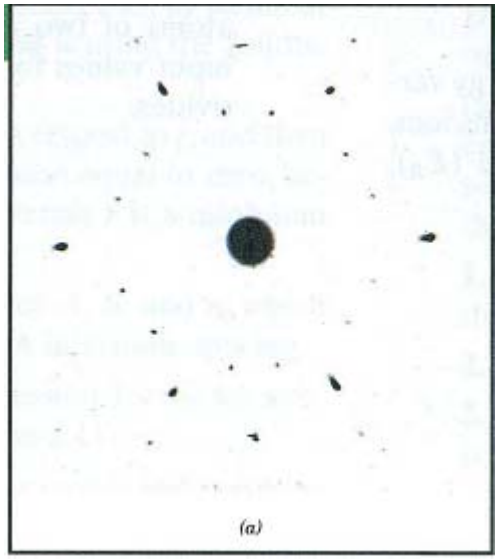
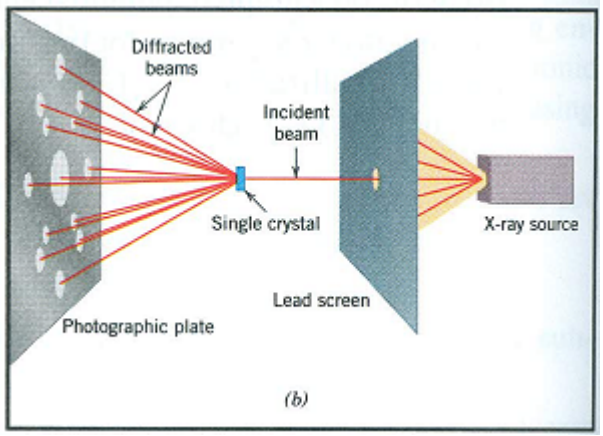
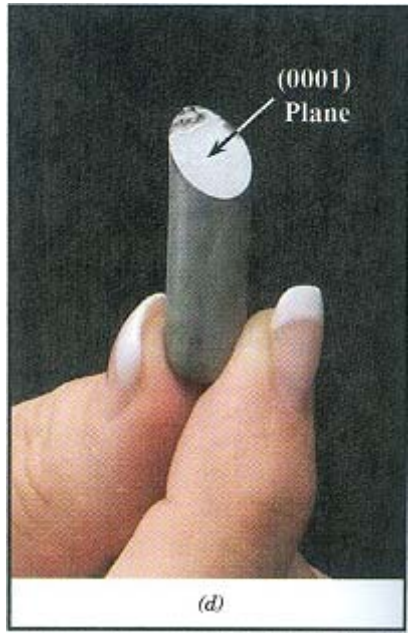
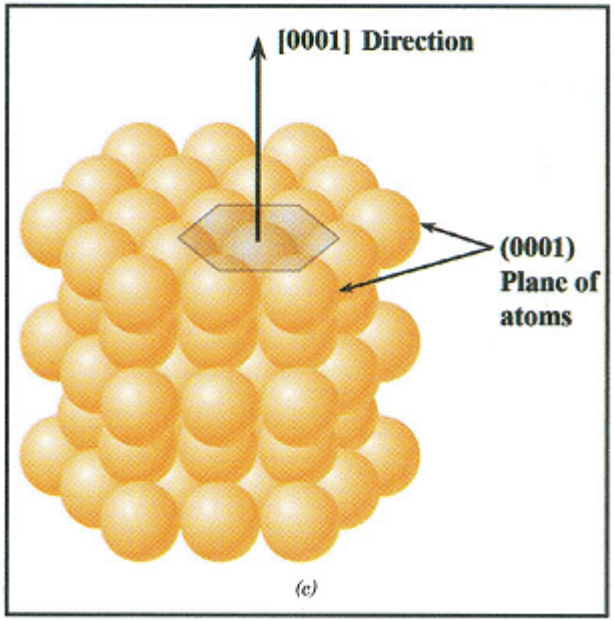
Structural metallic materials









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Structural metallic materials

2.1 FUNDAMENTAL CONCEPTS

Crystalline: In which the atom are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three-dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms.

Crystal structure: the manner in which atoms, ions or molecules are spatially arranged.

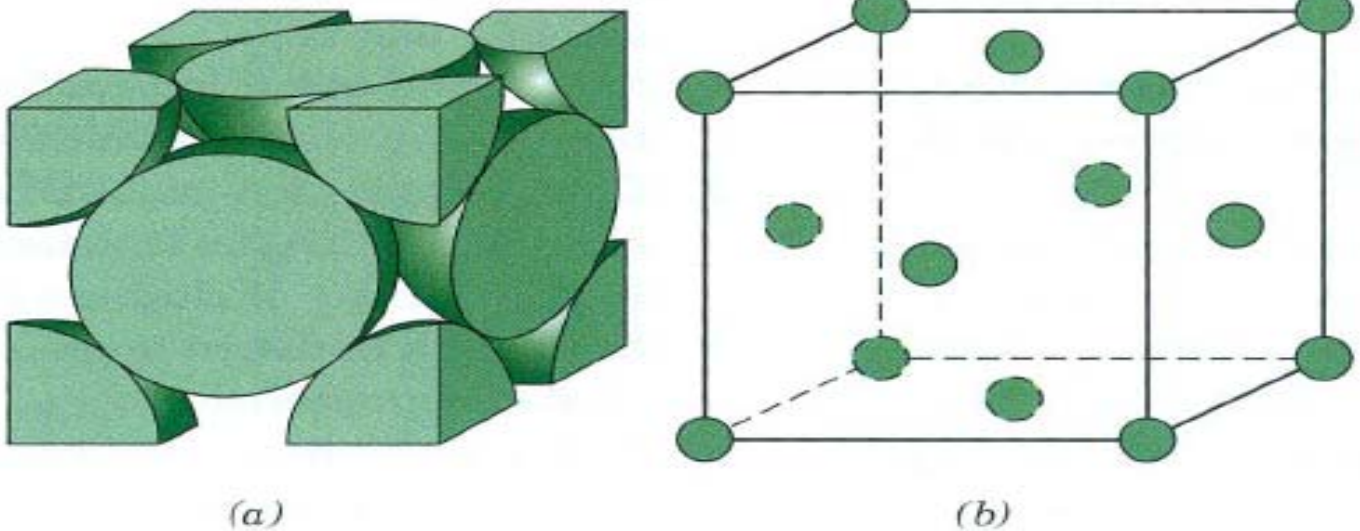
Structural metallic materials

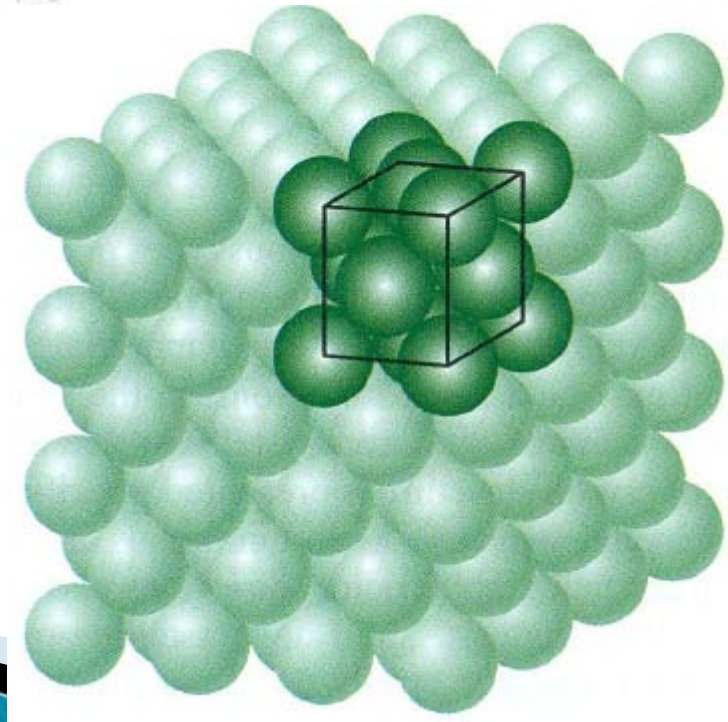
2.1 FUNDAMENTAL CONCEPTS

lattice: the regular geometrical arrangement of points in crystal space

Unit cell: the basic structural unit of a crystal structure. It is generally defined in terms of atom (or ion) positions within a parallelepiped volume

Structural metallic materials





2.2Face centered cubic crystal structure

Structural metallic materials

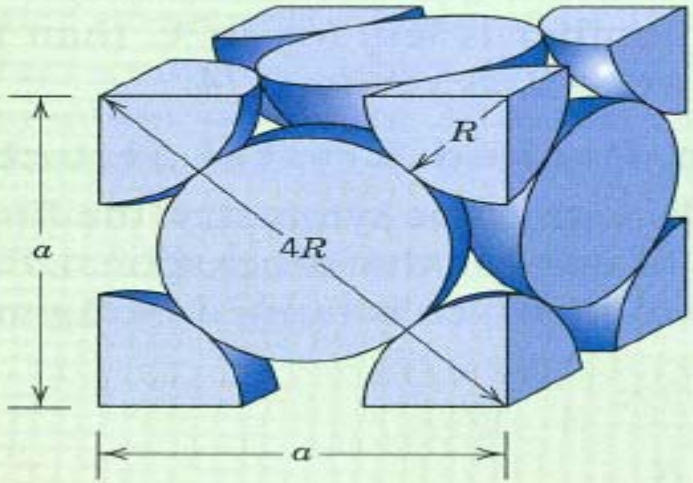
2.2 Face centered cubic crystal structure

Determination of FCC Unit Cell Volume

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

Solution

In the FCC unit cell illustrated,



$$a^2 + a^2 = (4R)^2$$

$$a = 2R\sqrt{2}$$

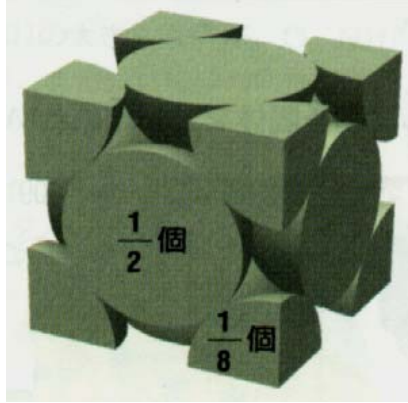
The FCC unit cell volume V_C may be computed from

$$V_C = a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$

Structural metallic materials

Face centered cubic crystal structure

Computation of the atomic packing factor for FCC



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

Solution

The APF is defined as the fraction of solid sphere volume in a unit cell, or

$$\text{APF} = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

Both the total atom and unit cell volumes may be calculated in terms of the atomic radius R. The volume for a sphere is $\frac{4}{3}\pi R^3$, and because there are four atoms per FCC unit cell, the total FCC atom (or sphere) volume is

$$V_S = (4)\tfrac{4}{3}\pi R^3 = \tfrac{16}{3}\pi R^3$$

From Example Problem 3.1, the total unit cell volume is

$$V_C = 16R^3\sqrt{2}$$

Therefore, the atomic packing factor is

$$\text{APF} = \frac{V_S}{V_C} = \frac{(\frac{16}{3})\pi R^3}{16R^3\sqrt{2}} = 0.74$$

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Structural metallic materials

Face centered cubic crystal structure

DENSITY COMPUTATIONS

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.

Solution

Equation 3.5 is employed in the solution of this problem. Because the crystal structure is FCC, n, the number of atoms per unit cell, is 4. Furthermore, the atomic weight A_{Cu} is given as 63.5 g/mol. The unit cell volume V_C for FCC was determined in Example Problem 3.1 as $16R^3\sqrt{2}$, where R, the atomic radius, is 0.128 nm.

Substitution for the various parameters into Equation 3.5 yields

$$\rho = \frac{nA_{Cu}}{V_C N_A} = \frac{nA_{Cu}}{(16R^3\sqrt{2})N_A}$$

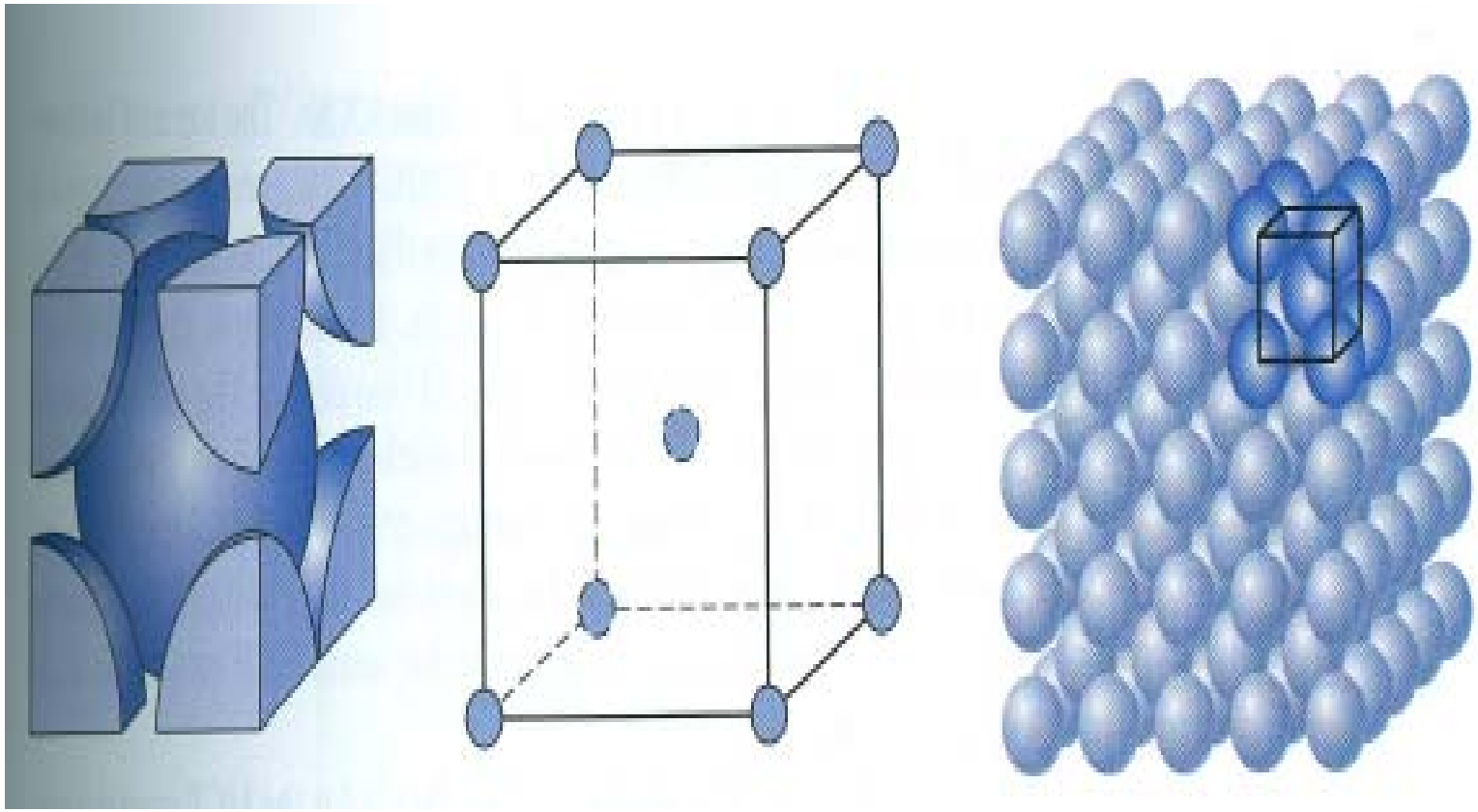
$$= \frac{(4 \text{ atoms/unit cell})(63.5 \text{ g/mol})}{[16\sqrt{2}(1.28 \times 10^{-8} \text{ cm})^3/\text{unit cell}](6.022 \times 10^{23} \text{ atoms/mol})}$$

$$= 8.89 \text{ g/cm}^3$$

The literature value for the density of copper is 8.94 g/cm^3, which is in very close agreement with the foregoing result.

Structural metallic materials

2.3 Body-centered cubic crystal structure



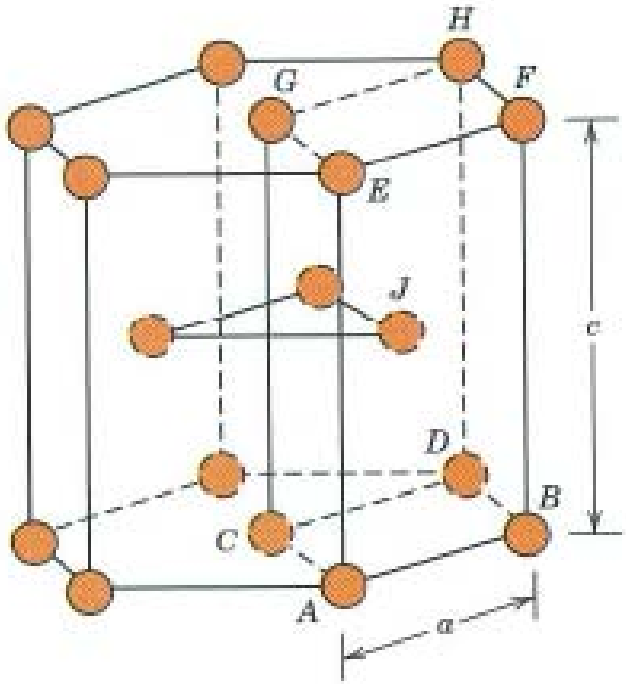
Structural metallic materials

Body-centered cubic crystal structure

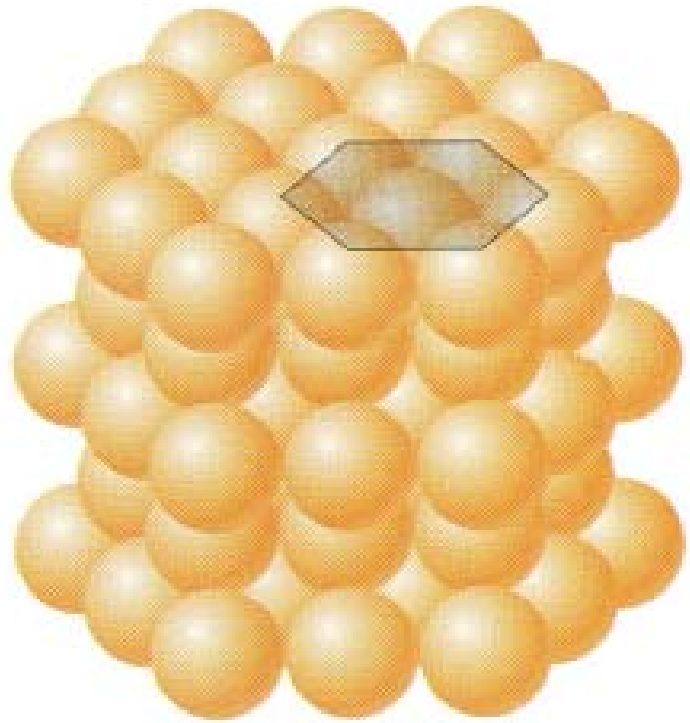
- the cubic edge length a
- The cubic –diagonal length r= $\sqrt{3}$ /4(a)
- atom per BCC=8*(1/8)+1=2
- APF=nV1/V=0.68

Structural metallic materials

2.4 Hexagonal close-packed crystal structure



(a)



(b)

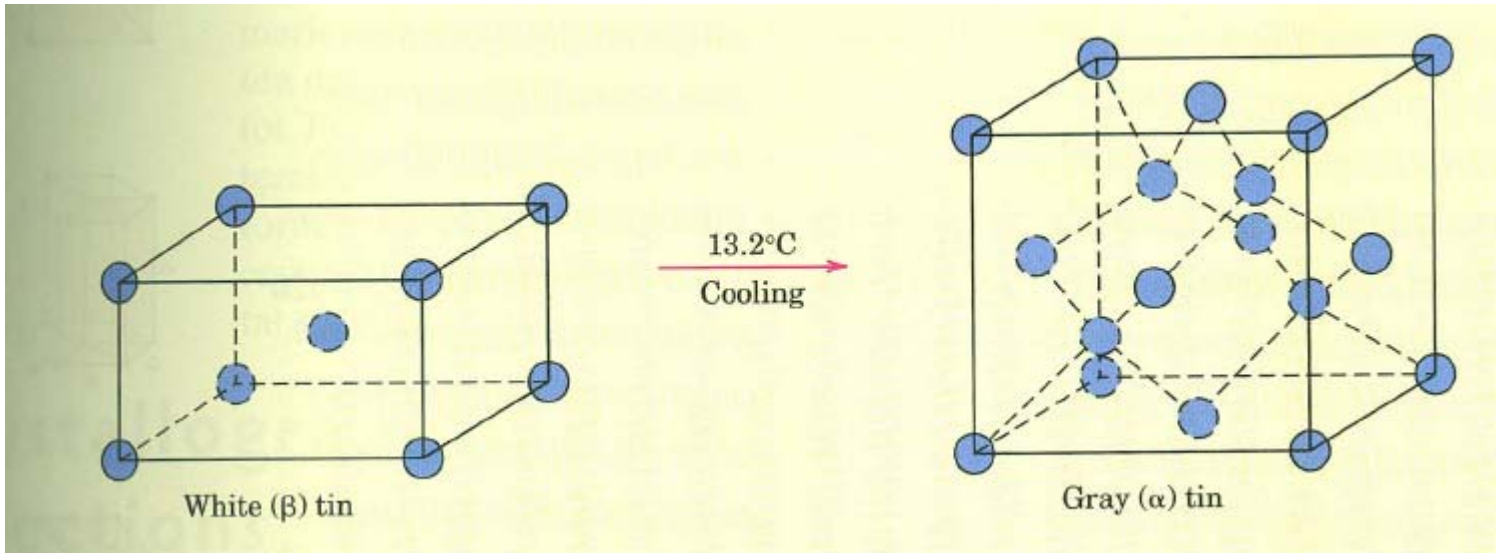
Structural metallic materials

Hexagonal close-packed crystal structure

- the HCP edge length a and c
- r= a/2
- atom per HCP=12*(1/6)+3+1/2*2=6
- APF=nV1/V=0.74

Structural metallic materials

2.5 Tin (Its Allotropic Transformation)



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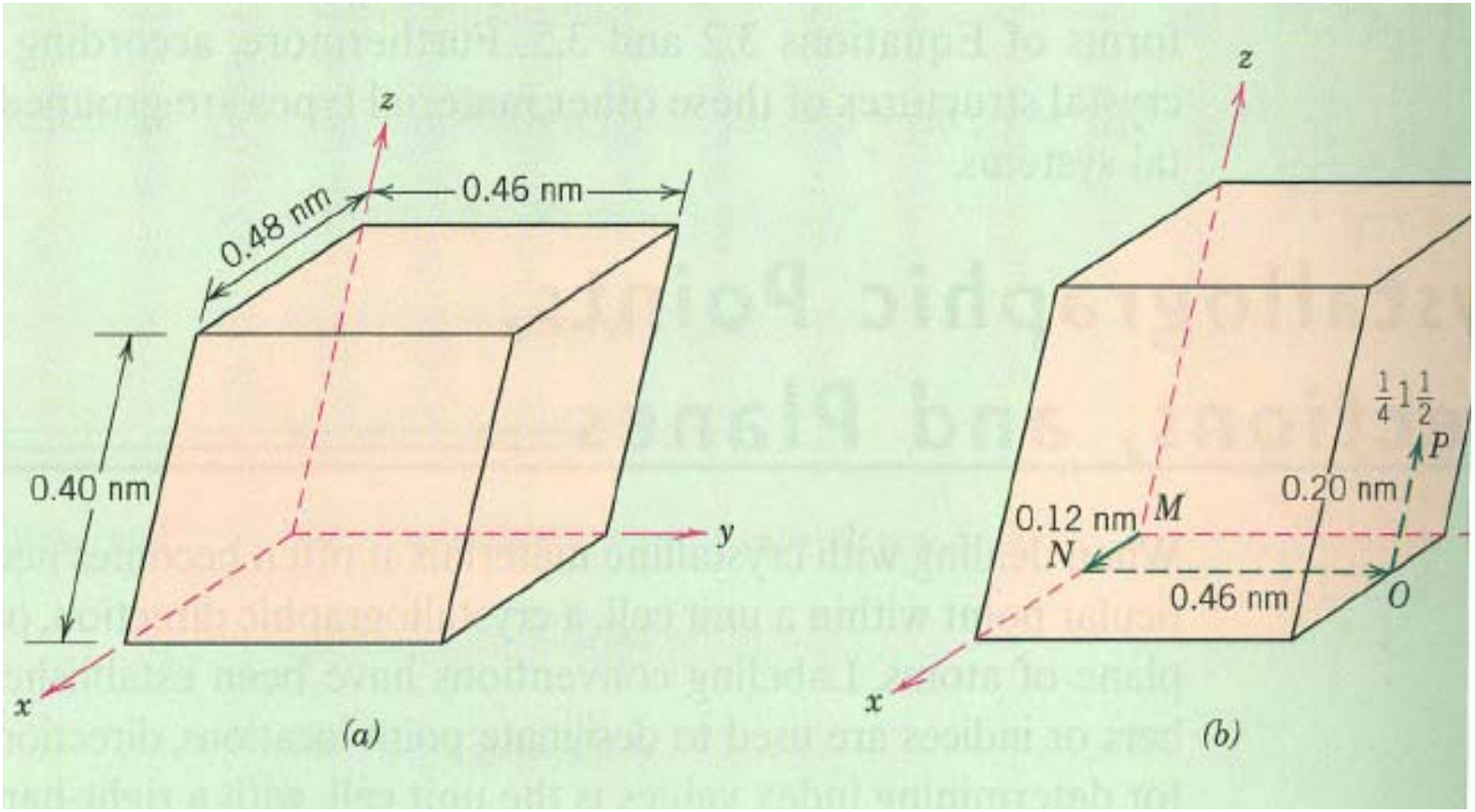
Structural metallic materials

2.6 crystallographic points, direction and planes

POINTCOORDINATES



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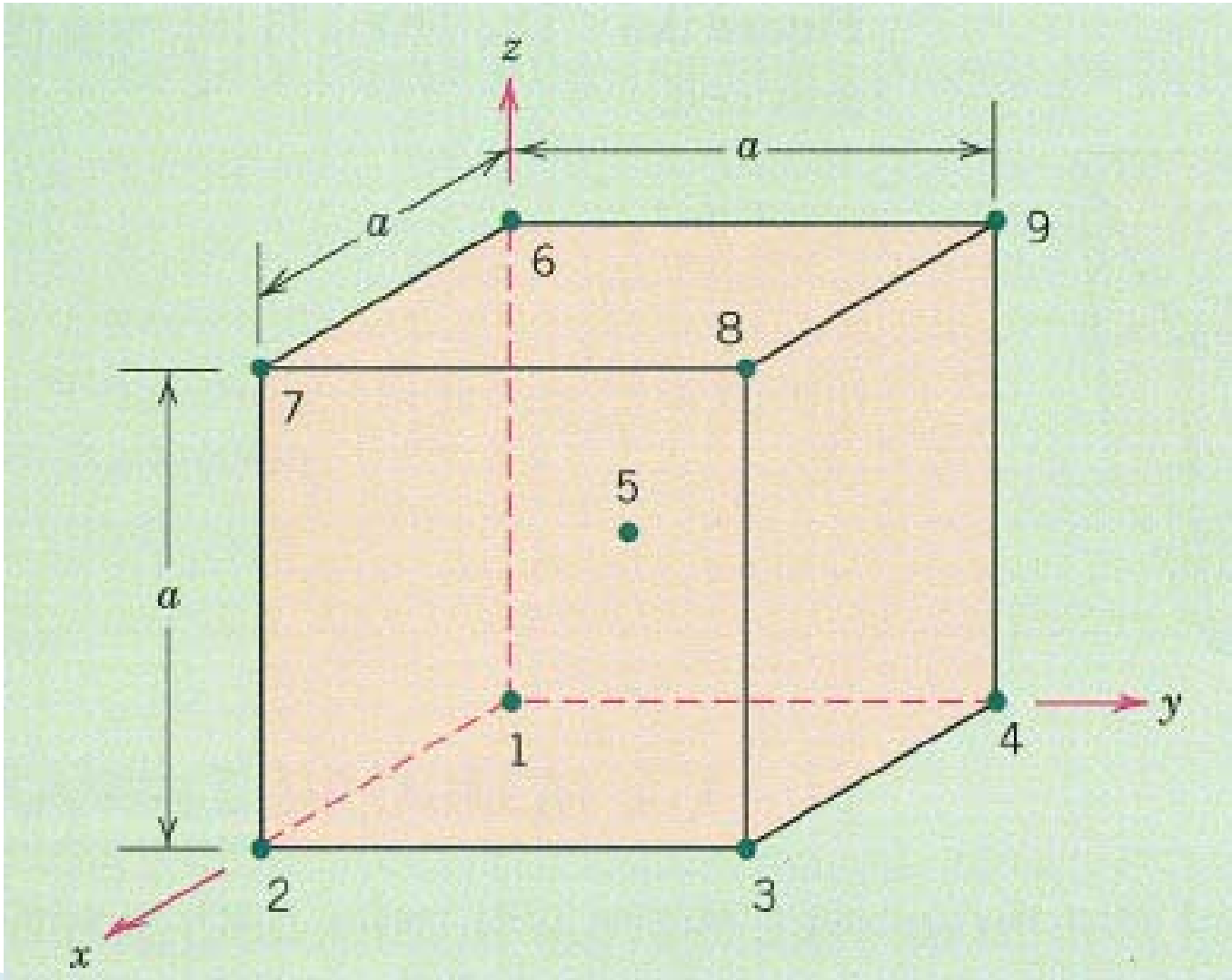
Structural metallic materials

2.6 crystallographic points, direction and planes



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Structural metallic materials

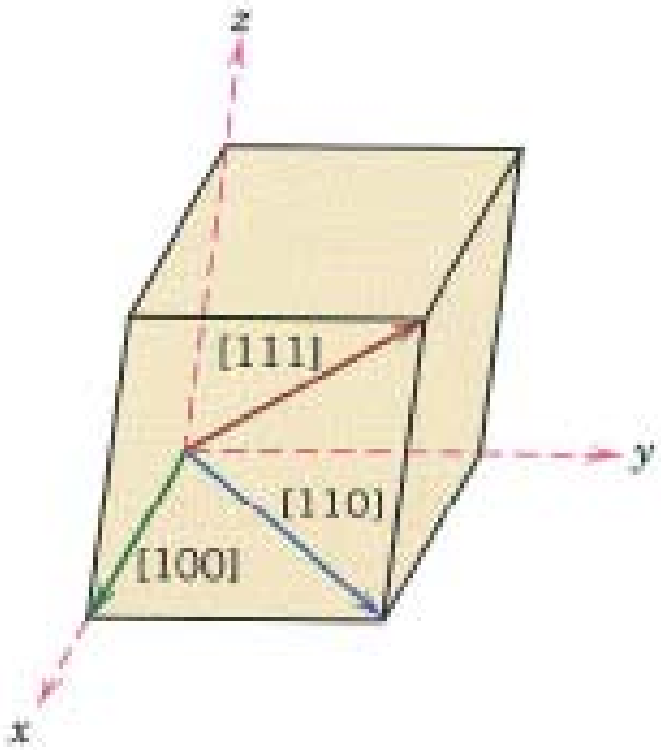
2.6 crystallographic points, direction and planes

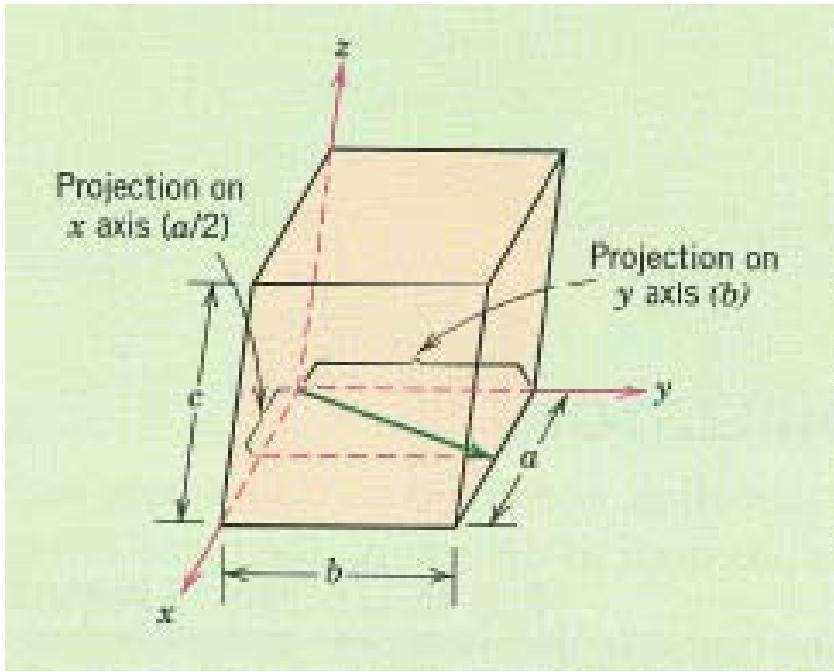
Point Number	Fractional Lengths			Point Coordinates
	x axis	y axis	Z axis	
1	0	0	0	0 0 0
2	1	0	0	1 0 0
3	1	1	0	1 1 0
4	0	1	0	0 1 0
5	½	½	½	½ ½ ½
6	0	0	1	0 0 1
7	1	0	1	1 0 1
8	1	1	1	1 1 1
9	0	1	1	0 1 1

Structural metallic materials

2.6 crystallographic points, direction and planes

CRYSTALLOGRAPHIC DIRECTIONS





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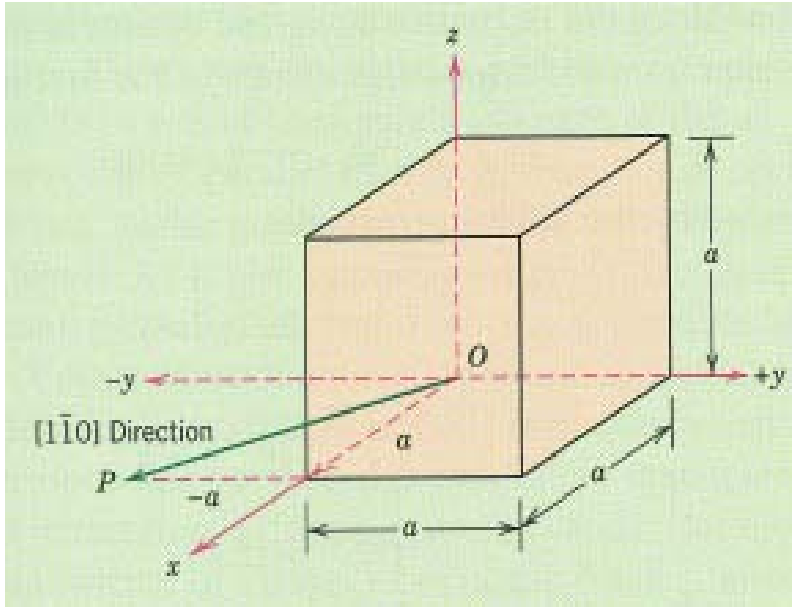
Structural metallic materials

2.6 crystallographic points, direction and planes

	x	y	z
Projections	a/2	b	0_c
Projections(in terms of a,b,andc)	1/2	1	0
Reduction	1	2	0
Enclosure		[120]	



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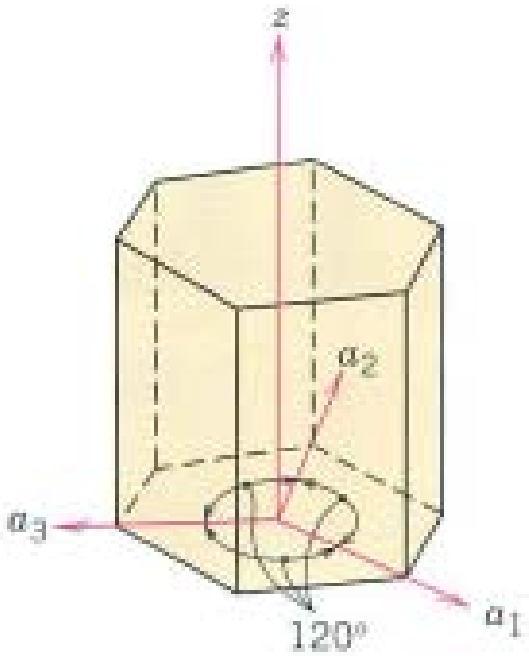
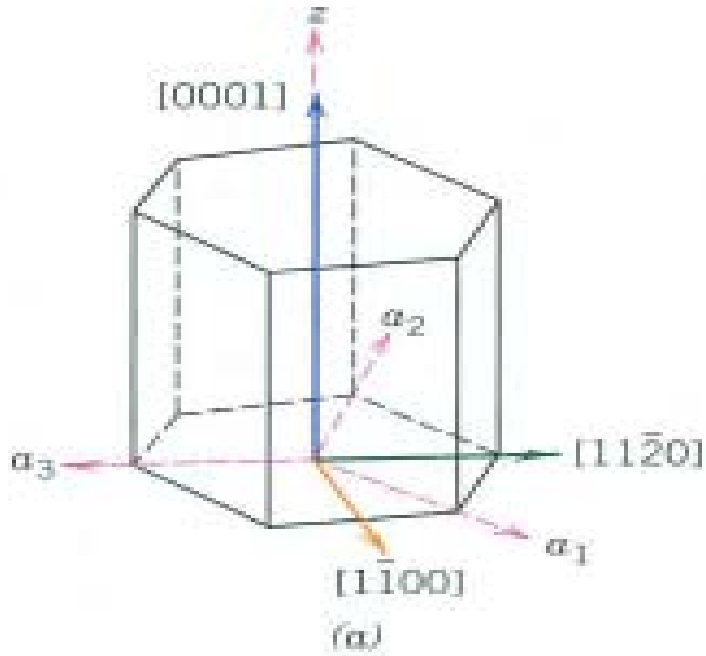
Structural metallic materials

2.6 crystallographic points, direction and planes





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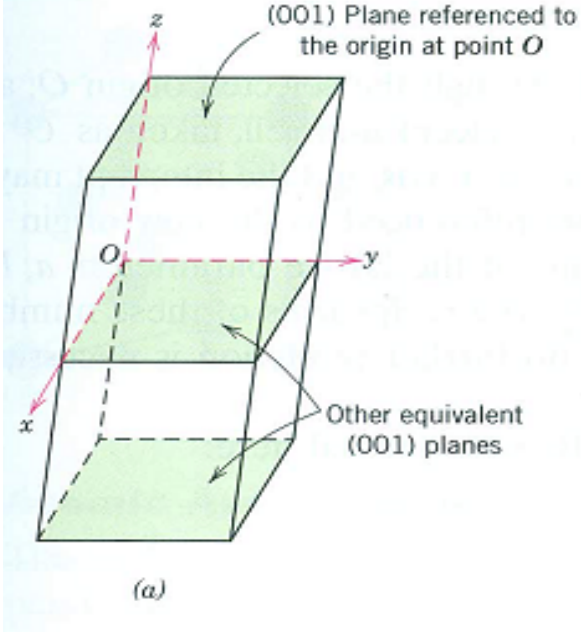
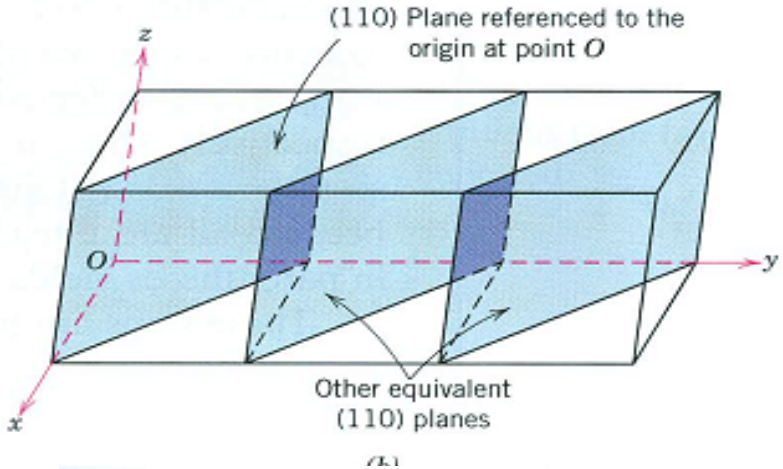
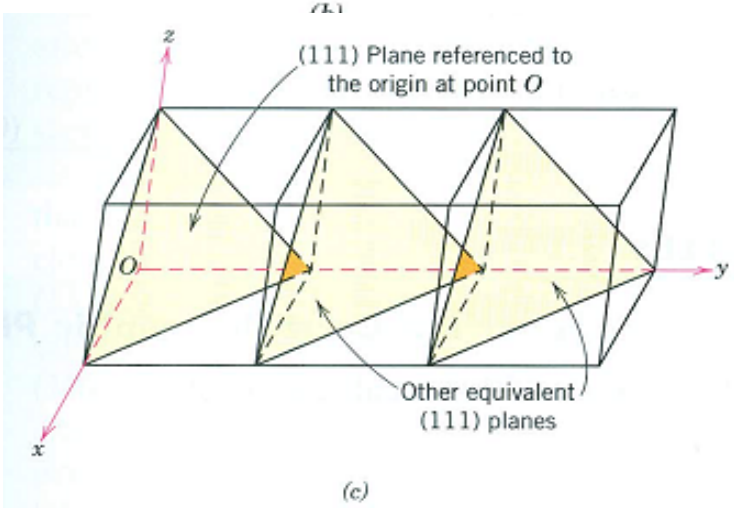
Structural metallic materials

2.6 crystallographic points, direction and planes

CRYSTALLOGRAPHIC PLANES







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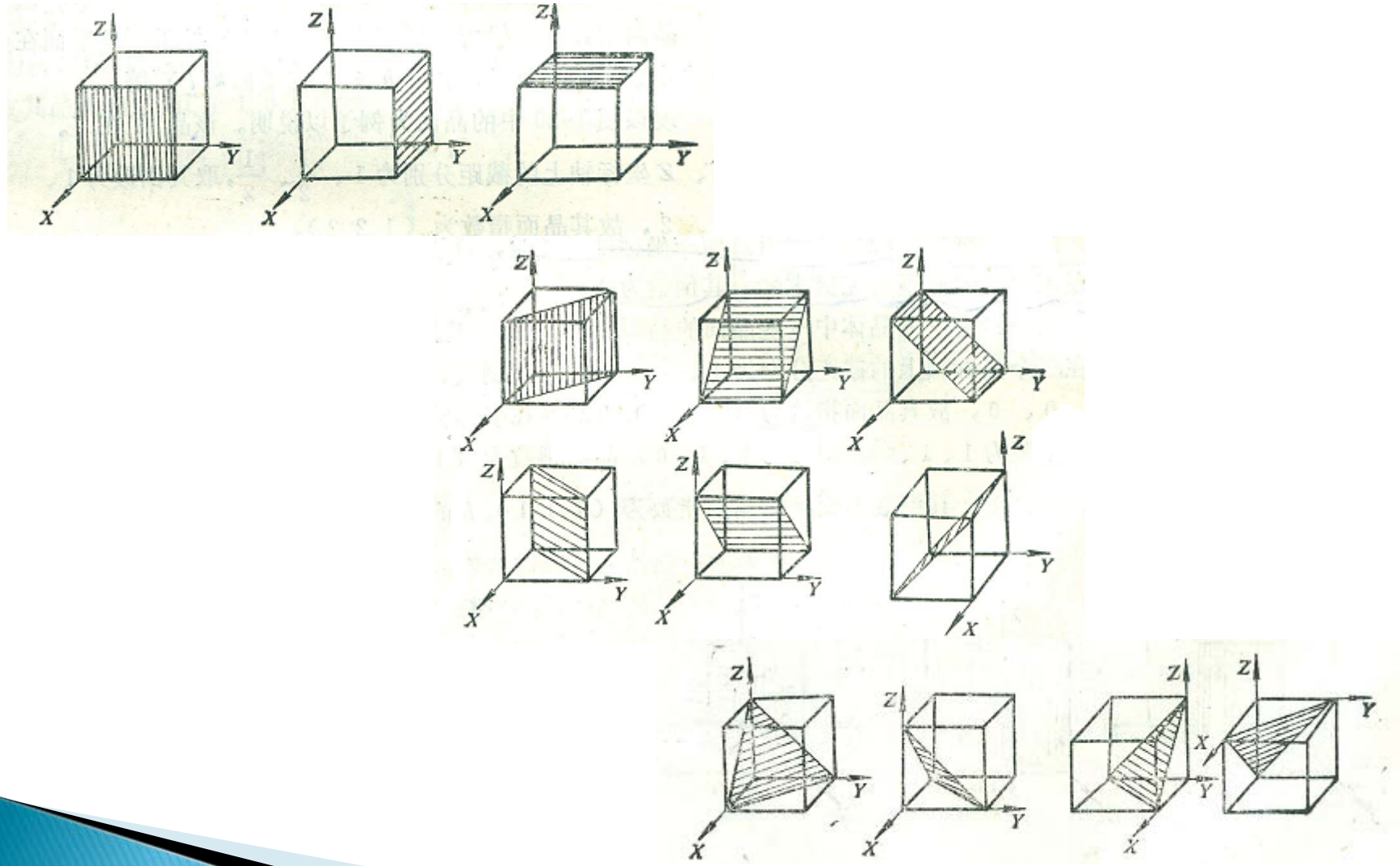
Structural metallic materials

2.6 crystallographic points, direction and planes



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Structural metallic materials

2.6 crystallographic points, direction and planes

$$\{1\ 0\ 0\} = (1\ 0\ 0) + (0\ 1\ 0) + (0\ 0\ 1)$$

$$\{1\ 1\ 1\} = (1\ 1\ 1) + (1\ 1\ 1) + (1\ 1\ 1) + (1\ 1\ 1)$$

$$\{1\ 1\ 0\} = (1\ 1\ 0) + (1\ 0\ 1) + (0\ 1\ 1) + (1\ 1\ 0) + (1\ 0\ 1) + (0\ 1\ 1)$$

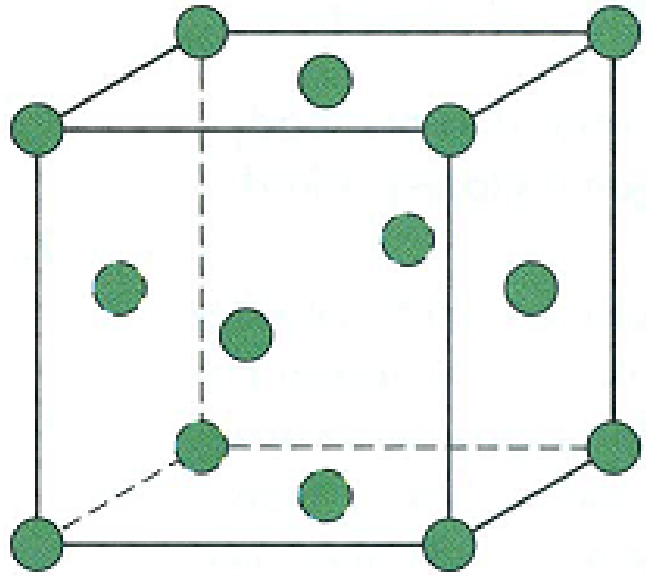
Structural metallic materials

QUESTION

If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.

(FCC crystal structure)

List the point coordinates for all atoms that are associated with the FCC unit cell



Structural metallic materials

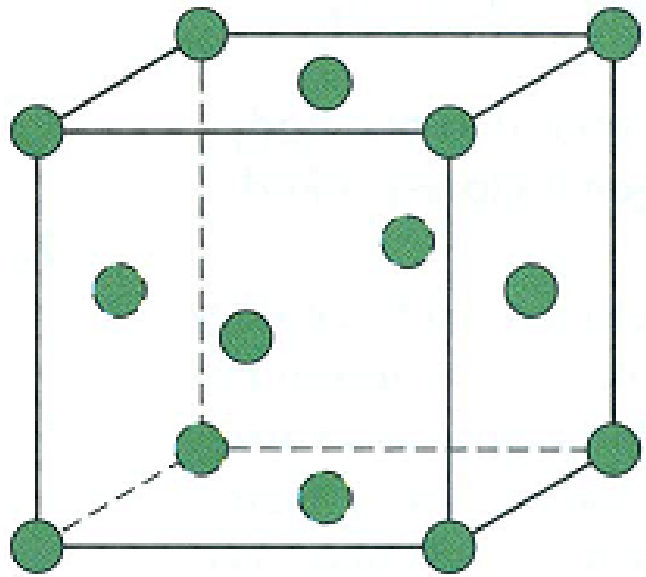
Answer

If the atomic radius of aluminum is 0.143 nm, calculate the volume of its unit cell in cubic meters.

(FCC crystal structure)

$6.62X10^{-29}m^3$

List the point coordinates for all atoms that are associated with the FCC unit cell



000,100,110,010,001,101,111,011,

1/2 ½ 0 ,1/2 ½ 1,1 ½ ½,

0 ½ ½,

1/2 0 ½, and ½ 1 ½