Lecture 2

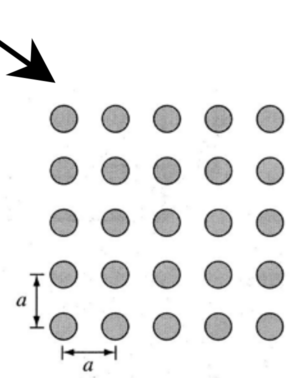
Unit Cells and Miller Indexes

Reading:

(Cont'd) Pierret 1.1, 1.2, 1.4, 2.1-2.6

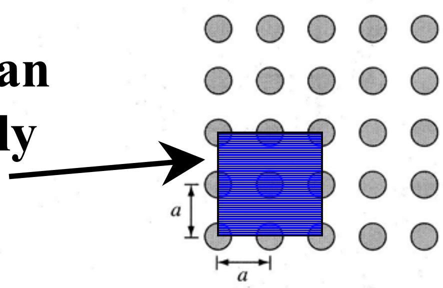
Unit Cell Concept

The crystal lattice consists of a periodic array of atoms.



Unit Cell Concept

A "building block" that can be periodically duplicated to result in the crystal lattice is known as the "unit cell".



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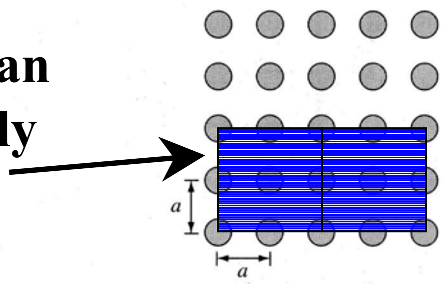

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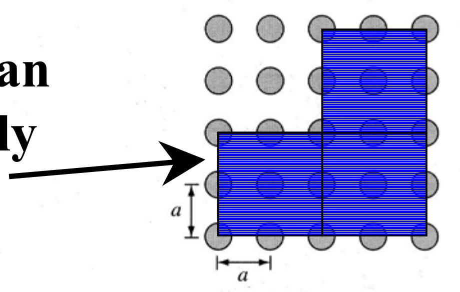

Unit Cell Concept

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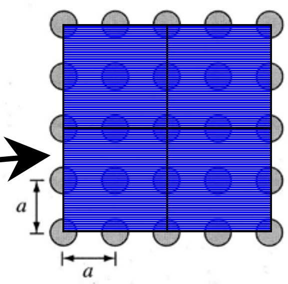
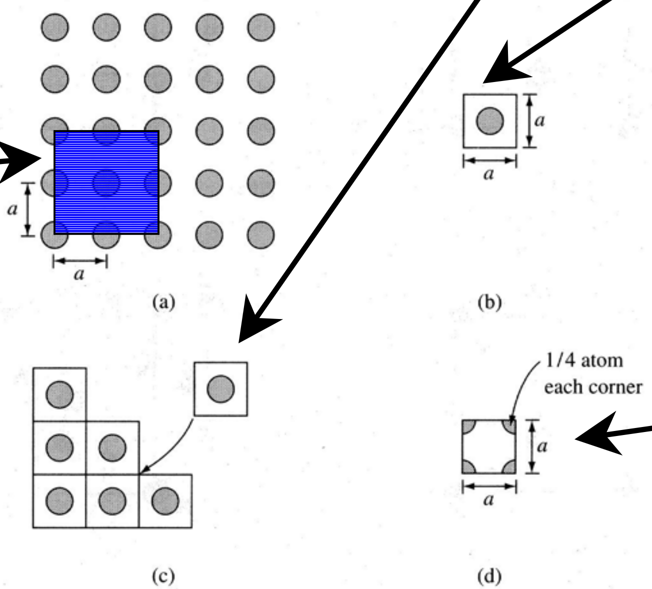


Unit Cell Concept

The crystal lattice consists of a periodic array of atoms.

The smallest "building block" that can be periodically duplicated to result in the crystal lattice is known as the "primative unit cell".

A "building block" that can be periodically duplicated to result in the crystal lattice is known as the "unit cell".



The unit cell may not be unique.

Figure 1.2 Introduction to the unit cell method of describing atomic arrangements within crystals. (a) Sample two-dimensional lattice. (b) Unit cell corresponding to the part (a) lattice. (c) Reproduction of the original lattice. (d) An alternative unit cell.

Unit Cell Concept

Lattice Constant: A length that describes the unit cell. It is normally given in Å, angstroms = 1e-10 meters.

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Diamond Structure: Constructed by 2 "inter-penetrating" FCC Lattices

QuickTime Movie

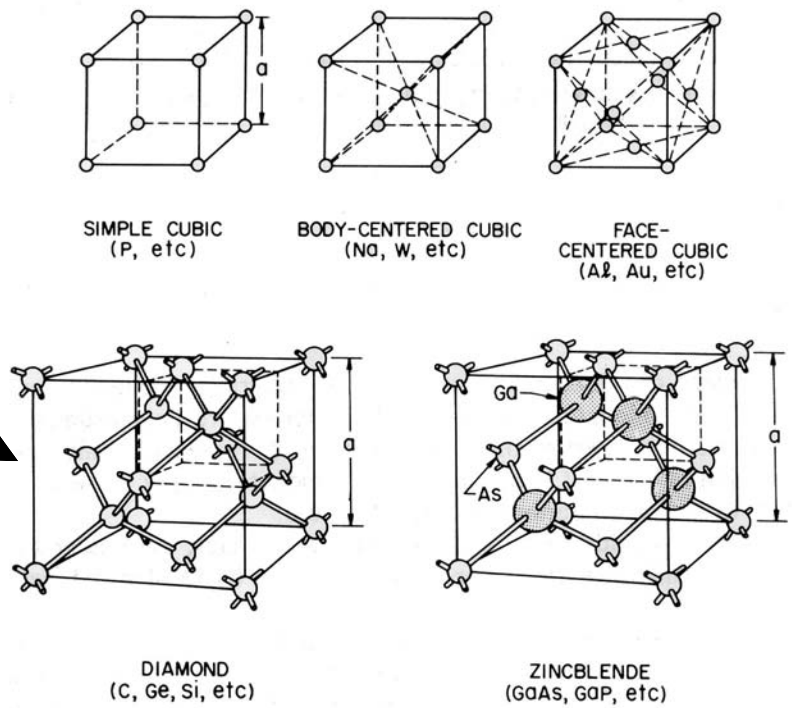


Fig. 1 Some important unit cells (direct lattices) and their representative elements or compounds; a is the lattice constant.

Zincblende is a diamond structure with every other atom a different element. Example: Ga only bonds to As and As only bonds to Ga.

Unit Cell Concept

Some unit cells have hexagonal symmetry.

Rocksalt unit cells are one of the simplest practical unit cells.

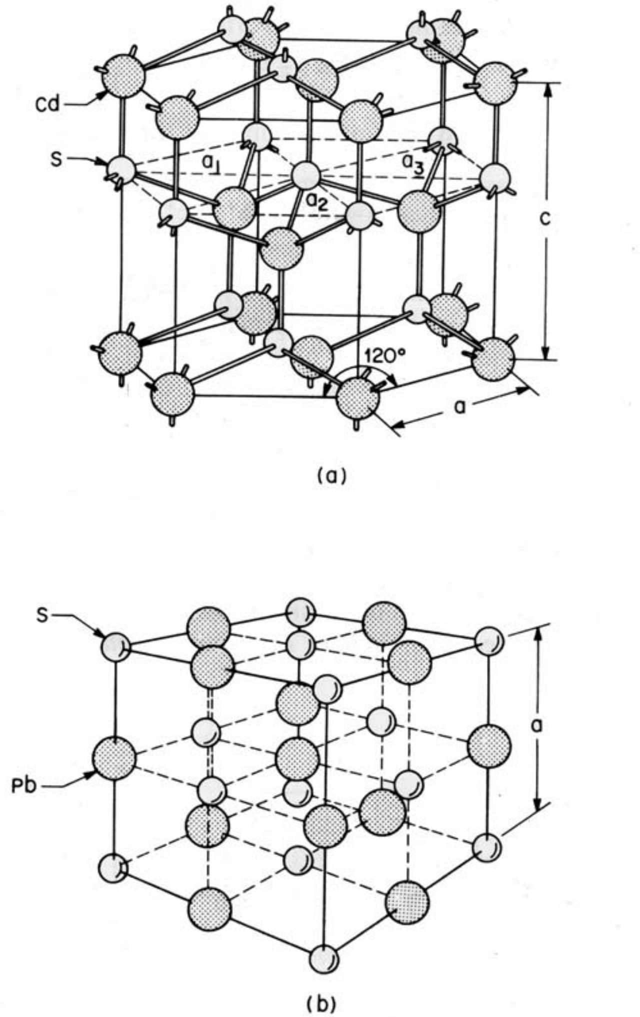
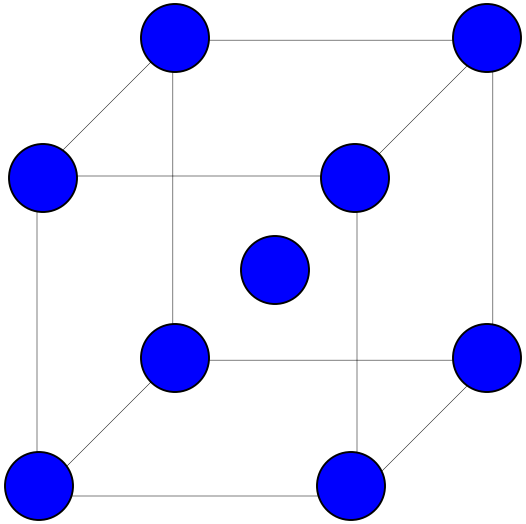


Fig. 2 Two unit cells of compound semiconductors. (*a*) Wurtzite lattice (CdS, ZnS, etc.). (*b*) Rock-salt lattice (PbS, PbTe, etc.).

Atomic Density

What is the atomic density of a BCC material with lattice constant 5.2 angstroms?

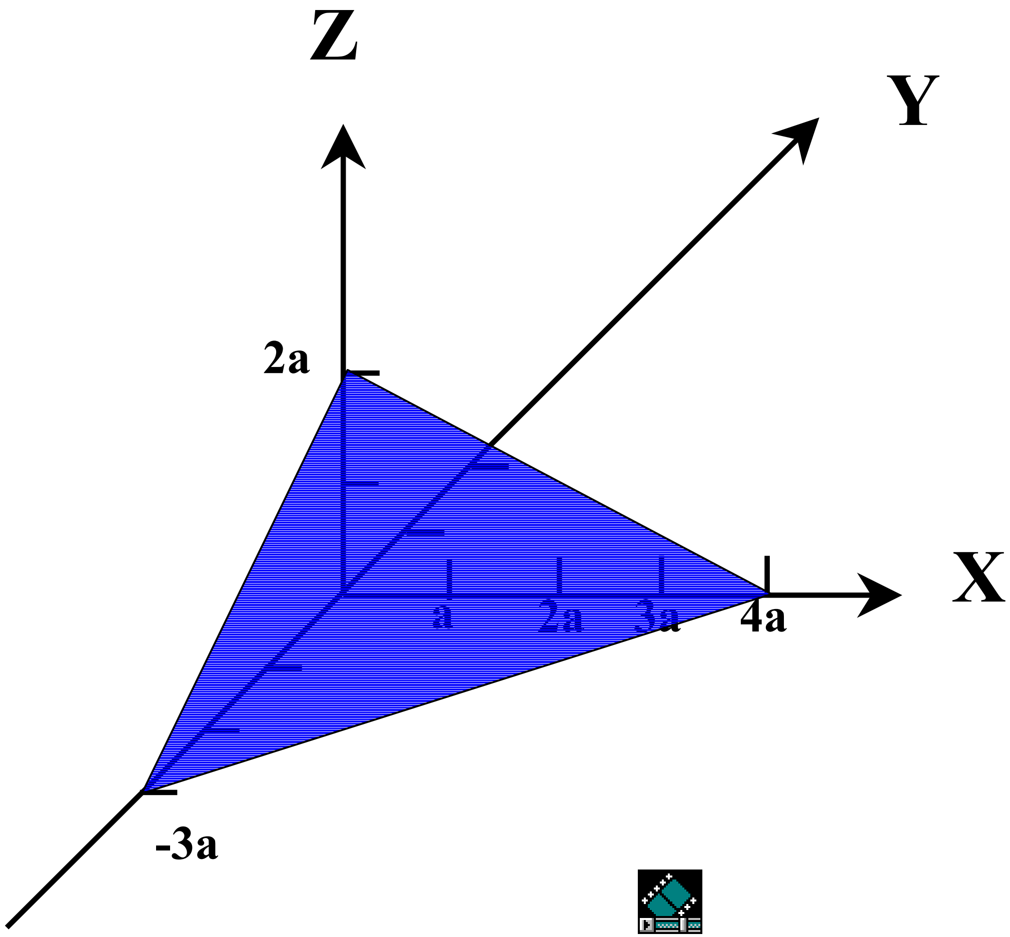


$$Number\ of\ \ Atoms\ \ per\ unit\ cell = 2$$

$$Volume\ of\ \ unit\ cell = a^3 = (5.2e-8\ cm)^3 = 1.41e-22\ cm^3$$

$$Density = \frac{Number\ of\ \ Atoms\ \ per\ unit\ cell}{Volume\ of\ \ unit\ cell} = 1.4e22\ \frac{atoms}{cm^3}$$

Crystalline Planes and Miller Indices



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Identify Intercepts in x,y,z order = 4a, -3a, 2a

Divide by unit cell length in each direction x,y,z order = 4, -3, 2

Invert the values = 1/4, -1/3, 1/2

Multiply by a number (12 in this example) to give smallest whole number set = 3, -4, 6

Place any minus signs over their index and place set in parenthesis = $(3\bar{4}6)$

Crystalline Planes and Miller Indices: Planes and directions

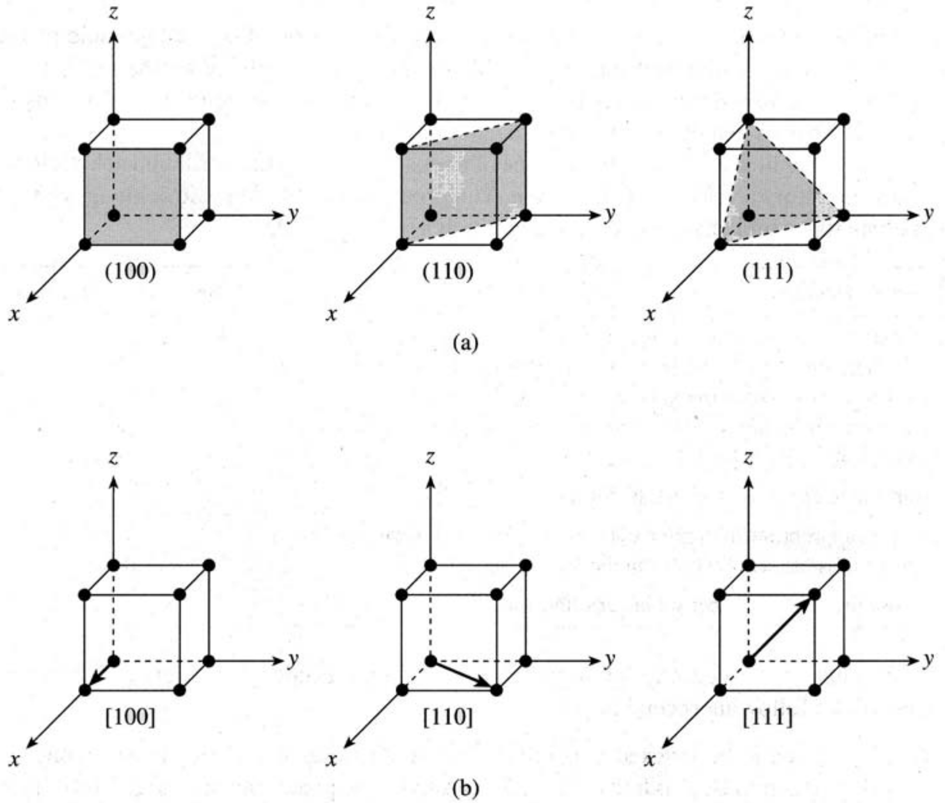
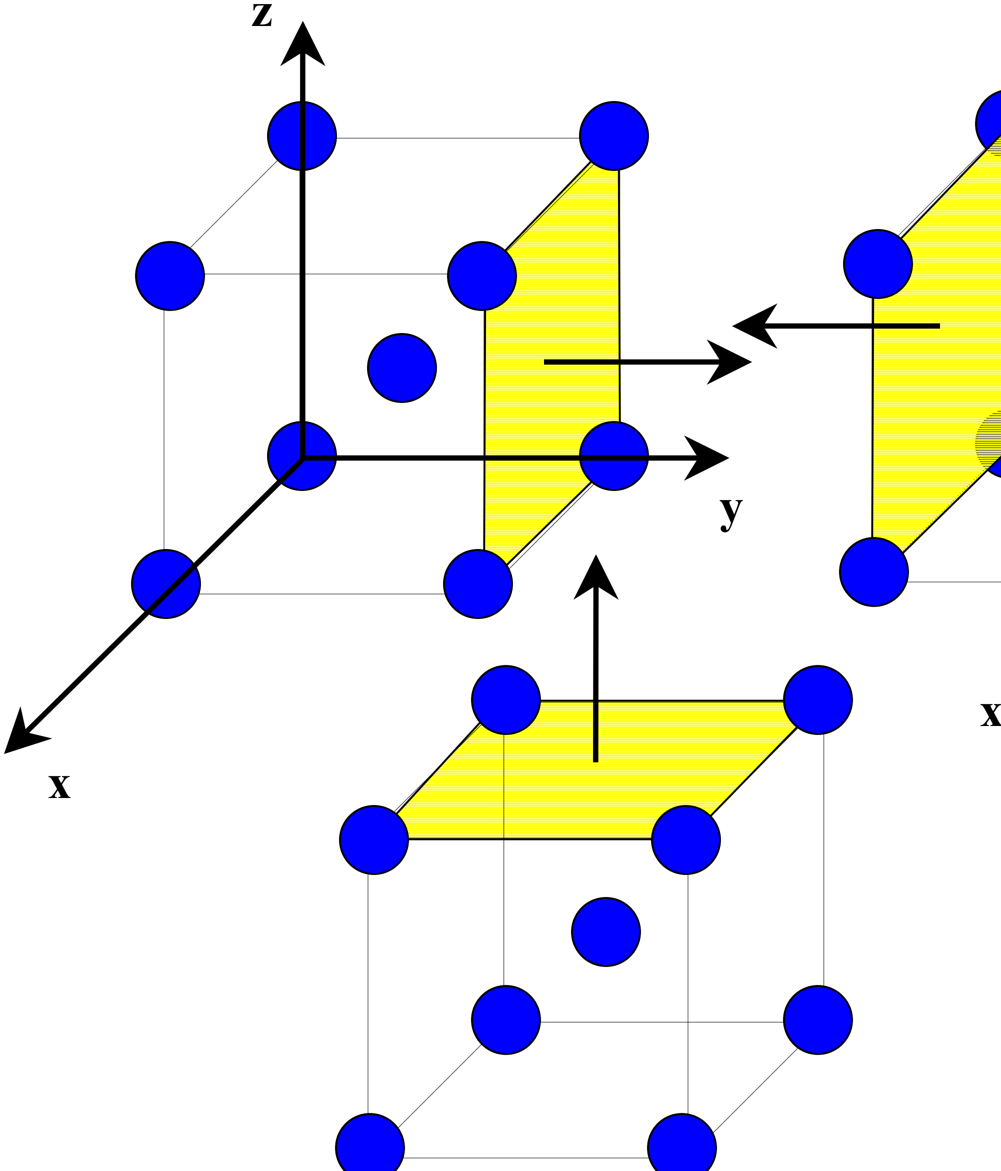
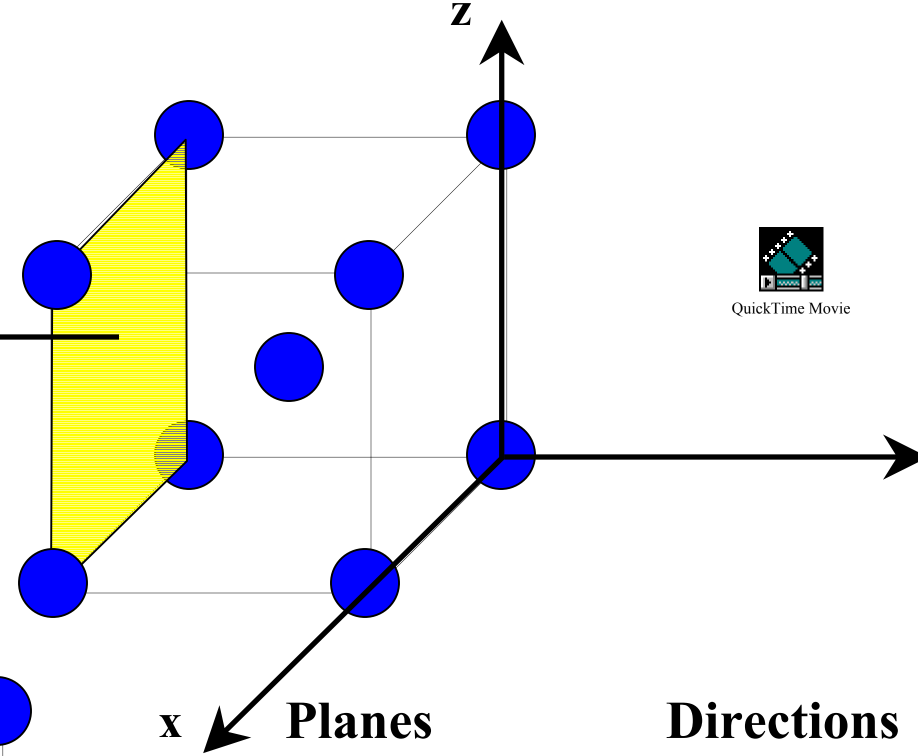


Figure 1.7 Visualization and Miller indices of commonly encountered (a) crystalline planes and (b) direction vectors.

Crystalline Planes and Miller Indices:

Equivalent Planes and directions





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Planes	Directions
{100} =	[100] =
$(100), (\bar{1}00)$	$<100>, <\bar{1}00>$
$(010), (0\bar{1}0)$	$<010>, <0\bar{1}0>$
$(001), (00\bar{1})$	$<001>, <00\bar{1}>$