SOLUTIONS: ECE 305 Homework 1: Week 1

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1) Ge has the same crystal structure (diamond) as Si, with a lattice constant of *a* = 5.64 Angstroms = 0.564 nm. Find the atomic density (atoms/cm^3) and the spacing between nearest-neighbor atoms in Ge. Recall that 1 nm = 1x10^{-7} cm.

Solution:

Volume of the cubic unit cell: $V_u = a^3$ $\quad$ ($a = 0.564 \times 10^{-7}$ cm)

Number of atoms in the cubic unit cell: $N_u = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$

(Eight on the corners, shared with 8 neighbors + 6 on the faces, each one shared with a nearest neighbor + 4 in the interior.) See Fig. 1.4 Pierret.

Atomic density: $\frac{N_u}{V_u} = \frac{8}{a^3} = \frac{8}{\left(0.564 \times 10^{-7}\right)^3} = 4.46 \times 10^{22} \text{ atoms/cm}^3$

$$\boxed{\frac{N_u}{V_u} = 4.46 \times 10^{22} \text{ atoms/cm}^3}$$

Note: Proper MKS units would be atoms/m^3, but for semiconductor work, it is common to use cm. **Be careful about units!**

The nearest neighbor to an atom is ¼ of the body diagonal away. The body diagonal of a cube of side, *a*, is $\sqrt{3}a$, so the NN spacing is

$$d_{NN} = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3}\left(0.564 \text{ nm}\right)}{4} = 0.244 \text{ nm} \qquad \boxed{d_{NN} = 0.244 \text{ nm}}$$

2) Gallium arsenide (GaAs) has a zinc-blende crystal structure. Answer the following questions about GaAs. (Assume a lattice spacing of *a* = 5.65 Angstroms = 0.565 nm.)

   a) What is the density of GaAs in gm/cm^3?
   b) How many atoms/cm^3 are there in GaAs?
   c) How many valence electrons per cm^3 are there in GaAs?
   d) What is the closest spacing between adjacent arsenic atoms in GaAs?

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Solution:

2a)
8 atoms per unit cell: 4 Ga and 4 As
atomic weights:

Ga = 69.72 Da or u
As = 74.92
$1\text{ u} = 1.660\times10^{-27}\text{ kg}$

Total mass in unit cell: $M = 4\times(69.72+74.92)\times1.660\times10^{-27}\text{ kg}$

Density = mass/volume:

$$\rho = \frac{9.60\times10^{-25}\text{ kg}}{\left(5.65\times10^{-10}\right)^3} = 5.32\times10^3\text{ kg/m}^3$$

(These are proper MKS units. Also called International System of Units.)

$$\rho = 5.32\times10^3\,\frac{\text{kg}}{\text{m}^3}\times\frac{10^3\text{gm}}{\text{kg}}\times\frac{1}{\left(10^2\text{ cm/m}\right)^3} = 5.32\,\frac{\text{gm}}{\text{cm}^3}\qquad \boxed{\rho = 5.32\,\frac{\text{gm}}{\text{cm}^3}}$$

2b)

Atomic density: $\frac{N_u}{V_u} = \frac{8}{a^3} = \frac{8}{\left(0.565\times10^{-7}\right)^3} = 4.44\times10^{22}\text{ atom/cm}^3$ $\boxed{\frac{N_u}{V_u} = 4.44\times10^{22}\text{ atom/cm}^3}$

Note that GaAs and Ge have almost exactly the same lattice constant and the same crystal structure, so they have almost exactly the same atomic density.

2c)
Ga has 3 valence electrons (column III of periodic table)
As has 5 valence electrons (column IV of periodic table)

The unit cell has 4 Ga atoms and 4 As atoms

$$\frac{N_{ve}}{V_u} = \frac{4(3+5)}{a^3} = \frac{32}{\left(0.565\times10^{-7}\right)^3} = 1.77\times10^{23}\text{ valence electrons/cm}^3$$

$$\boxed{\frac{N_{ve}}{V_u} = 1.77\times10^{23}\text{ valence electrons/cm}^3}$$

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2d)

The nearest neighbor of an As atom is a Ga atom and vice versa. Consider Fig. 1.4(c) in SDF. If the atom in the **upper left** is As, then the nearest neighbor is the Ga atom in the middle. The nearest **As atom** is the one on the top face at the **back right** of the cube. The distance is

$$d_{As-As} = \frac{a}{\sqrt{2}} = \frac{0.565\text{ nm}}{\sqrt{2}} = 0.400\text{ nm} \qquad \boxed{d_{As-As} = 0.400\text{ nm}}$$

3) Silicon (Si) has a diamond crystal structure. Answer the following questions about Si. (Assume a lattice spacing of a = 5.42 Angstroms.)

   a) Compute the density of Si atoms per cm^2 on {100} planes.
   b) Treat atoms as rigid spheres with radii equal to one-half of the distance between nearest neighbors. Compute the percentage of volume occupied by the Si atoms.

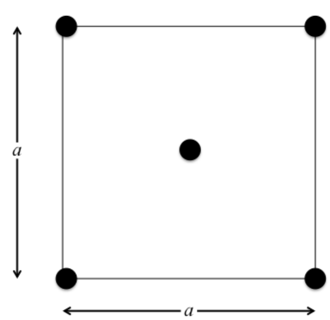
Solution:

3a)

Consider the top face of the unit cell in Fig. 1.4 (a). As shown below, there are 5 atoms on the face, but the 4 on the corners are shared between 4 adjacent unit cells, so the total number is $N = 4 \times \frac{1}{4} + 1 = 2$ per face of a cell. The density per unit area is

$$N_S = \frac{2}{a^3} = \frac{2}{\left(5.42\times10^{-8}\text{cm}\right)^2} = 6.81\times10^{14}\text{ cm}^{-2} \qquad \boxed{N_S = 6.81\times10^{14}\text{ cm}^{-2}}$$

Note that the corresponding answer for a (111) plane is $N_S = 7.86\times10^{14}\text{ cm}^{-2}$, but the geometry is a bit harder to visualize.



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3b)

The volume of each sphere is $V_{sphere} = \frac{4}{3}\pi R^3$

The radius is one-half the nearest neighbor distance, so

$$R = \frac{1}{2}\left(\frac{\sqrt{3}a}{4}\right) = \frac{\sqrt{3}a}{8}$$

$$V_{sphere} = \frac{4}{3}\pi R^3 = \frac{4}{3}\pi\left(\frac{\sqrt{3}a}{8}\right)^3 = \frac{4}{3}\pi\frac{3\sqrt{3}a^3}{64} = \frac{\pi\sqrt{3}a^3}{16}$$

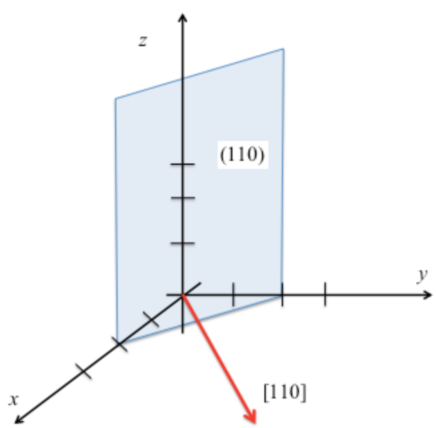
There are eight of these spheres in a unit cell, so the fraction of the unit cell volume filled (the packing fraction, *PF*,) is

$$PF = \frac{8V_{sphere}}{a^3} = \frac{\sqrt{3}\pi}{16} = 0.34 \qquad \boxed{PF = 0.34}$$

4) What is the angle between a [110] direction and a (110) plane?

Solution:

The plane and direction are shown below.



Note that the [110] direction is normal to the (110) plane. **The angle is 90 degrees.** In general, one can prove that a [hkl] direction is normal to an (hkl) plane.

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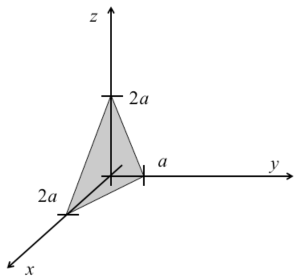
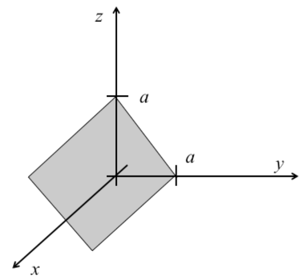
5) Determine the Miller indices for the following planes along with the directions normal to each plane. (Use the general result from problem 4.)

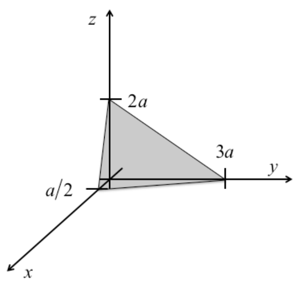
a)



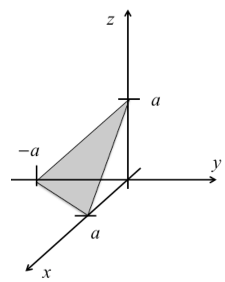
b)



c)



d)



Solution:

5a) Find the intercepts with the x, y, z, axes: 2, 1, 2 (in units of *a*)
invert the intercepts: 1/2, 1, 1/2
multiply by 2 to produce integers: 1, 2, 1
put in parentheses to denote a plane (1, 2, 1)
direction normal to this plane is [1, 2, 1]

(1 2 1) plane
[1 2 1] normal to the plane

5b) Find the intercepts with the x, y, z, axes: infinity, 1, 1 (in units of *a*)
invert the intercepts: 0, 1, 1
multiply by 1 to produce integers: 0, 1, 1
put in parentheses to denote a plane (0, 1, 1)
direction normal to this plane is [0, 1, 1]

(001) plane
[001] normal to the plane

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5c) Find the intercepts with the x, y, z, axes: 1/2, 3, 2 (in units of a)
invert the intercepts: 2, 1/3, 1/2
multiply by 6 to produce integers: 12, 2, 3
put in parentheses to denote a plane (12, 2, 3)
direction normal to this plane is [12, 2, 3]

$\boxed{\begin{array}{l}(12\ 2\ 3)\text{ plane}\\ [12\ 2\ 3]\text{ normal to the plane}\end{array}}$

5d) Find the intercepts with the x, y, z, axes: 1, -1, 1 (in units of a)
invert the intercepts: 1, -1, 1
multiply by 1 to produce integers: 1, -1, 1
put in parentheses to denote a plane (1, -1, 1)
direction normal to this plane is [1, -1, 1]

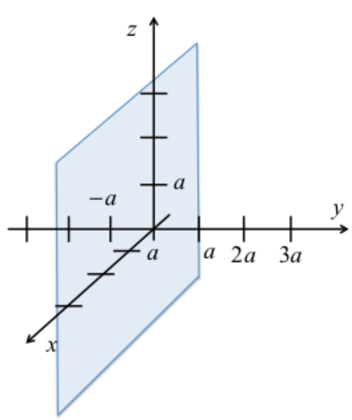
$\boxed{\begin{array}{l}(1\ \bar{1}\ 1)\text{ plane}\\ [1\ \bar{1}\ 1]\text{ normal to the plane}\end{array}}$

*** Note: when writing Miller indices, a bar over a number denotes a negative sign.

6) Sketch the following

a) (010)
b) $[010]$
c) (203)
d) $(\bar{1}1\bar{1})$

Solution:
6a) (010) is a plane



Note that a similar plane with a y-intercept at 2a, or 3a would also be an (010) plane.

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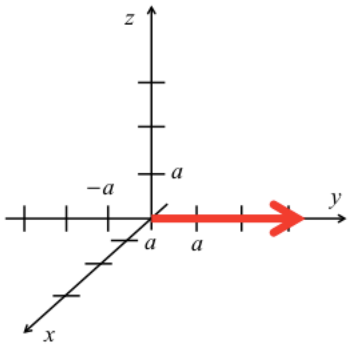
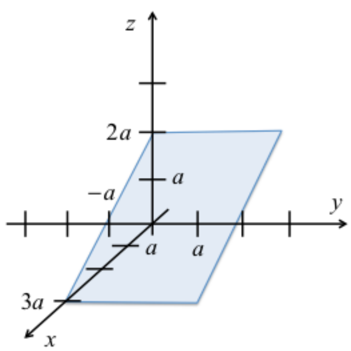
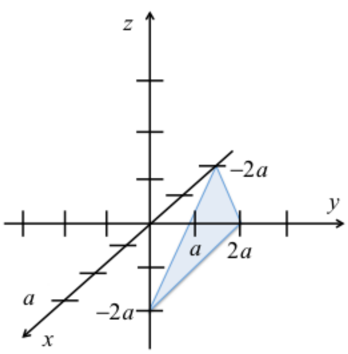
6b) [010] is a direction normal to the plane in 6a)



6c) (203) is a plane



6d) $\left(\bar{1}1\bar{1}\right)$ is a plane



Note that a similar plane with intercepts at $x=-a, y=a, z=-a$ would also be a $\left(\bar{1}1\bar{1}\right)$ plane. In general, {*h*, *k*, *l*} denotes a family of planes.

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7) Consider a hydrogen atom (1 electron orbiting one proton). Suppose that we excite the electron from the ground state to the first excited state (see Fig. 2.1).
   a) The electron relaxes to the ground state and emits a photon. What is the energy of this photon (in eV)?
   b) What is the wavelength, λ, of the photon in vacuum? It may be helpful to recall that $E = h\nu$, where h is Planck's constant and ν is the frequency, and $c = \lambda\nu$, where c is the speed of light. **Pay attention to units.**

Solution:

7a) From Fig. 2.1:

$E_0 = -13.6\text{ eV}$ (ground state)
$E_1 = -3.4\text{ eV}$ (first excited state)
(Note that $E = 0$ is the energy of the electron infinitely far away from the proton.

$E_{ph} = -3.4 - (-13.6) = 10.2\text{ eV}$ (photon energy) $\boxed{E_{ph} = 10.2\text{ eV}}$

b) $\lambda = \dfrac{c}{\nu} = \dfrac{c}{E_{ph}/h} = \dfrac{hc}{E_{ph}}$

$$\lambda = \frac{hc}{E_{ph}} = \frac{\left(6.626\times10^{-34}\text{ J-s}\right)\left(3\times10^{8}\text{ m/s}\right)}{9.8\times\left(1.6\times10^{-19}\right)\text{J}} = 1.27\times10^{-7}\text{ m}$$

Careful: Be sure to use MKS units – meters for distance, meters/second for velocity, and Joules for energy.

$\boxed{\lambda_{ph} = 127\text{ nm}}$

8) Consider Si ($E_G = 1.1\text{ eV}$), Ge ($E_G = 0.67\text{ eV}$) and GaAs ($E_G = 1.4\text{ eV}$).
   a) Using the same vertical scale , draw a simple energy band diagram (showing E_C and E_V) for each of the three materials.
   b) On the energy band diagram for Si, illustrate an electron in the conduction band.
   c) On the energy band diagram for Ge, illustrate a hole in the valence band.

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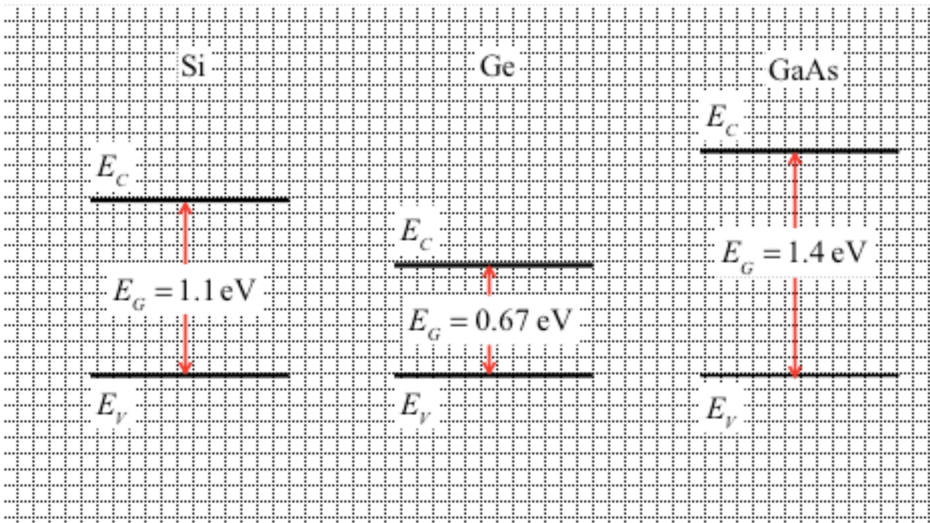
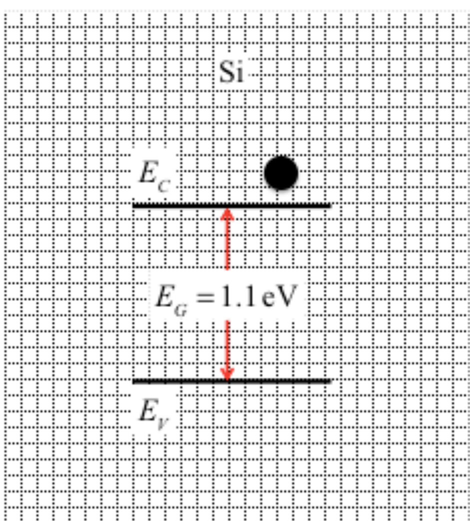
Solution:

a)



b) An electron in the conduction band is a filled state in the conduction band. It is a carrier of negative charge.



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c) A hole in the valence band is an empty state in the valence band. It is a carrier of positive charge.