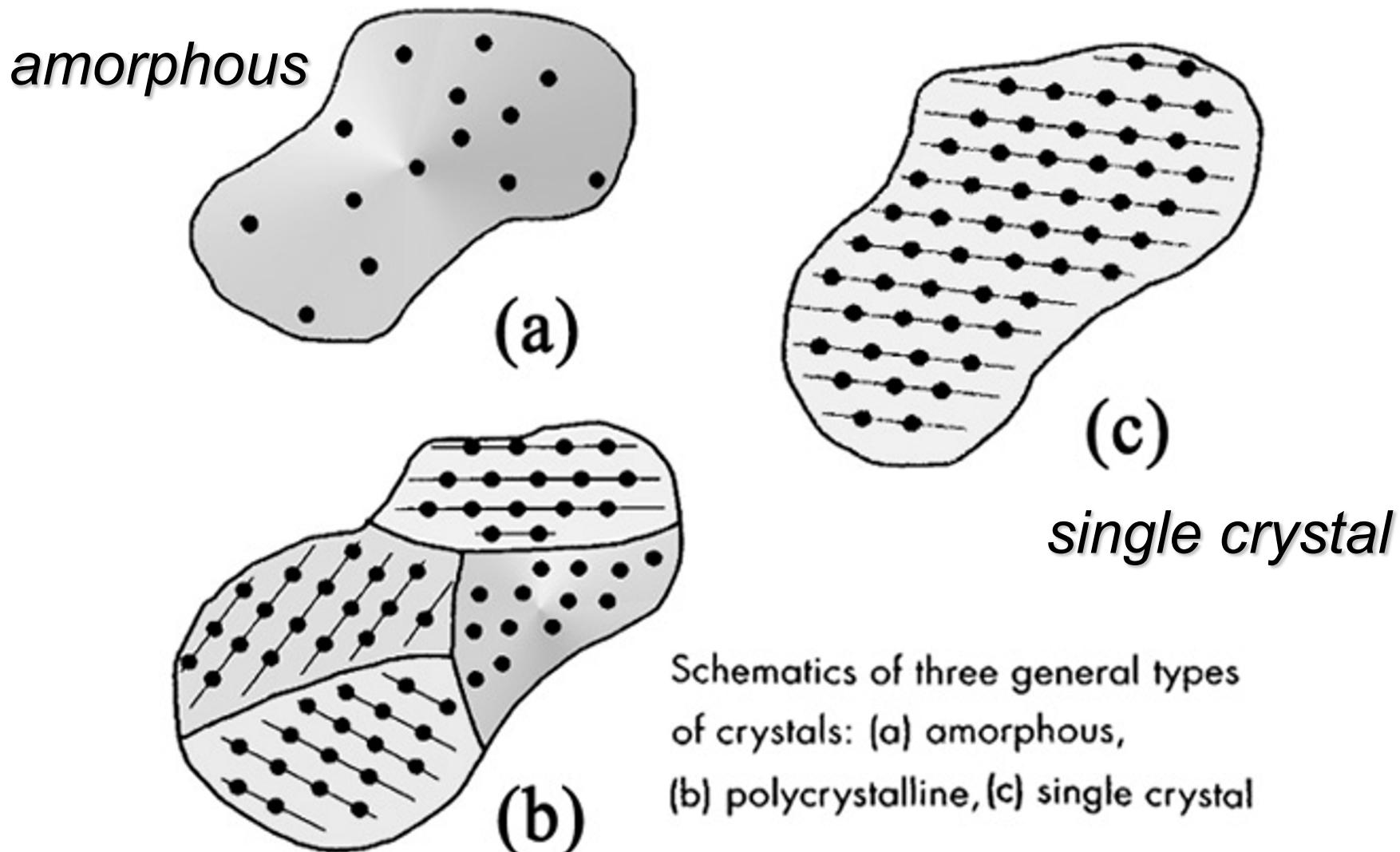


Lecture 3

2 SEMICONDUCTOR CRYSTAL STRUCTURE

2.1 Types of Solids

- Solids are characterized by the size of an ordered region within the material.
- The ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement, or periodicity.
- Three general types of solids (see Fig. 2.1)



Schematics of three general types
of crystals: (a) amorphous,
(b) polycrystalline, (c) single crystal

polycrystalline

Fig.2.1

- Amorphous materials

- Ordered region is only within a few atomic or molecular dimensions (a few to tens of angstrom; $1\text{\AA} = 10^{-10} \text{ m}$)

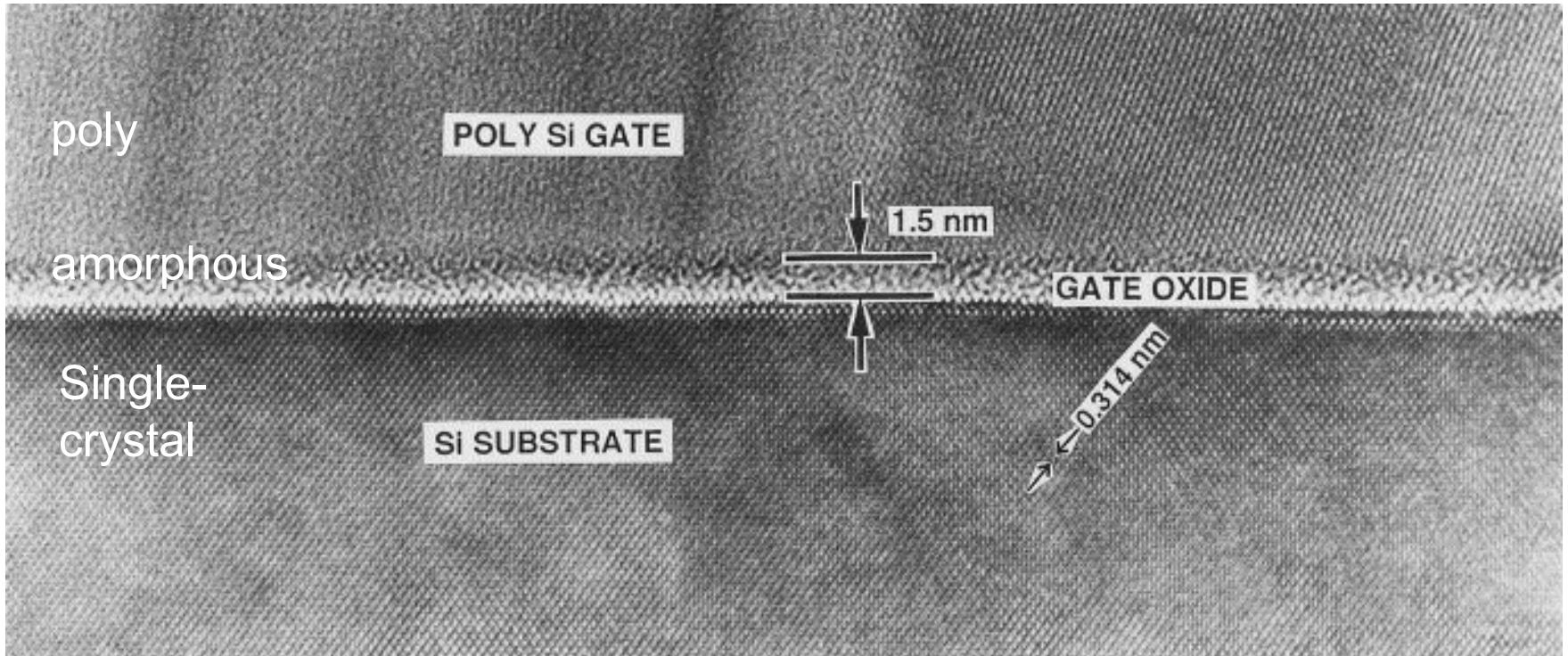
- Polycrystalline materials

- High degree of order over many atomic or molecular dimensions
- Ordered regions (or single crystal regions) vary in size & orientation with respect to one another.
- These single crystal regions are called *grains* & are separated from one another by grain boundaries.

- Single crystal

- High degree of order, or regular geometric periodicity, throughout entire volume of material
- Electrical properties are superior to those of non-single crystal materials (because grain boundaries degrade electrical characteristics)

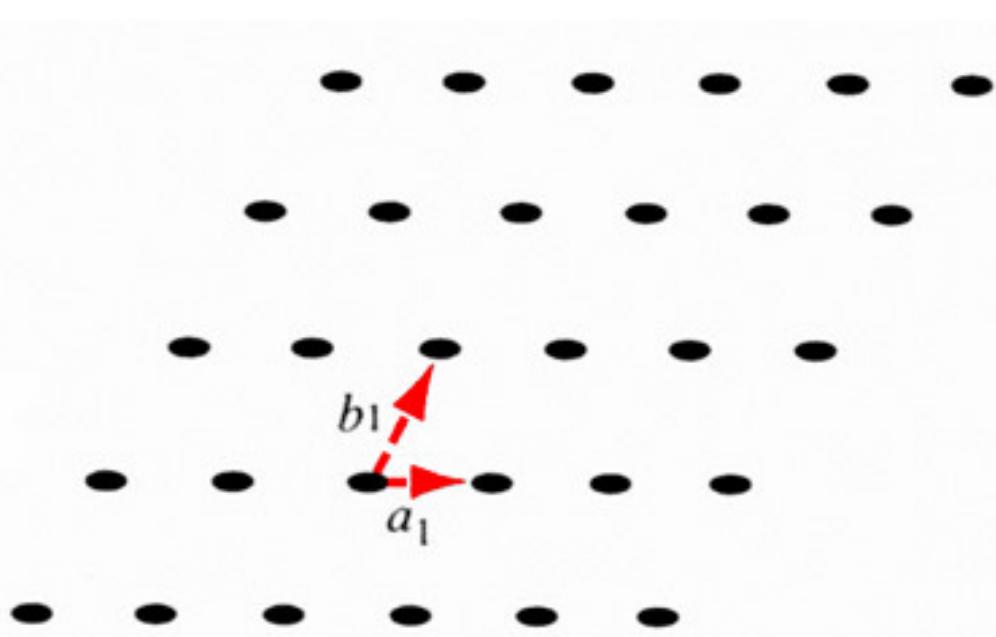
Image of an MOS capacitor



Momose et al, Microelectronics Reliability, Volume 38, Issue 9,
September 1998, Pages 1413–1423

2.2 Space Lattice, Primitive and Unit Cell

- Consider a single crystal
- Periodic arrangement of points in a space is called a lattice. The point is called a lattice point.



Two-dimensional representation
of a single-crystal lattice

Fig. 2.2 shows an infinite 2-D array of lattice points.

- Each lattice point can be translated a distance a_1 and a distance b_1 in a second non-colinear direction to generate the 2-D lattice.
- A third non-colinear translation will produce the three dimensional (3-D) lattice. The lattice directions need not be perpendicular
- A crystal structure is formed when an atom, group of atoms/molecules is attached identically to each lattice point

When considering a lattice,

- Do not need to consider the entire lattice. Need to look only at a fundamental unit that is being repeated
- A unit cell is a small volume of crystal that can be used to reproduce the entire crystal. It is a representative of the entire lattice. We can generate the entire lattice by repeating the unit cell throughout the crystal
 - A unit cell is not unique entity
 - Several possible unit cell in 2-D lattice is shown in Fig. 2.3

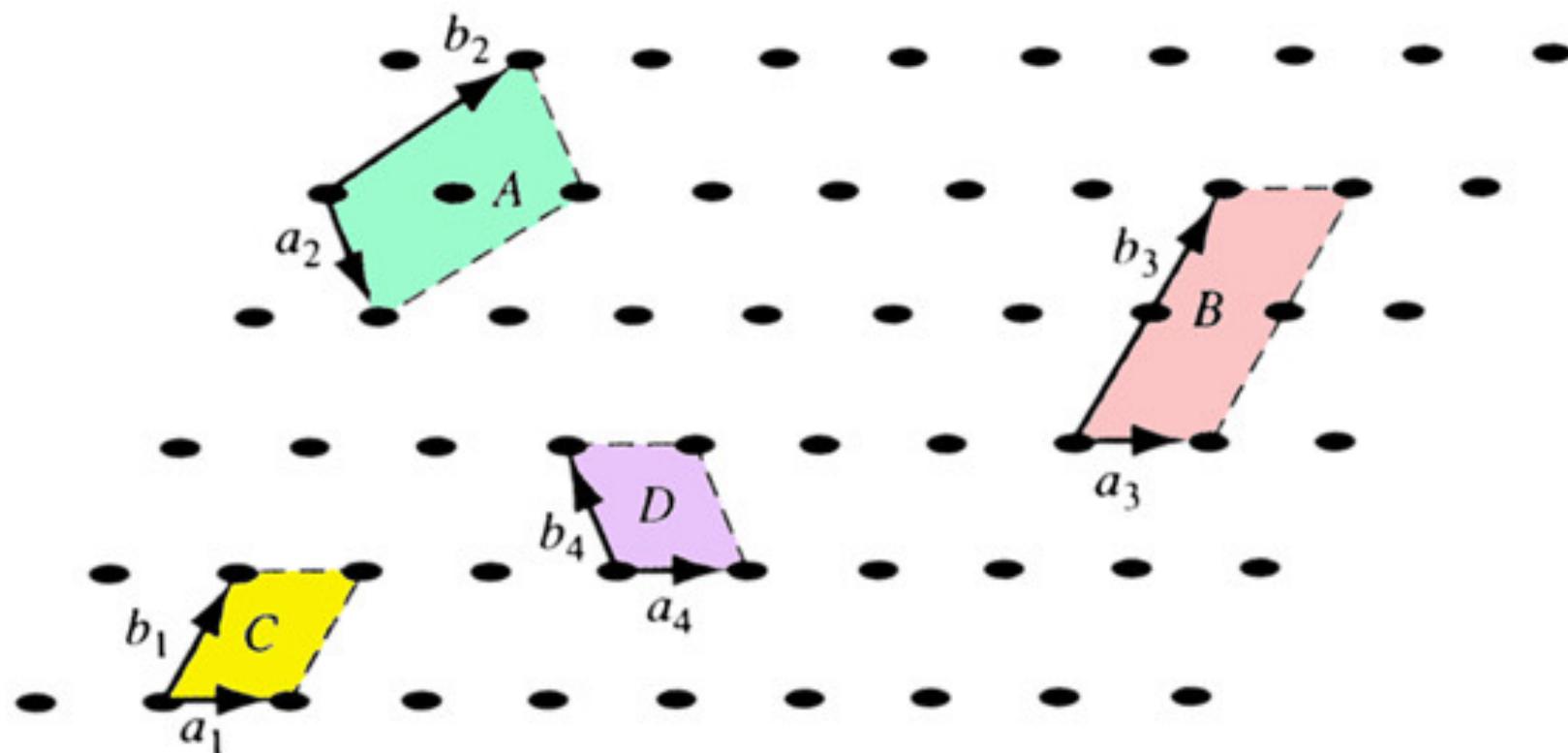


Fig. 2.3

Two-dimensional representation of a single-crystal lattice showing various possible unit cells

- A primitive cell is the smallest unit cell that can be repeated to form lattice
- In many cases, more convenient to use a unit cell
 - They can be chosen to have orthogonal sides, whereas sides of primitive cell may not be orthogonal as shown in Fig. 2.4.

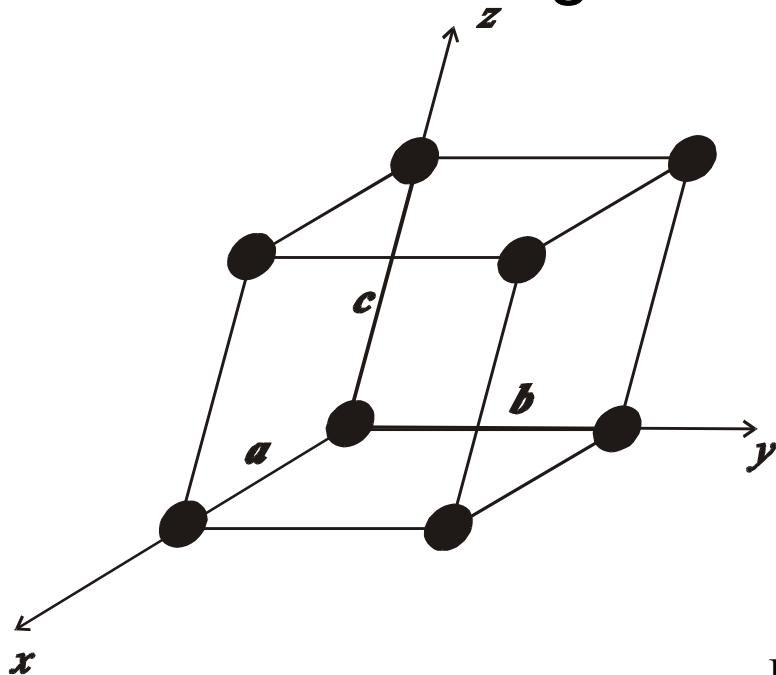
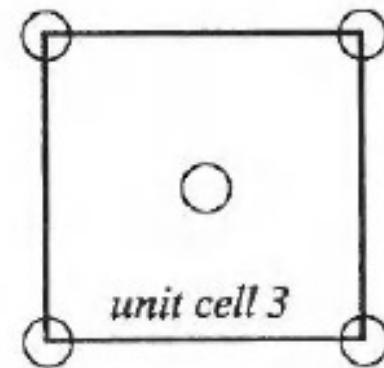
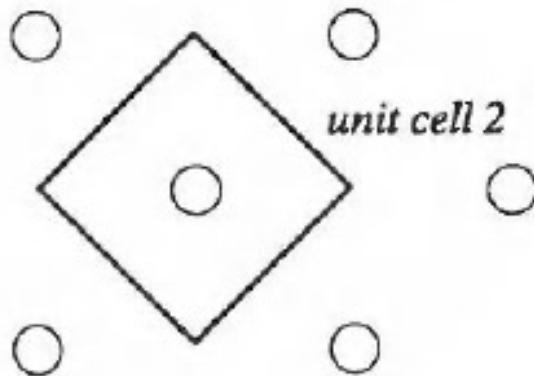
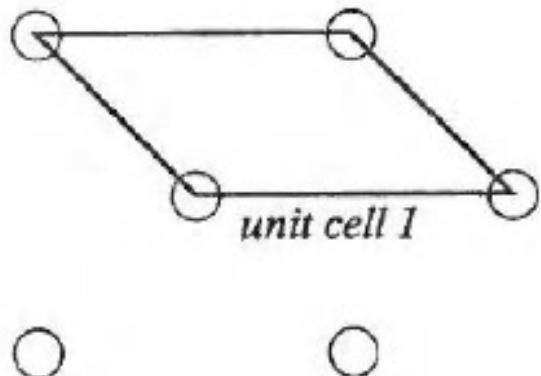


Fig. 2.4 A generalized primitive unit cell

Question (BG Streetman)

Which of the following three unit cells are *primitive cells* for the two-dimensional lattice? Circle the correct combination **in bold** below.

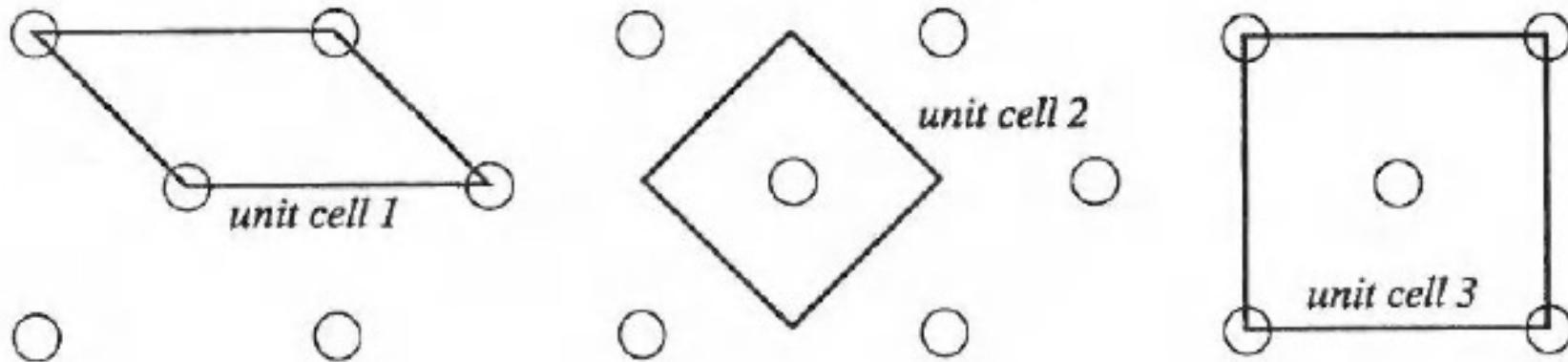
1 / 2 / 3 / 1 and 2 / 1 and 3 / 2 and 3 / 1, 2, and 3



Question (BG Streetman)

Which of the following three unit cells are *primitive cells* for the two-dimensional lattice? Circle the correct combination **in bold** below.

1 / 2 / 3 / 1 and 2 / 1 and 3 / 2 and 3 / 1, 2, and 3



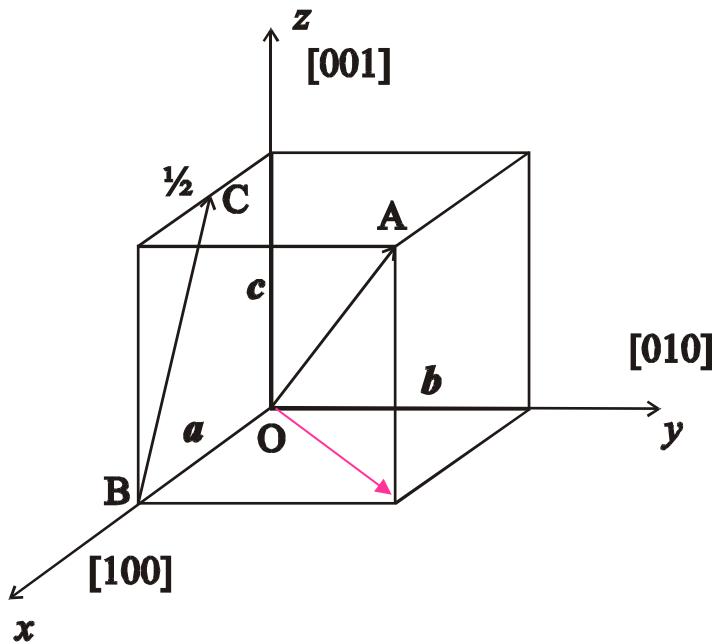
1 and 2: 1 and 2 each contain a single atom and may be repeated to form the lattice. 3 may be repeated to form the lattice, but it contains 2 atoms.

2.3 Crystallographic directions and planes

- Consider a unit cell defined by 3 vectors \mathbf{a} , \mathbf{b} and \mathbf{c} . The dimensions a , b and c are unit cell dimensions or lattice constant. For cubic unit cell the dimensions $a = b = c$.
- A crystallographic direction is defined as a line between two points, a vector. To determine the crystallographic directions:
 - determine the origin
 - determine the initial and the final positions of the vector in terms of the lattice constant a , b and c

- determine the vector: (final position) – (initial position)
- write down the vector in terms of the numbers of the lattice constant
- multiply or divide these numbers by a common factor to reduce them to the smallest integer values
- the three indices are enclosed in square brackets $[uvw]$. The u , v and w integers correspond to the reduced projections along x , y and z
- negative indices are represented by a bar over the appropriate index

Examples 2.1



In most Si transistor, current flows in the [110] direction

Vector OA

	x	y	z
Final position	$1a$	$1b$	$1c$
Initial position	$0a$	$0b$	$0c$
Vector OA	$1a$	$1b$	$1c$
Vector OA (numbers only)	1	1	1
Reduction	1	1	1
Enclosure	[111]		

Vector BC

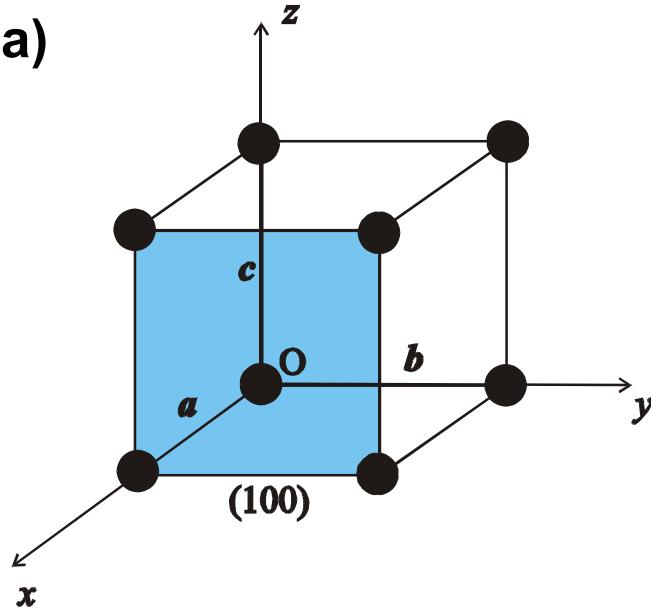
	x	y	z
Final position	$1/2a$	$0b$	$1c$
Initial position	$1a$	$0b$	$0c$
Vector BC	$-1/2a$	$0b$	$1c$
Vector BC (numbers only)	$-1/2$	0	1
Reduction	-1	0	2
Enclosure	[$\bar{1}02$]		

- Planes in a crystal are specified by Miller indices (hkl).
- To determine the Miller indices of the planes:
 - determine the origin, make sure that the planes do not pass through the origin
 - determine the intercepts on the axes in terms of the lattice constant a , b and c
 - write down the intercepts in terms of the numbers of the lattice constant

- take the reciprocal of these numbers
- multiply or divide the reciprocal to reduce them to usually smallest three integers
- the integers are enclosed in parentheses (hkl)
- again, negative indices are represented by a bar over the appropriate index

Example 2.2

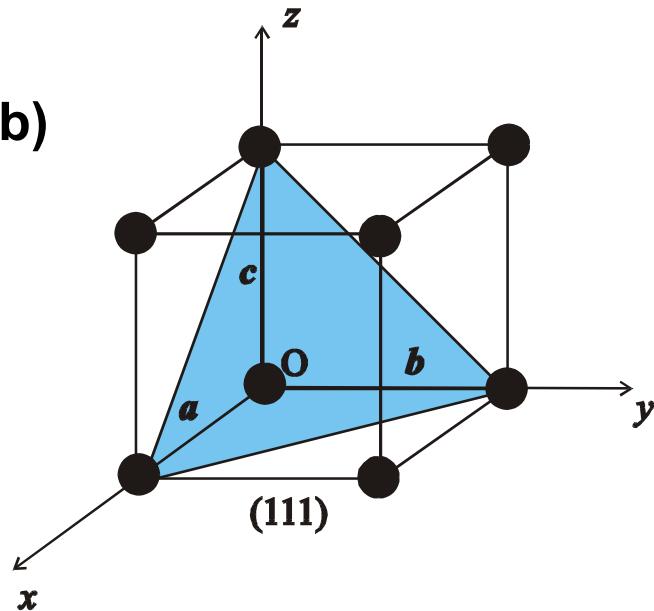
(a)



(100) plane (origin at O)

	x	y	z
Intercepts	$1a$	∞b	∞c
Intercepts (numbers only)	1	∞	∞
Reciprocal	1	0	0
Reduction	1	0	0
Enclosure	(100)		

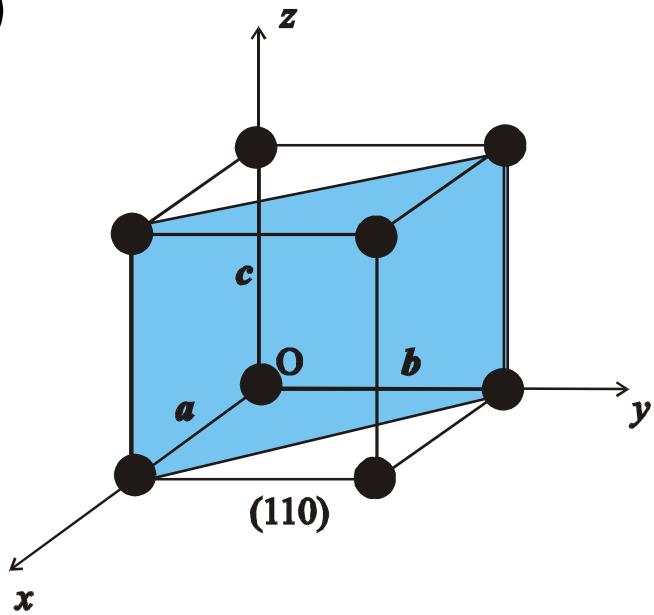
(b)



(111) plane (origin at O)

	x	y	z
Intercepts	$1a$	$1b$	$1c$
Intercepts (numbers only)	1	1	1
Reciprocal	1	1	1
Reduction	1	1	1
Enclosure	(111)		

(c)



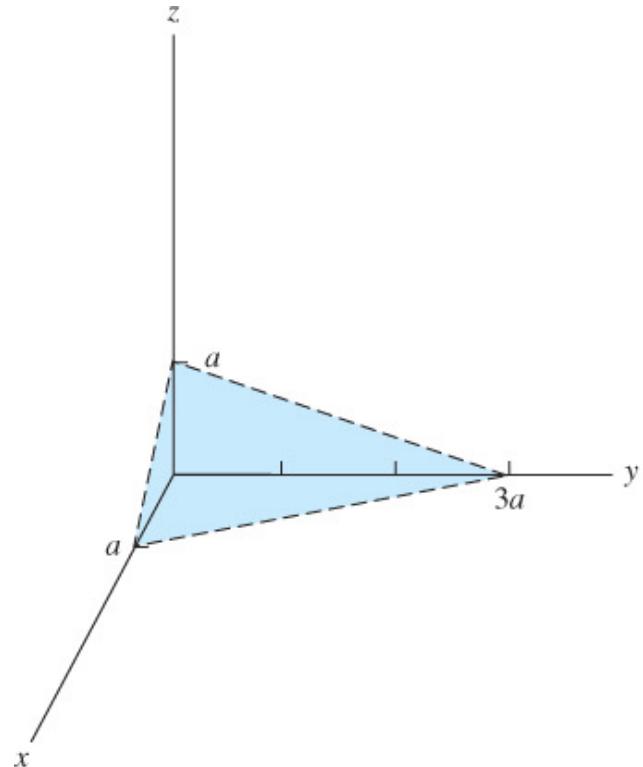
(110) plane (origin at O)

	x	y	z
Intercepts	$1a$	$1b$	∞c
Intercepts (numbers only)	1	1	∞
Reciprocal	1	1	0
Reduction	1	1	0
Enclosure	(110)		

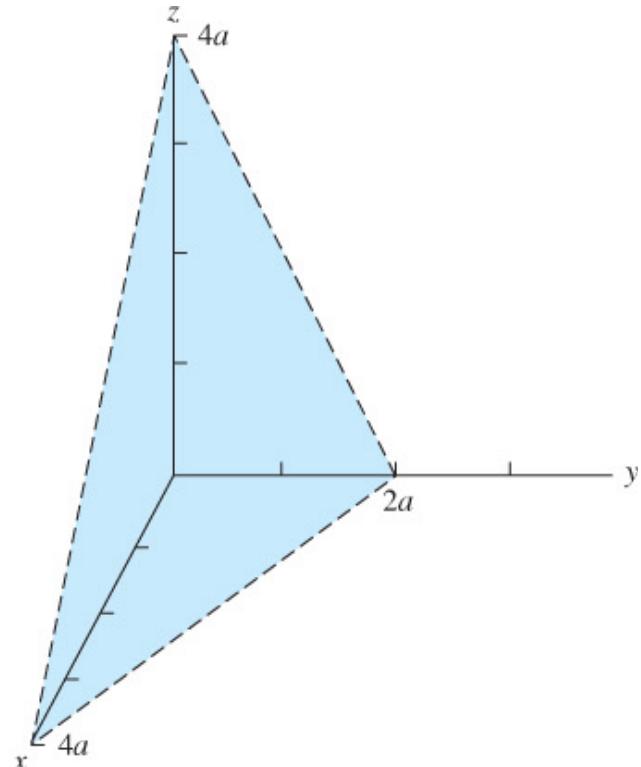
Silicon wafer surface is classified as (100) or (111)

Problem 1

Determine the Miller indices for the planes shown below. [1.16]



(a)



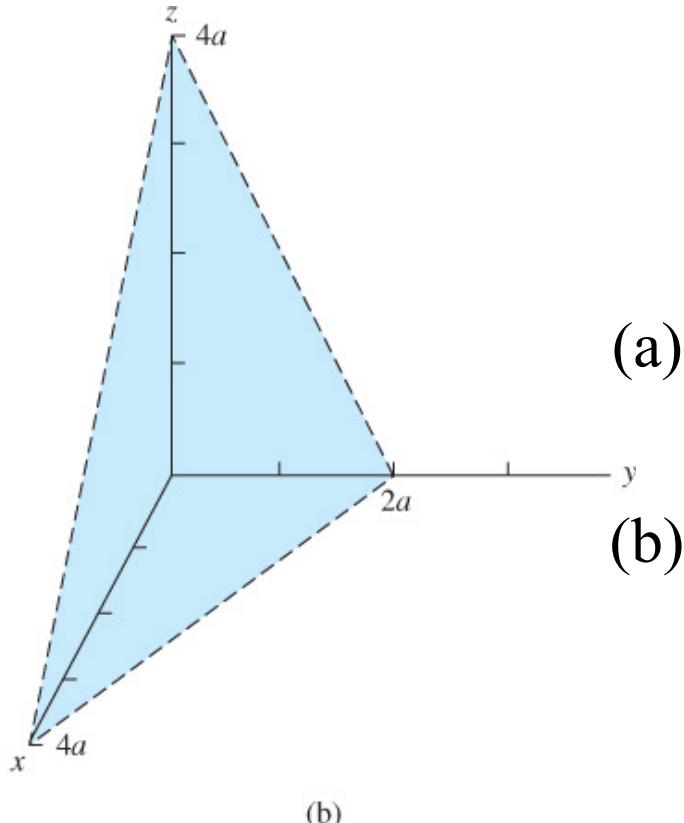
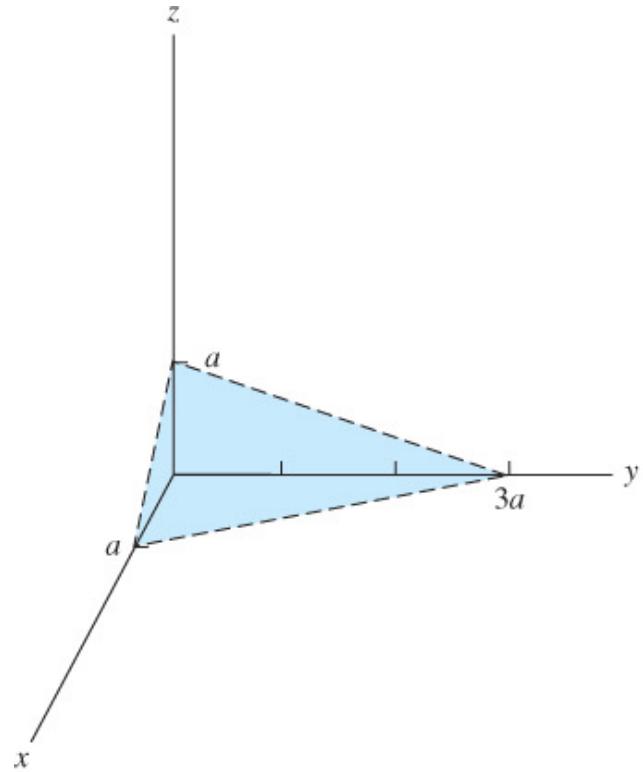
(b)

Figure P1.16 | Figure for Problem 1.16.



Problem 1

Determine the Miller indices for the planes shown below. [1.16]

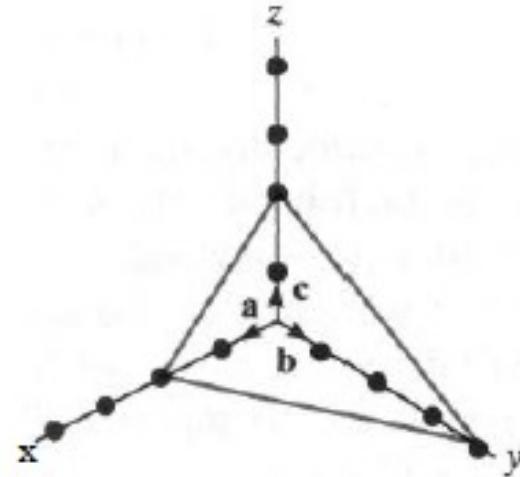
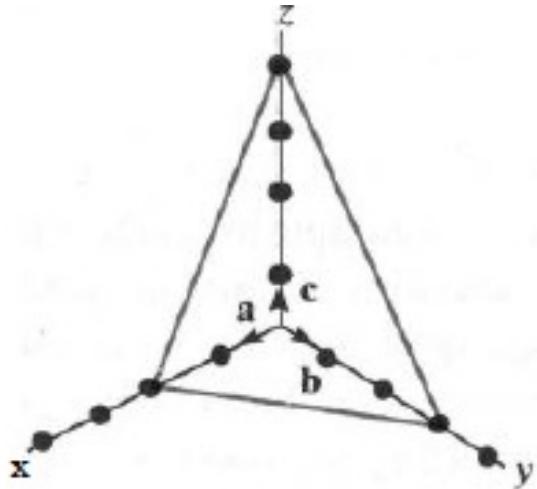


$$(a) \left(\frac{1}{1}, \frac{1}{3}, \frac{1}{1} \right) \Rightarrow (313)$$
$$(b) \left(\frac{1}{4}, \frac{1}{2}, \frac{1}{4} \right) \Rightarrow (121)$$

Figure P1.16 | Figure for Problem 1.16.

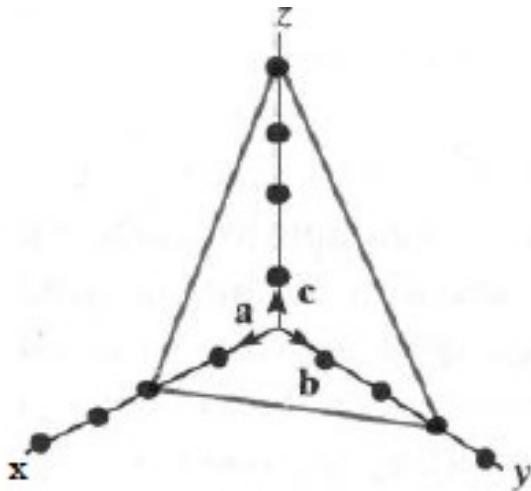
Problem 2

Determine the Miller indices for the planes shown below.

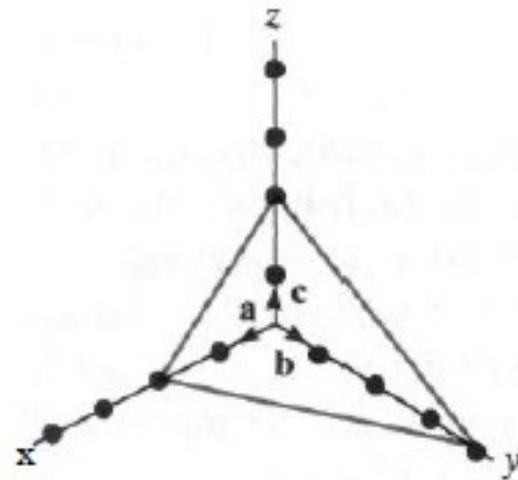


Problem 2

Determine the Miller indices for the planes shown below.



x	y	z
2	3	4
1/2	1/3	1/4
6	4	3



x	y	z
2	4	2
1/2	1/4	1/2
2	1	2

How do you determine the Miller indices for a plane that intercepts the origin?

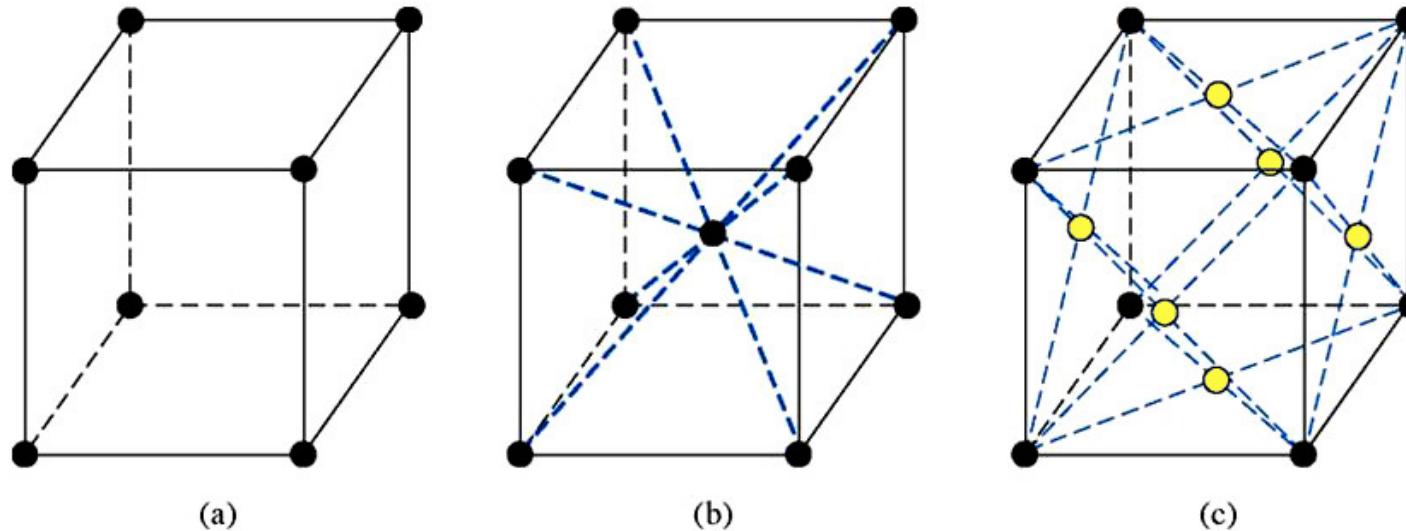
Key takeaways (Lecture #3)

- Types of solid:
 - Amorphous, poly-crystalline, crystalline
- A unit cell is a small volume of crystal that can be used to reproduce the entire crystal.
- A crystallographic direction is defined as a line between two points, a vector.
- Planes in a crystal are specified by Miller indices.

Lecture 4

2.4 Basic Crystal Structures

Three simple structures are shown in Fig. 2.6:



Three lattice types: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic

<http://www.dawgsdk.org/crystal/en/library/>

Fig. 2.6

The vectors \mathbf{a} , \mathbf{b} and \mathbf{c} of the unit cells are perpendicular to each other and have equal lengths.

- for simple cubic crystal structure
 - *one lattice point located at each corner of the cube*
- for body-centered cubic crystal structure
 - *one lattice point located at each corner of the cube & an additional lattice point at the center of the cube*
- for face-centered cubic crystal structure
 - *one lattice point located at each corner of the cube & additional lattice points on each face plane*

- To have a crystal, one or more atoms/molecules can be placed identically at each lattice point
- Length of the cube side is termed as the **lattice constant**
- By knowing the crystal structure & the lattice dimensions, we are able to determine the *surface density* (# atoms/cm²) & *volume density* of atoms (# atoms/cm³)

Problems

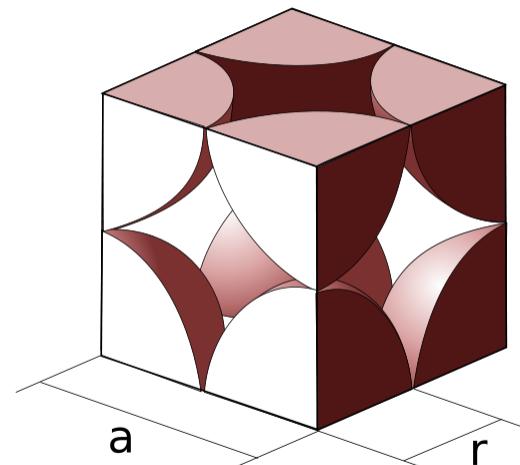
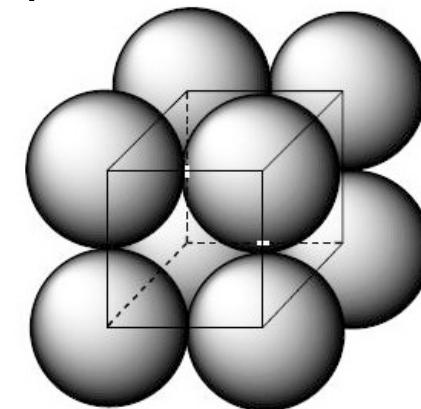
Q1: The volume density of atoms for a simple cubic lattice is $4 \times 10^{22} \text{ cm}^{-3}$. Assume that the atoms are hard spheres with each atom touching its nearest neighbor. Determine the lattice constant and the radius of the atom. (TYU 1.1)

$$\text{Number of atoms per unit cell} = 8 \times \frac{1}{8} = 1$$

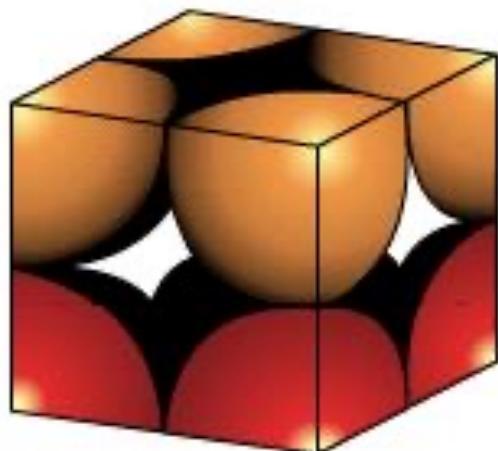
$$\text{Volume Density} = 4 \times 10^{22} = \frac{1}{a^3}$$

$$\Rightarrow a = 2.92 \times 10^{-8} \text{ cm} = 2.92 \text{ } \overset{\circ}{\text{\AA}}$$

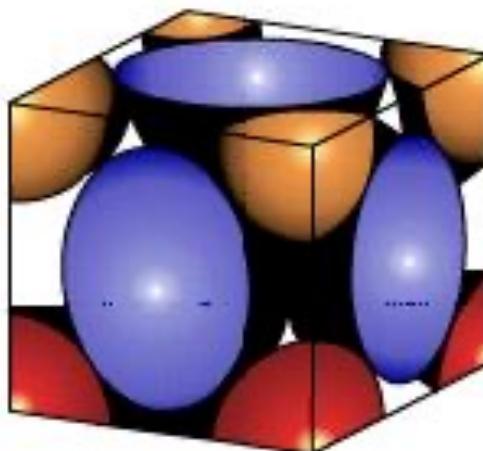
$$\text{Radius} = r = a/2 = 1.46 \text{ } \overset{\circ}{\text{\AA}}$$



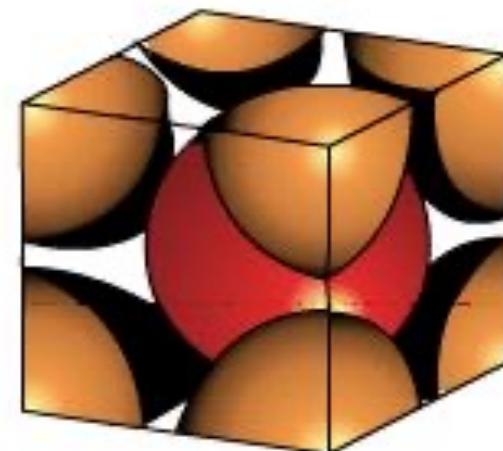
Effective number of atom



(a) Simple cubic



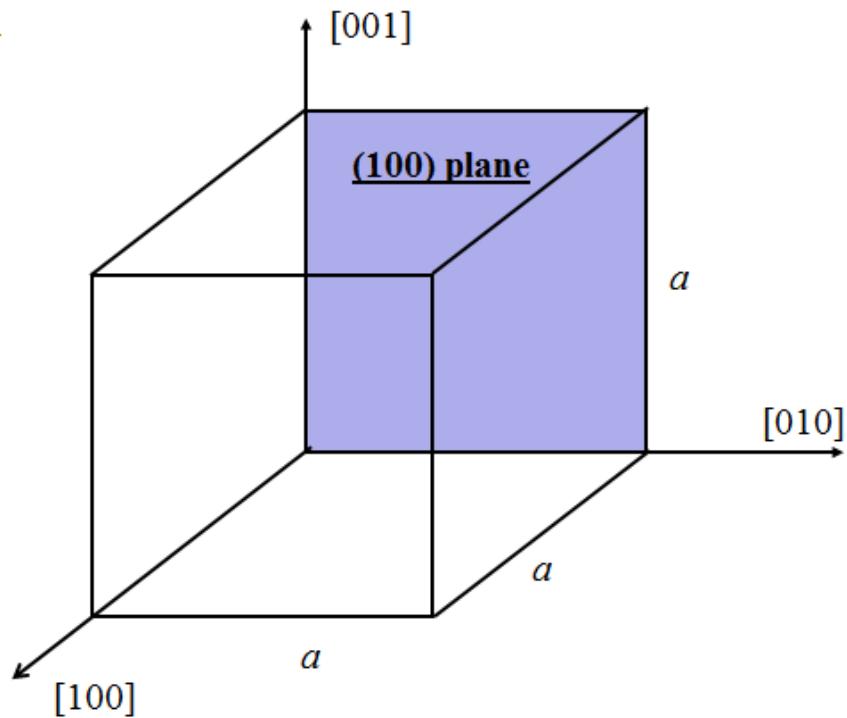
(b) Face centred cubic



(c) Body centred cubic

Three dimensional view showing the number of atoms per unit cell

Q2: Consider a simple cubic structure with a lattice constant of $a = 4.56\text{\AA}$. Determine the surface density of atoms in the (a) (100) plane, (b) (110), plane and (c) (111) plane. (TYU 1.2)



Number of atoms per (100) lattice plane

$$= 4 \times \frac{1}{4} = 1$$

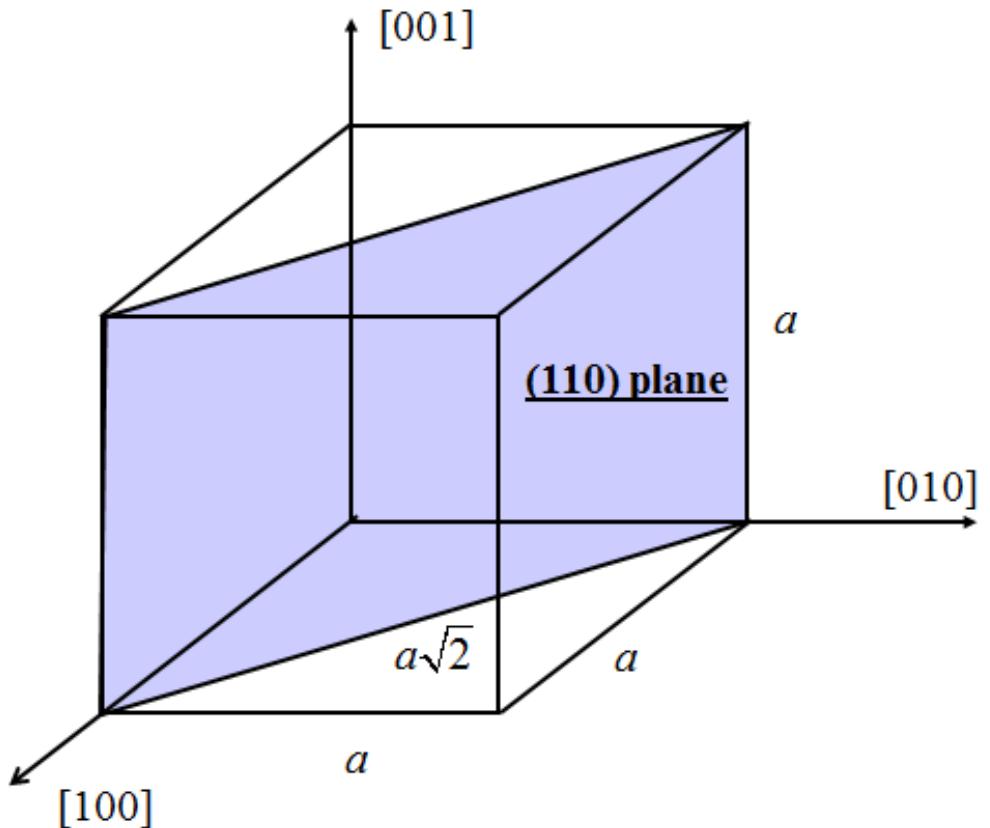
$$\begin{aligned}\text{Surface Density} &= \frac{1}{a^2} = \frac{1}{(4.65 \times 10^{-8})^2} \\ &= 4.62 \times 10^{14} \text{ cm}^{-2}\end{aligned}$$

(b) Number of atoms per (110) lattice plane

$$= 4 \times \frac{1}{4} = 1$$

Surface Density

$$\begin{aligned} &= \frac{1}{(a)(a\sqrt{2})} = \frac{1}{(4.65 \times 10^{-8})^2 \sqrt{2}} \\ &= 3.27 \times 10^{14} \text{ cm}^{-2} \end{aligned}$$



(c) Number of atoms per (111) lattice plane

$$= 3 \times \frac{1}{6} = \frac{1}{2}$$

$$\text{Lattice plane area} = \frac{1}{2} b h$$

$$\text{where } b = a\sqrt{2}$$

$$h = \left[(a\sqrt{2})^2 - \left(\frac{1}{2} a\sqrt{2} \right)^2 \right]^{1/2}$$

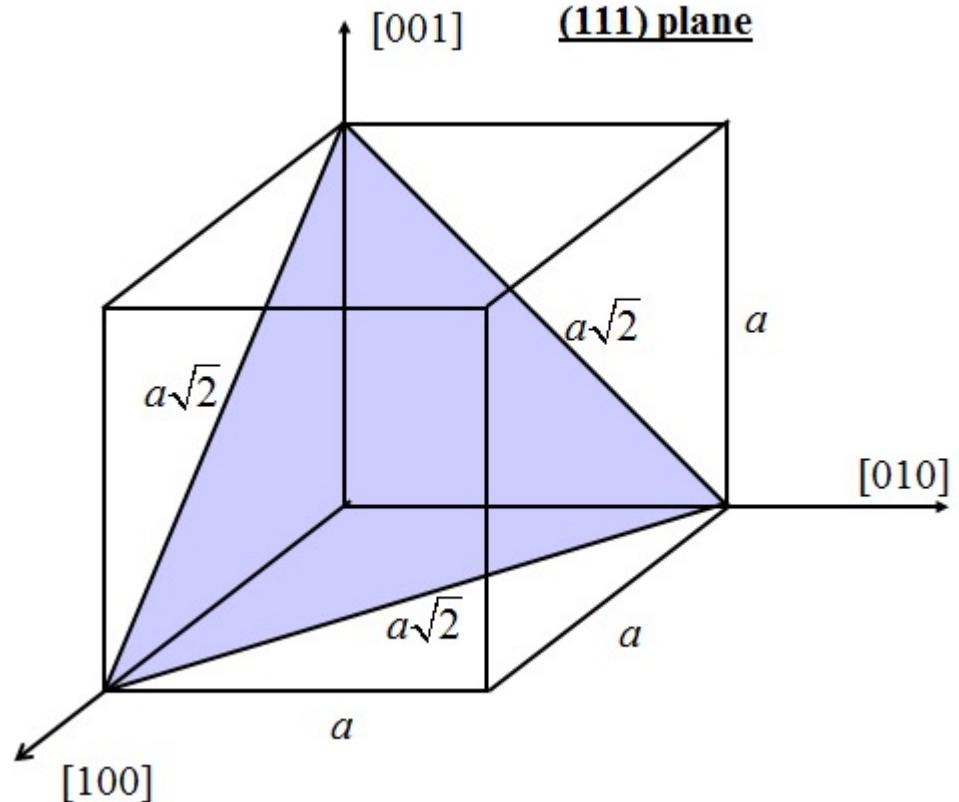
$$= \left[2a^2 - \frac{1}{2}a^2 \right]^{1/2} = a\sqrt{\frac{3}{2}}$$

Then lattice plane area

$$= \frac{1}{2} \left(a\sqrt{2} \right) \left(a\sqrt{\frac{3}{2}} \right) = \frac{\sqrt{3}}{2} a^2$$

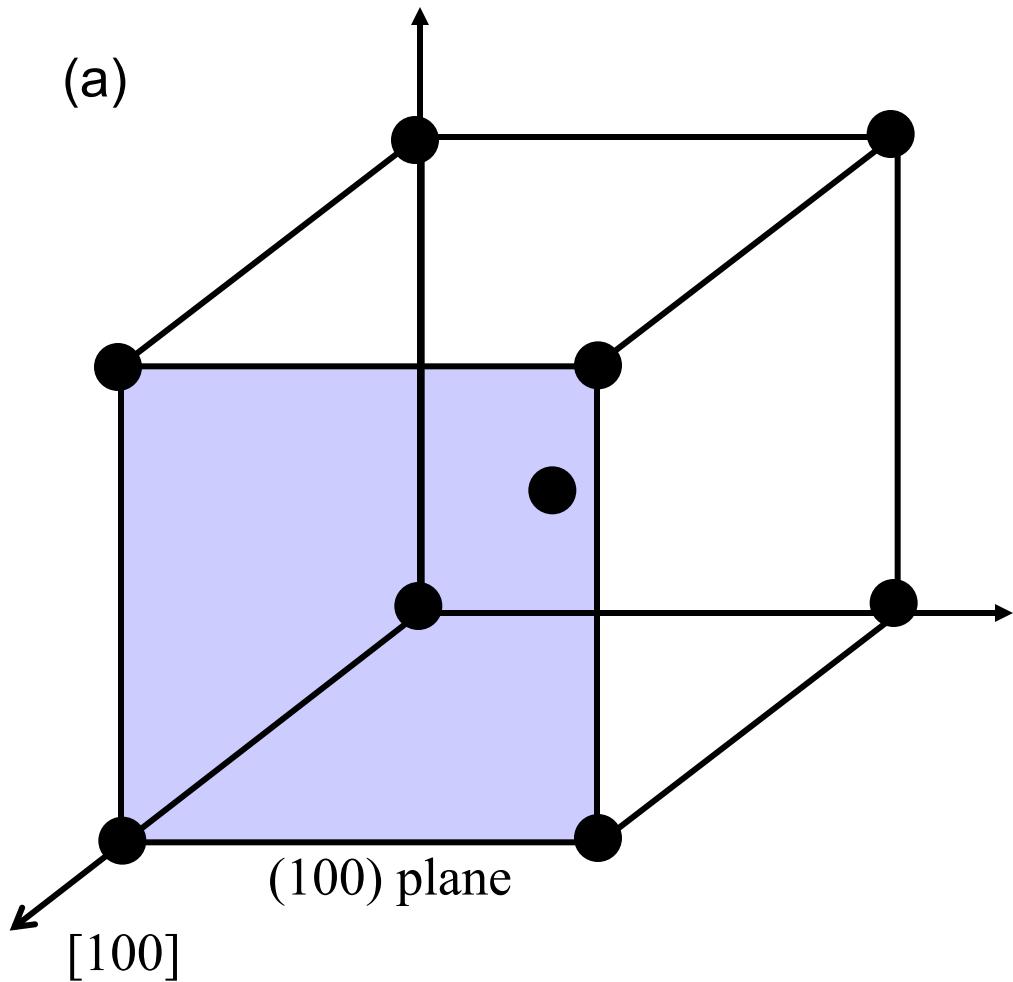
Surface Density

$$= \frac{\frac{1}{2}}{\frac{\sqrt{3}}{2} (4.65 \times 10^{-8})^2} = 2.67 \times 10^{14} \text{ cm}^{-2}$$

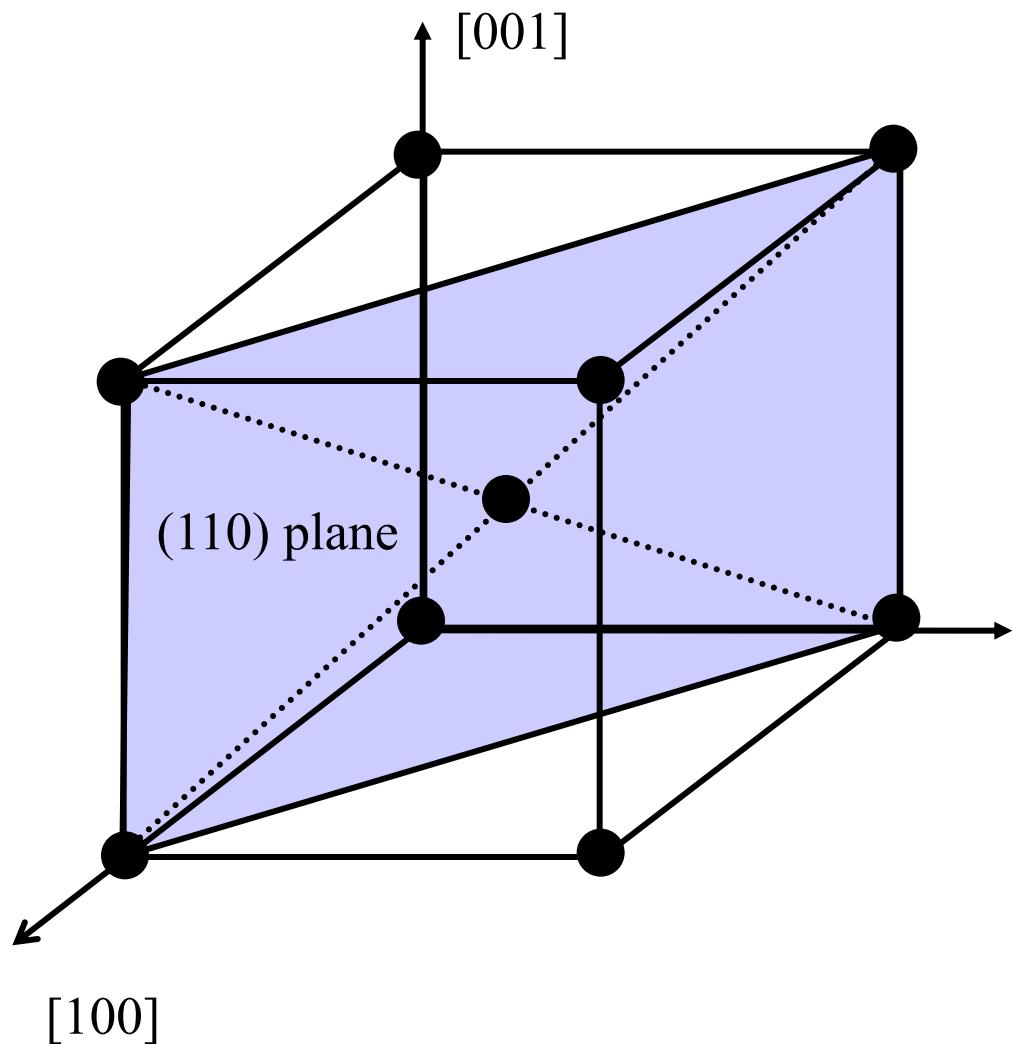


For SC, (100) has the highest surface density of atoms. How about BCC and FCC? (See Tutorial 1)

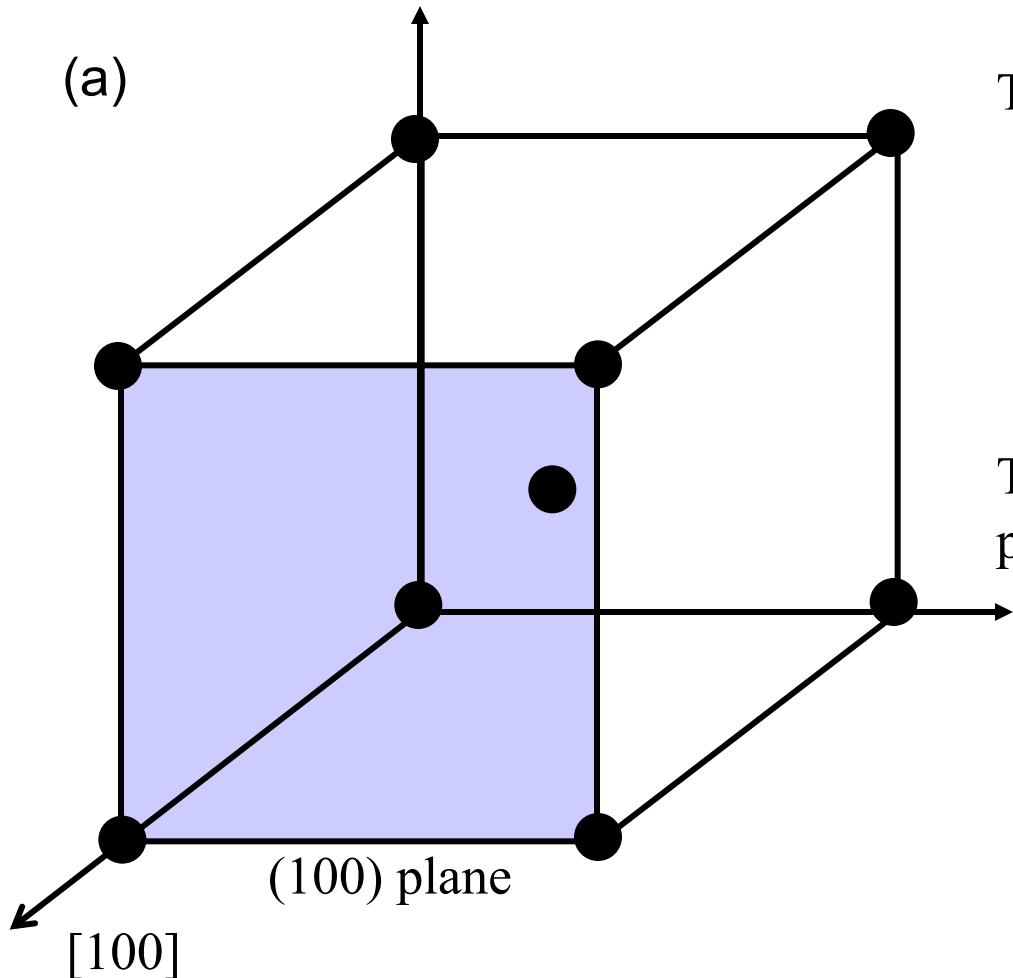
Q3. The lattice constant of a body-centered cubic structure is 4 Å. Calculate the surface density of atoms for (a) a (100) plane and (b) a (110) plane.



(b)



Q3. The lattice constant of a body-centered cubic structure is 4 Å. Calculate the surface density of atoms for (a) a (100) plane and (b) a (110) plane.



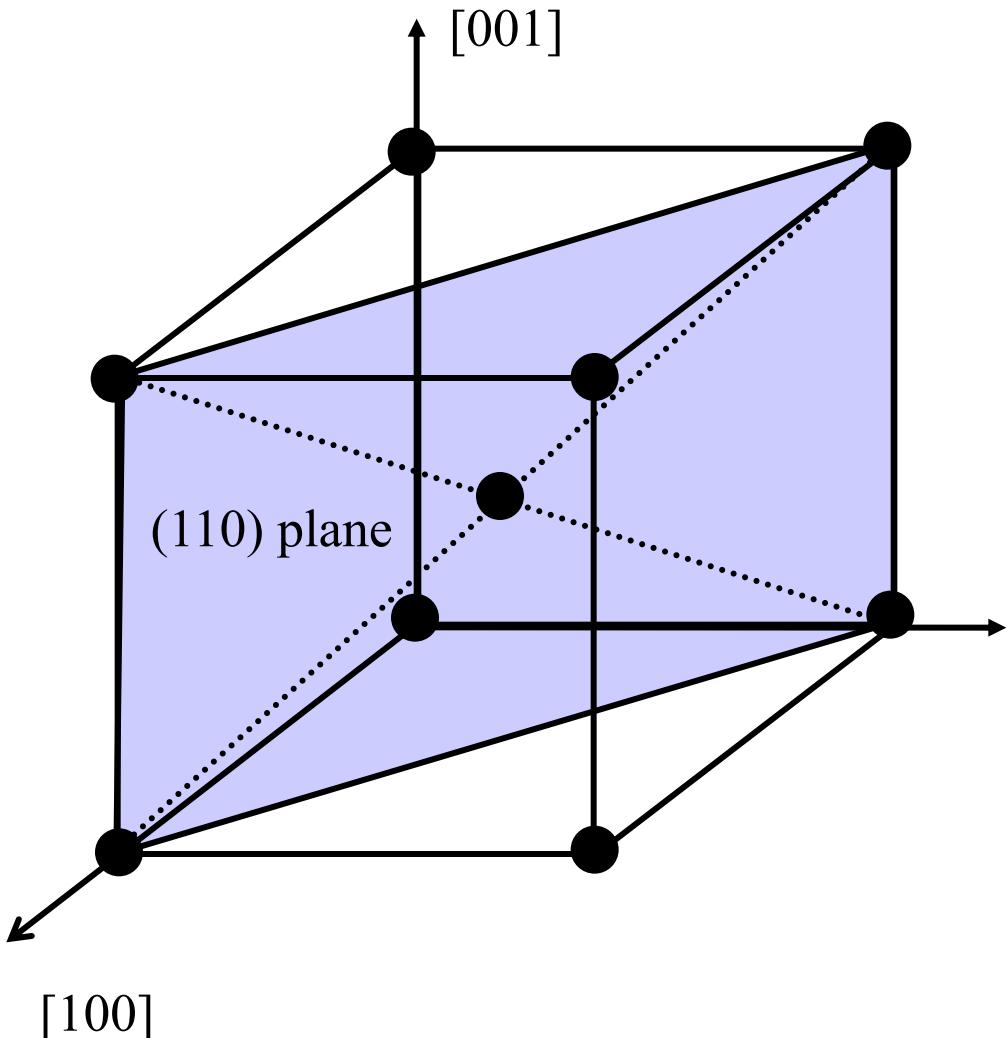
The surface area of (100) plane =

$$(4 \times 10^{-8})^2 = 1.6 \times 10^{-15} \text{ cm}^2$$

The surface density of atoms on (100) plane =

$$\frac{4 \times 1/4}{1.6 \times 10^{-15}} = 6.25 \times 10^{14} / \text{cm}^2$$

(b)



The surface area of (110) plane =

$$(4 \times 10^{-8}) (4\sqrt{2} \times 10^{-8}) = 2.26 \times 10^{-15} \text{ cm}^2$$

The surface density of atoms on (110) plane =

$$\frac{4 \times 1/4 + 1}{2.26 \times 10^{-15}} = 8.85 \times 10^{14} / \text{cm}^2$$

2.5 Semiconductor Crystals

Fig. 2.7 shows diamond crystal structure

- Silicon and Germanium have this structure
- All atoms are of the same species
- Any atom within the diamond structure will have four nearest neighboring atoms
 - they are bonded by covalent bonding

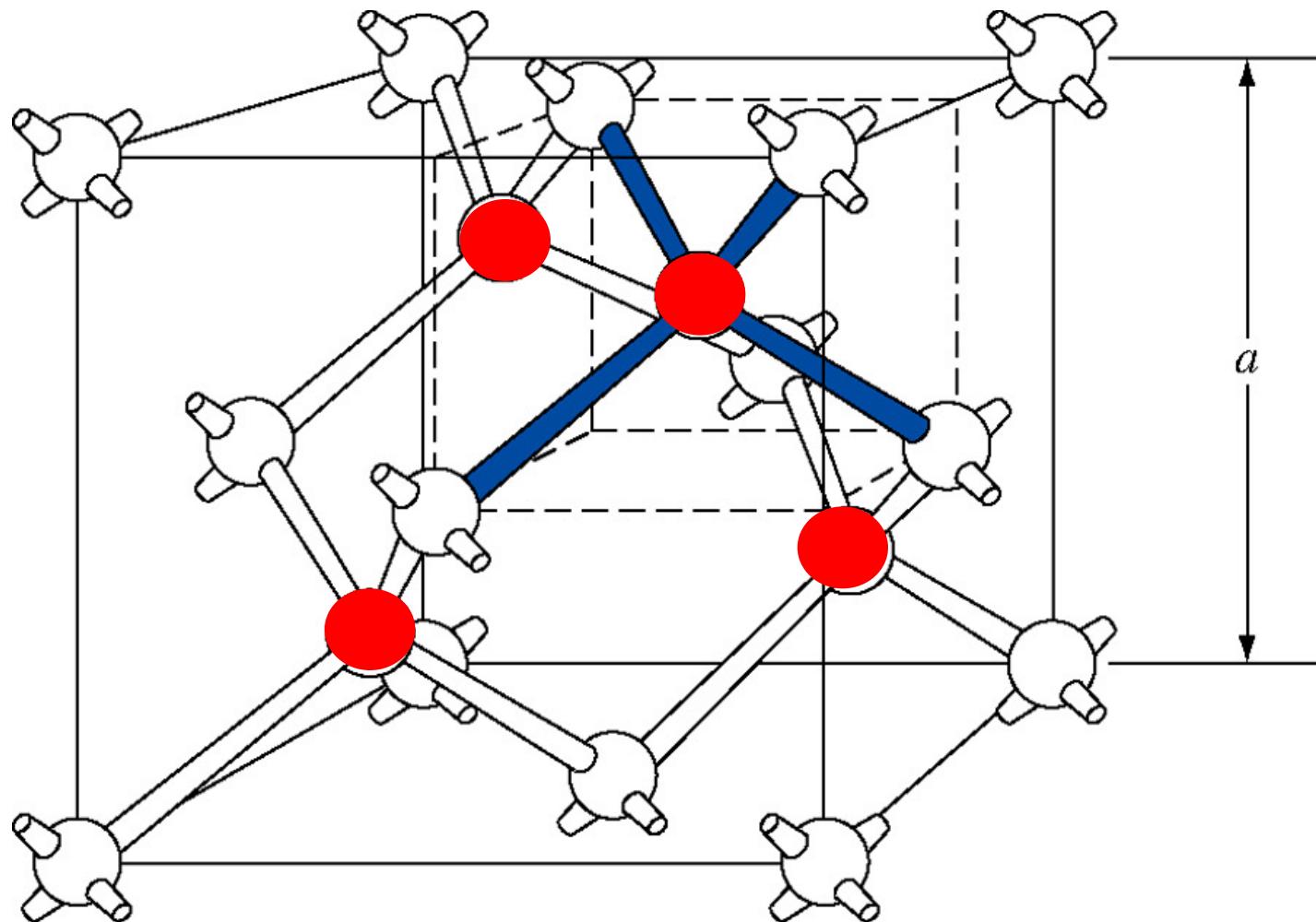


Fig. 2.7 The diamond structure

<http://www.dawgsdk.org/crystal/en/library/>

- Silicon crystal can be regarded as a face-centered cubic structure with 2 silicon (Si) atoms at each lattice point
 - the relative position of the Si atoms at each lattice point are $(0,0,0)$ and $(a/4,a/4,a/4)$

Fig. 2.8

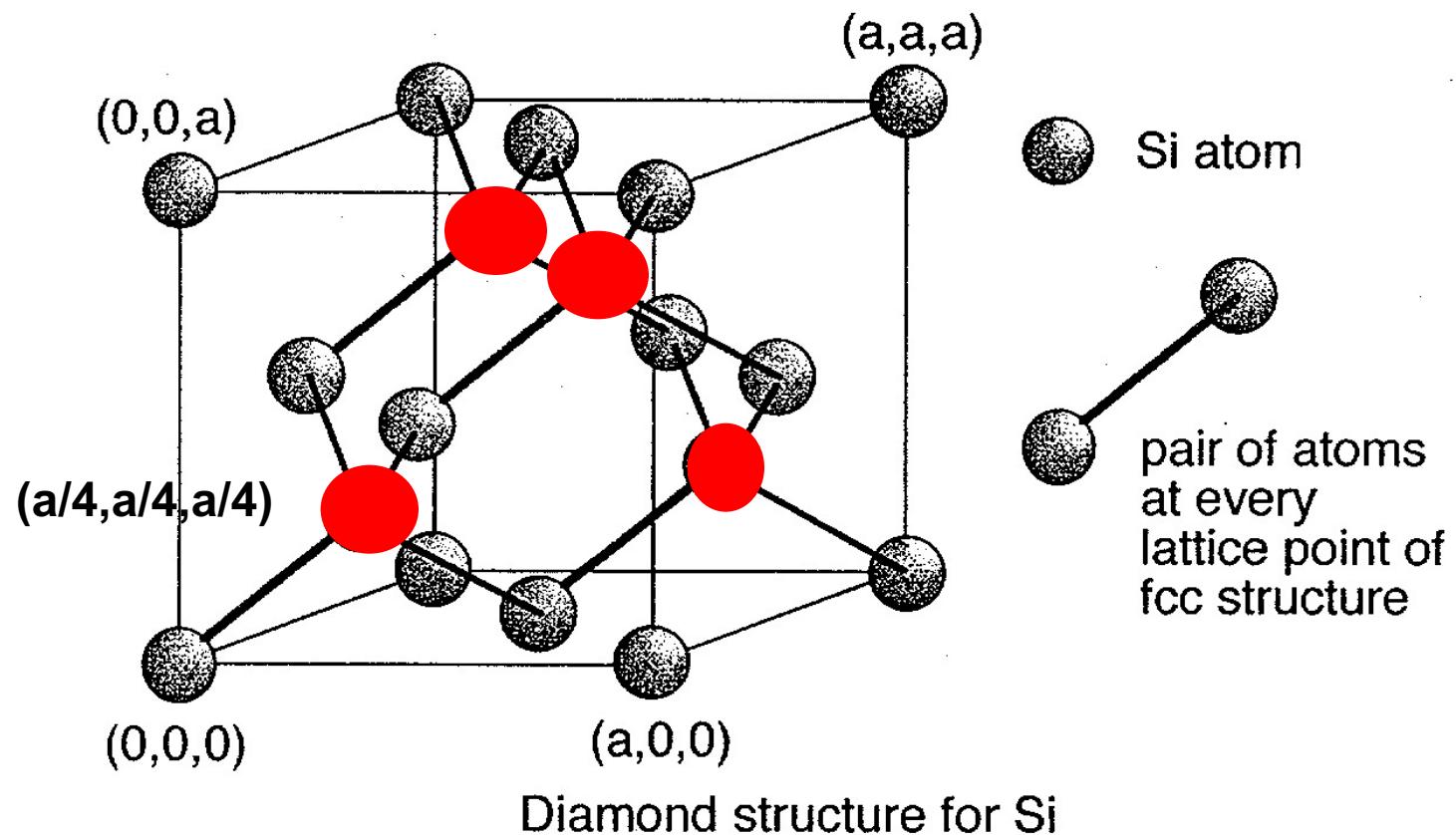


Fig. 2.9 shows a zincblende (sphalerite) crystal structure:

- This structure differs from the diamond structure only in that there are two different types of atoms in the lattice
- Most compound semiconductors, e.g. GaAs (gallium arsenide) and InP (indium phosphide) have this structure
- For a GaAs crystal, each Ga atom has 4 nearest As neighbors and each As atom has 4 nearest Ga neighbors
 - they are bonded by covalent bonding

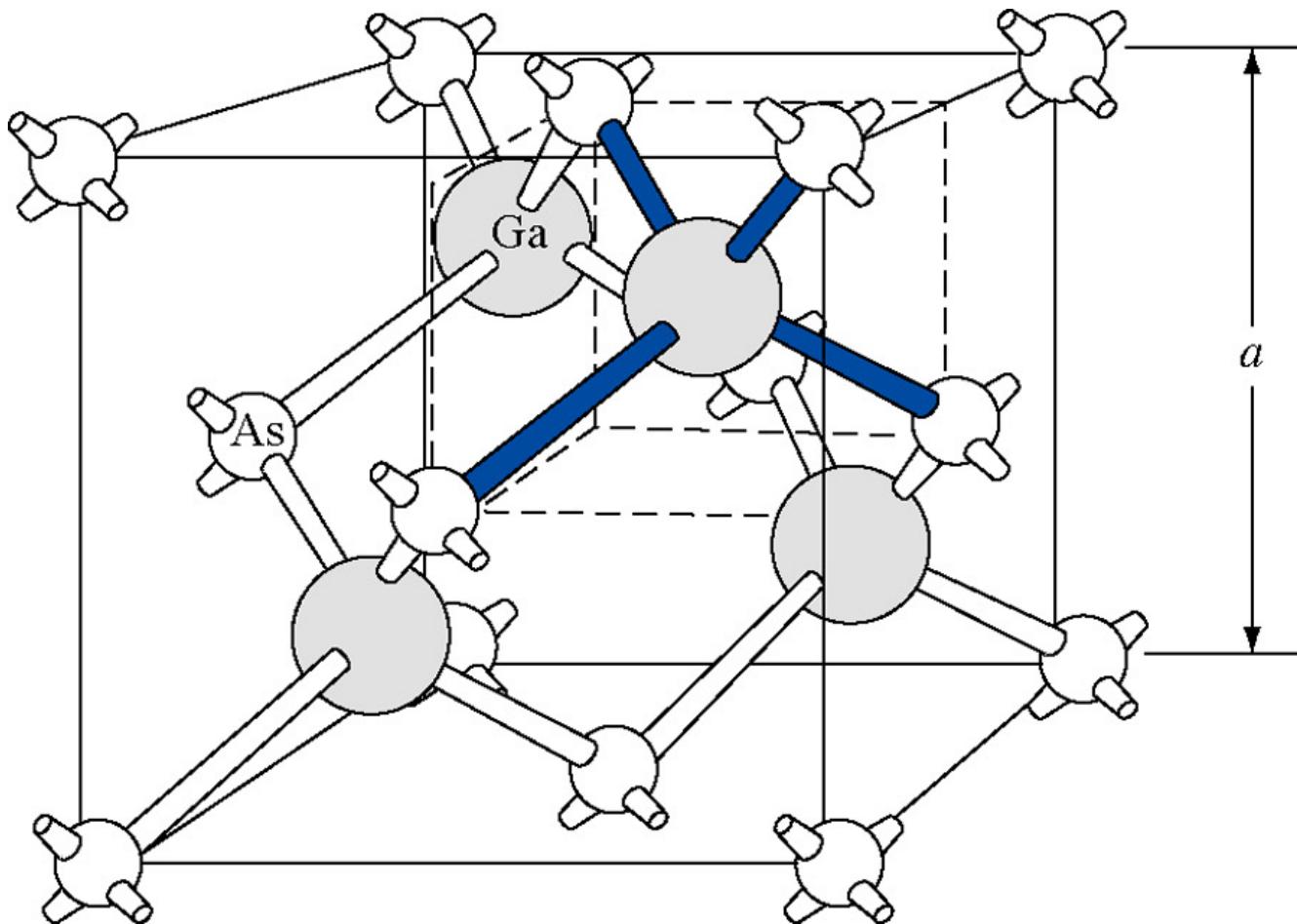
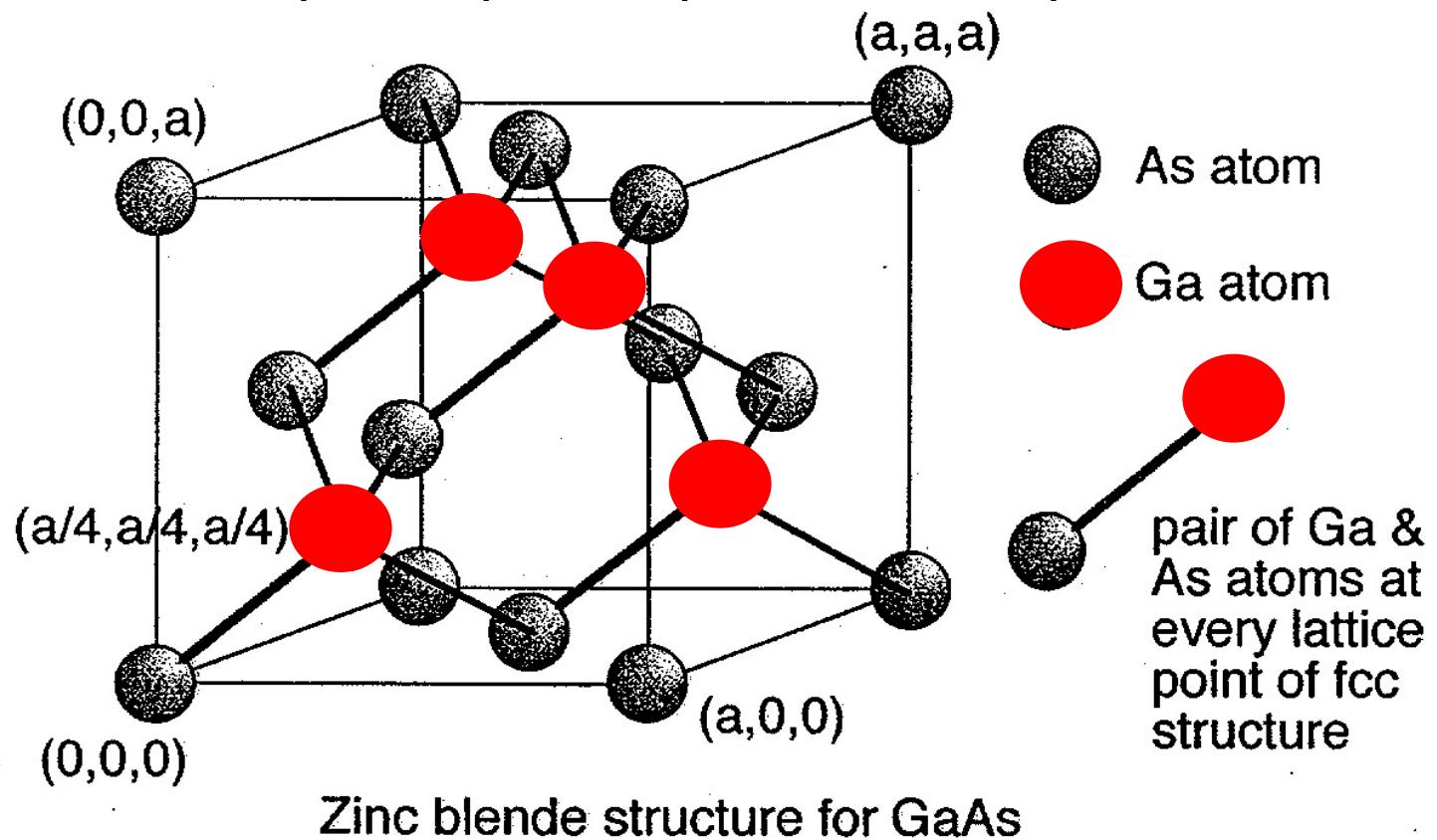


Fig. 2.9 The zincblende (sphalerite) lattice of GaAs

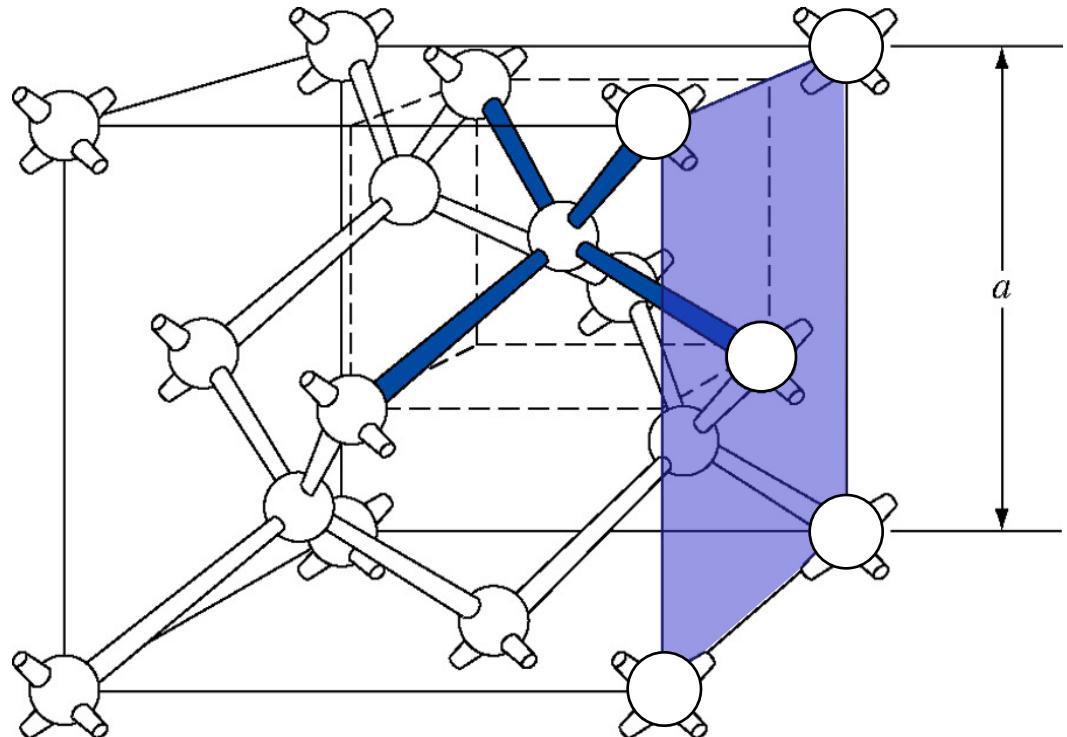
<http://www.dawgsdk.org/crystal/en/library/>

- GaAs crystals can also be considered as face-centered cubic with one Ga atom and one As atom at each lattice point
 - the relative position of the Ga and As atoms at each lattice point are $(0,0,0)$ and $(a/4,a/4,a/4)$

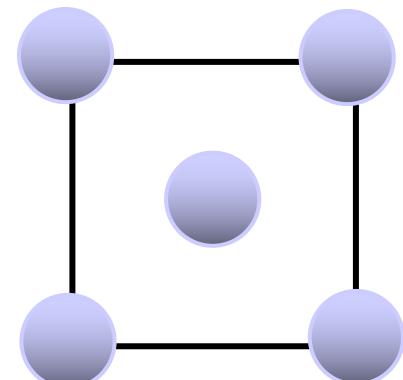


Example 2.3

Calculate the surface density of atoms (# atoms/cm²) on the shaded plane [(010) plane] of a silicon crystal shown. The lattice constant for silicon is 5.43Å (1Å = 10⁻¹⁰ m).



The silicon crystal has the face-centered cubic structure. The indicated plane can be redrawn as :



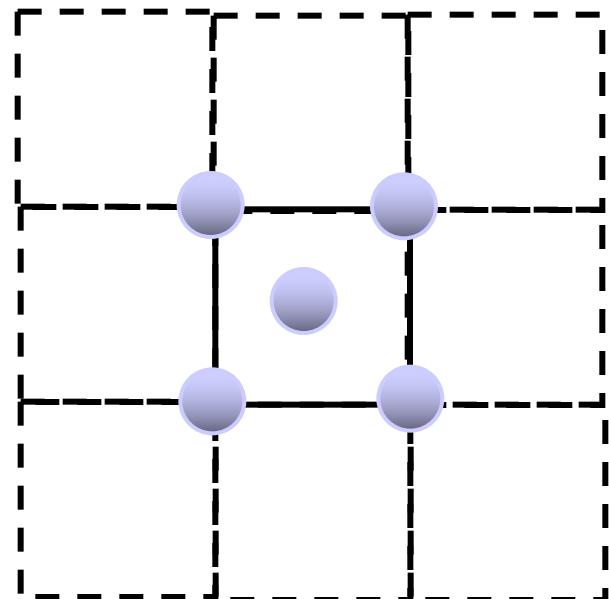
Notice that the atom at each corner is shared by 4 similar equivalent lattice planes, so each corner atom effectively contributes $1/4$ atom to the indicated lattice plane.

The atom in the middle of the plane is not shared by any other plane.

Hence, no. of atoms on the plane is
 $4(1/4) + 1 = 2$ atoms

Therefore,

$$\text{Surface density} = \frac{\text{No. of atoms}}{a^2} = \frac{2}{(5.43 \times 10^{-8} \text{ cm})^2}$$
$$= 6.78 \times 10^{14} \text{ atoms/cm}^2$$



Problems

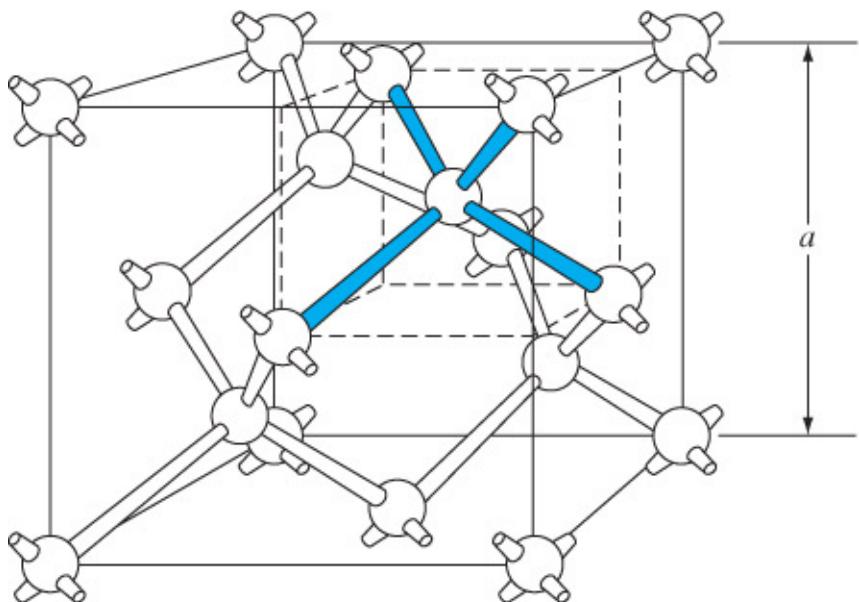


Figure 1.11 | The diamond structure.

Q1: Consider the diamond unit cell shown in Fig. 1.11. Determine the (a) number of corner atoms, (b) number of face-centered atoms, and (c) number of atoms totally enclosed in the unit cell. (TYU 1.4)

- (a) 8 corner atoms
- (b) 6 face-centered atoms
- (c) 4 atoms totally enclosed

Q2: The lattice constant of silicon is 5.43Å. Calculate the volume density of silicon atoms.

Number of atoms in the unit cell

$$= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$$

$$\begin{aligned}\text{Volume Density} &= \frac{8}{a^3} = \frac{8}{(5.43 \times 10^{-8})^3} \\ &= 5 \times 10^{22} \text{ cm}^{-3}\end{aligned}$$

Q3: Calculate the density of valence electrons in silicon. (1.22)

Density of silicon atoms = $5 \times 10^{22} \text{ cm}^{-3}$ and
4 valence electrons per atom, so

Density of valence electrons = $2 \times 10^{23} \text{ cm}^{-3}$

Q4: The structure of GaAs is the zincblende lattice. The lattice constant is 5.65Å. Calculate the valence electrons in GaAs. (1.23)

Density of GaAs atoms

$$= \frac{8}{(5.65 \times 10^{-8})^3} = 4.44 \times 10^{22} \text{ cm}^{-3}$$

An average of 4 valence electrons per atom,

So

Density of valence electrons

$$= 1.77 \times 10^{23} \text{ cm}^{-3}$$

Q5: Calculate the mass density of GaAs. The lattice constant is 5.65Å.

GaAs: $a = 5.65 \cdot 10^{-8}$ cm, 4 each Ga, As atoms/cell

$$\frac{4}{a^3} = \frac{4}{(5.65 \cdot 10^{-8} \text{ cm})^3} = 2.22 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{2.22 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot (69.7 + 74.9) \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 5.33 \frac{\text{g}}{\text{cm}^3}$$

Key takeaways (Lecture #4)

- Three basic types of crystal structure:
 - SC, BCC, FCC
- It is essential to determine the effective number of atoms on a surface and within the unit cell
- Silicon and Germanium both have the diamond structure, while GaAs has the zinc blonde structure