SOLUTIONS: ECE 305 Homework 1: Week 1

Mark Lundstrom
Purdue University

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 = 1×10^{-7} cm.

Solution:

Volume of the cubic unit cell: $V_u = a^3$ ($a = 0.564\times10^{-7}$ 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, SDF.

Atomic density: $\frac{N_u}{V_u}=\frac{8}{a^3}=\frac{8}{\left(0.564\times10^{-7}\right)^3}=4.46\times10^{22}\text{ atoms/cm}^3$

$$\boxed{\frac{N_u}{V_u}=4.46\times10^{22}\text{ atoms/cm}^3}$$

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?

ECE 305 Homework 1 SOLUTONS: Week 1 (continued)
Solution:

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

Ga = 69.72 Da or u
As = 74.92
$1\ \text{u} = 1.660 \times 10^{-27}\ \text{kg}$

Total mass in unit cell: $M = 4 \times (69.72 + 74.92) \times 1.660 \times 10^{-27}\ \text{kg}$ $M = 9.60 \times 10^{-25}\ \text{kg}$

Density = mass/volume:

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

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

$$\rho = 5.32 \times 10^3 \frac{\text{kg}}{\text{m}^3} \times \frac{10^3\text{gm}}{\text{kg}} \times \frac{1}{(10^2\ \text{cm/m})^3} = 5.32 \frac{\text{gm}}{\text{cm}^3}$$

$$\boxed{\rho = 5.32 \frac{\text{gm}}{\text{cm}^3}}$$

2b)

Atomic density: $\frac{N_u}{V_u} = \frac{8}{a^3} = \frac{8}{(0.565 \times 10^{-7})^3} = 4.44 \times 10^{22}\ \text{atom/cm}^3$ $\boxed{\frac{N_u}{V_u} = 4.44 \times 10^{22}\ \text{atom/cm}^3}$

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

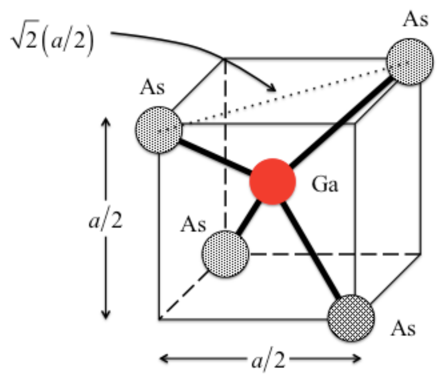
$$\frac{N_{ve}}{V_u} = \frac{4(3+5)}{a^3} = \frac{32}{(0.565 \times 10^{-7})^3} = 1.77 \times 10^{23}\ \text{valence electrons/cm}^3$$

$$\boxed{\frac{N_{ve}}{V_u} = 1.77 \times 10^{23}\ \text{valence electrons/cm}^3}$$

ECE 305 Homework 1 SOLUTIONS: Week 1 (continued)
2d)

The nearest neighbor of an As atom is a Ga atom and vice versa. Consider Fig. 1.4(c) in Pierret, SDF. This is the sub-cube (top corner)shown in the dotted lines of the diamond lattice in Fig. 1.4(a) on the upper left or equivalently the same sub-cube in the zinc blend lattice shown in Fig. 1.4(b).

Figure 1.4(c) is shown below.



If the atom in the **upper left** of the sub-cube is As, then the nearest neighbor is the Ga atom in the center of this sub-cube. The nearest **As atom** is the one on the top face center of the big cube or the one at the **back right** of the sub-cube shown above. The distance is

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

Because of the symmetry of the lattice, the atom in the middle of the sub-cube above could be an As atom and the atoms at the corners would then be Ga atoms (we would just be moving the origin of the coordinate system). We conclude the the distance between nearest Ga atoms is the same as the distance between nearest As atoms.

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.

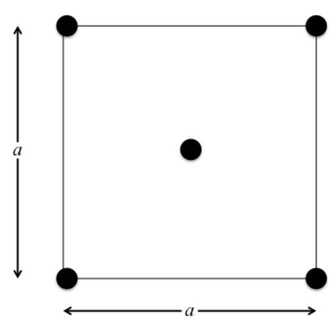
ECE 305 Homework 1 SOLUTIONS: Week 1 (continued)
Solution:

3a)

Consider the top face of the unit cell in Fig. 1.4 (a) of Pierret, SDF. 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

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

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.



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

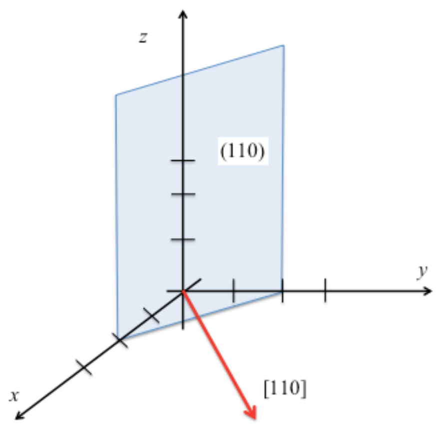
$$PF = \frac{8V_{sphere}}{a^3} = \frac{\sqrt{3}\pi}{16} = 0.34 \qquad \boxed{PF = 0.34}$$

ECE 305 Homework 1 SOLUTIONS: Week 1 (continued)

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

Solution:

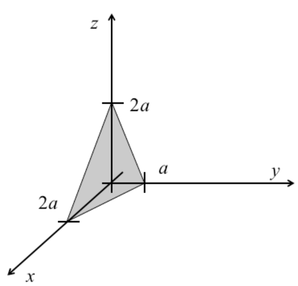
The plane and direction are shown below.



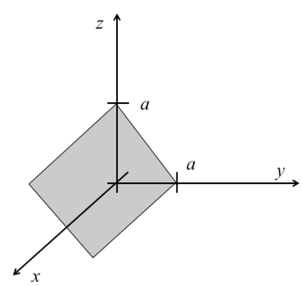
Note that the [110] direction is normal to the (110) plane. **The angle is 90 degrees.** In general, one can prove that a [hkl] direction is normal to an (hkl) plane.

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

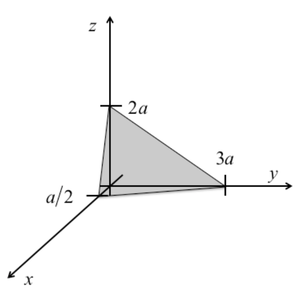
a)



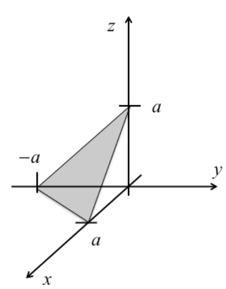
b)



c)



d)



ECE 305 Homework 1 SOLUTIONS: Week 1 (continued)
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]

(0 1 1) plane
[0 1 1] normal to the plane

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]

(12 2 3) plane
[12 2 3] normal to the plane

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]

$(1\,\bar{1}\,1)$ plane
$[1\,\bar{1}\,1]$ normal to the plane

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