Homework Solution #1

1. COMMON UNITS OF MEASUREMENT IN SEMICONDUCTORS

(A). This problem simply involves the conversion from Å^{-3} to nm^{-3} and cm^{-3}:

$$1 \text{ Å} = 1 \times 10^{-8} \text{ cm} \Rightarrow 5\text{Å}^{-3} = 5\left(10^{-8} \, cm\right)^{-3} = \boxed{5 \times 10^{24} \, cm^{-3}} \tag{1.1}$$

$$1 \text{ Å} = 0.1 \text{ nm} \Rightarrow 5\text{Å}^{-3} = 5\left(10^{-1} \, nm\right)^{-3} = \boxed{5 \times 10^{3} \, nm^{-3}} \tag{1.2}$$

(B). The conversion from eV to Joules and vice versa can be calculated from the fact that a Joule is the work required to move an electric charge of 1 Couloumb through an electric potential difference of 1 volt. Since the charge of an electron is approximately 1.602×10^{-19} C, an eV is simply the amount of energy gained or lost by moving a single electron across a potential difference of 1 volt.

$$\text{Energy} = \text{charge} \cdot \text{potential difference} \Rightarrow 1.602 \times 10^{-19} \text{ C} \cdot 1 \text{ V} = 1.602 \times 10^{-19} \text{ J} == 1 \text{ eV} \tag{1.3}$$

Therefore:

$$\boxed{1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}} \tag{1.4}$$

and

$$\boxed{1 \text{ J} = 6.242 \times 10^{18} \text{ eV}} \tag{1.5}$$

(C).

$$
\begin{aligned}
k &= 1.38 \times 10^{-23} \text{ J/K} \\
T &= 300 \text{ K} \\
kT &= 4.14 \times 10^{-21} \text{ J}
\end{aligned}
\tag{1.6}
$$

Converting from joules to eV using the calculated conversion value from Eq. 1.5 gives:

$$\boxed{kT = 0.0259 \text{ eV} = 25.9 \text{ meV}} \tag{1.7}$$

This is a very important value and you will use it continuously throughout the semester, so be sure to memorize it!

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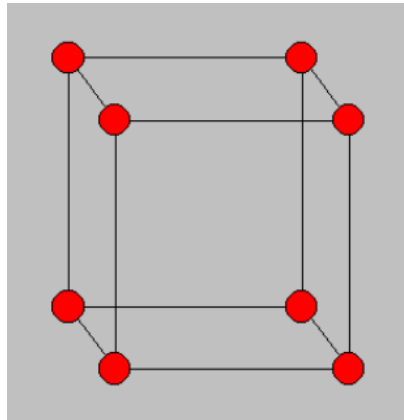## 2. LATTICES AND CRYSTAL STRUCTURES

(A). **SC Lattice:**

Figure 2.1: Simple cubic unit cell in real space.

First, it is important to note that each corner atom is only 1/8th contained in a single unit cell (that is, a corner atom is shared by 8 unit cells), so:

$$8 \text{ corner atoms} \Rightarrow \frac{1}{8} \cdot 8 = \boxed{1 \text{ atom in the SC unit cell}} \tag{2.1}$$
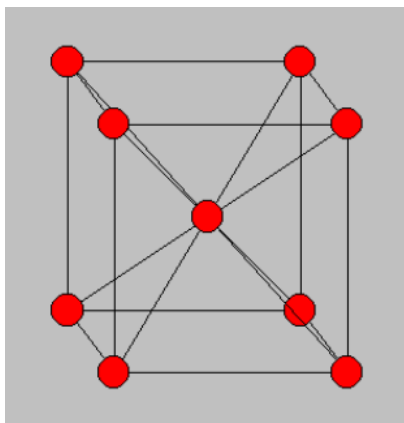
BCC Lattice:

Figure 2.2: BCC unit cell in real space.

Remembering that each corner atom contributes 1/8th of an atom, also notice that the center atom (the body portion

of BCC) contributes a full atom since it isn't shared with any other neighboring unit cells, so:

$$8 \text{ corner atoms}$$
$$1 \text{ center atom}$$
$$\frac{1}{8} \cdot 8 + 1 = \boxed{2 \text{ atoms in the BCC unit cell}}$$
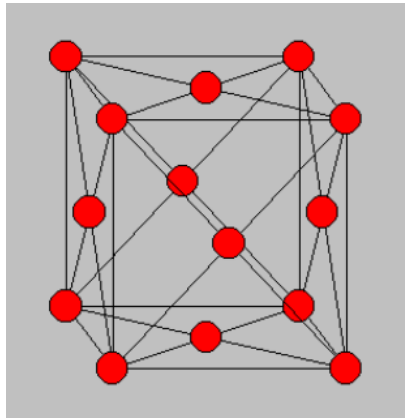
(2.2)

FCC Lattice:

Figure 2.3: FCC unit cell in real space.

Remembering that each corner atom contributes 1/8th of an atom, but that the atom on each face is shared by only 2 unit cells, so each contributes 1/2 of a full atom, so:

$$8 \text{ corner atoms}$$
$$6 \text{ face atoms}$$
$$\frac{1}{8} \cdot 8 + \frac{1}{2} \cdot 6 = \boxed{4 \text{ atoms in the FCC unit cell}}$$

(2.3)

Diamond Crystal Structure: A diamond crystal structure consists of two interpenetrating FCC lattices, separated by a distance in real space of {a/4, a/4, a/4}. Remembering that one FCC lattice contributes 4 atoms to the unit cell, we can see that the second FCC lattice has been shifted such that there are 4 whole atoms within a single unit cell that are not shared, so:

$$8 \text{ corner atoms}$$
$$6 \text{ face atoms}$$
$$4 \text{ atoms from interpenetrating FCC lattice}$$
$$\frac{1}{8} \cdot 8 + \frac{1}{2} \cdot 6 + 4 = \boxed{8 \text{ atoms in the diamond unit cell}}$$

(2.4)

Zinc Blende Crystal Structure: The zinc blende crystal structure is the same as the diamond crystal structure in terms of the number of atoms per unit cell (meaning it has 8 atoms per unit cell). However, it is important to note that the two interpenetrating FCC lattices that form this crystal structure are composed of different atoms (for example, Ga on one FCC lattice and As on the other FCC lattice). However, the math to find the total number of

atoms per unit cell follows the same logic as the diamond crystal structure:

$$8 \text{ corner atoms}$$

$$6 \text{ face atoms}$$

$$4 \text{ atoms from interpenetrating FCC lattice} \tag{2.5}$$

$$\frac{1}{8} \cdot 8 + \frac{1}{2} \cdot 6 + 4 = \boxed{8 \text{ atoms in the zinc blende unit cell}}$$

(B). **SC Lattice Nearest Neighbor:** In the simple cubic lattice is it apparent that the nearest neighbor to any atom you select in the unit cell is simply an atom at an adjacent corner along the edge of the unit cell. So:

$$\boxed{\text{SC nearest neighbor distance} = a} \tag{2.6}$$

BCC Lattice Nearest Neighbor: Looking at the bottom left corner atom of Fig. 2.2, the nearest neighbor is the central atom, which is a distance $a/2$ away in the x, y, and z directions, so:

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = \sqrt{\left(\frac{3a^2}{4}\right)} = \frac{a\sqrt{3}}{2} \tag{2.7}$$

$$\boxed{\text{BCC nearest neighbor distance} = \frac{a\sqrt{3}}{2}} \tag{2.8}$$

FCC Lattice Nearest Neighbor: Looking at the bottom left corner atom of Fig. 2.3, the nearest neighbor is an atom on the face, which is $a/2$ away in the x and y directions (or permutation of 2 of the x, y, and z directions), so:

$$\sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = \sqrt{\left(\frac{2a^2}{4}\right)} = \frac{a\sqrt{2}}{2} \tag{2.9}$$

$$\boxed{\text{FCC nearest neighbor distance} = \frac{a\sqrt{2}}{2}} \tag{2.10}$$

Diamond Nearest Neighbor: The nearest neighbor from the bottom left corner atom is a/4 away in all directions. To visualize this, remember that the diamond (and zinc blende) structures are composed of two interpenetrating FCC lattices offset by a/4 in all directions. So:

$$\sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2} = \sqrt{\left(\frac{3a^2}{16}\right)} = \frac{a\sqrt{3}}{4} \tag{2.11}$$

$$\boxed{\text{Diamond nearest neighbor distance} = \frac{a\sqrt{3}}{4}} \tag{2.12}$$

Zinc Blende Nearest Neighbor: As with the number of atoms per unit cell in part (a), the nearest neighbor distance in the zinc blende structure is exactly the same as in the diamong crystal structure, so:

$$\boxed{\text{Zinc Blende nearest neighbor distance} = \frac{a\sqrt{3}}{4}} \tag{2.13}$$

(C). For the packing fraction, we assume that all atoms in the unit cell are hard, non-overlapping spheres. To be non-overlapping yet maximize the total volume enclosed in each unit cell, the radius of each sphere must be exactly half of the nearest neighbor distance you calculated in part (b). It is also important to note that the **total volume** of the unit cell for each lattice and crystal structure is always a^3.

The equation for the packing fraction is as follows:

$$\text{Packing fraction (PF)} = \frac{\text{number of atoms per unit cell} \cdot \text{volume of sphere}}{\text{volume of unit cell}} \tag{2.14}$$

SC Lattice Packing Fraction:

$$\text{sphere radius} = \frac{a}{2}$$
$$\text{volume of sphere} = \frac{4}{3}\pi\left(\frac{a}{2}\right)^3 \tag{2.15}$$
$$\text{atoms per unit cell} = 1$$

$$\text{PF} = \frac{\pi}{6} \approx 0.52 = 52\% \tag{2.16}$$

BCC Lattice Packing Fraction:

$$\text{sphere radius} = \frac{a\sqrt{3}}{4}$$
$$\text{volume of sphere} = \frac{4}{3}\pi\left(\frac{a\sqrt{3}}{4}\right)^3 \tag{2.17}$$
$$\text{atoms per unit cell} = 2$$

$$\text{PF} = \frac{\pi\sqrt{3}}{8} \approx 0.68 = 68\% \tag{2.18}$$

FCC Lattice Packing Fraction:

$$\text{sphere radius} = \frac{a\sqrt{2}}{4}$$
$$\text{volume of sphere} = \frac{4}{3}\pi\left(\frac{a\sqrt{2}}{4}\right)^3 \tag{2.19}$$
$$\text{atoms per unit cell} = 4$$

$$\text{PF} = \frac{\pi\sqrt{2}}{6} \approx 0.74 = 74\% \tag{2.20}$$

Diamond Packing Fraction:

$$\text{sphere radius } = \frac{a\sqrt{3}}{8}$$

$$\text{volume of sphere } = \frac{4}{3}\pi \left(\frac{a\sqrt{3}}{8}\right)^3 \tag{2.21}$$

$$\text{atoms per unit cell } = 8$$

$$\boxed{\text{PF} = \frac{\pi\sqrt{3}}{16} \approx 0.34 = 34\%} \tag{2.22}$$

Zinc Blende Packing Fraction: The zinc blende packing fraction is more difficult to calculate due to the different weights that need to be assigned to the spheres of different atoms, such as Ga and As, meaning that the packing fraction for a zinc blende structure will differ on a per alloy basis.

(D). The atomic density is simply:

$$\frac{\text{number of atoms per unit cell}}{\text{volume of the unit cell}} \tag{2.23}$$

Given a lattice constant of a, the volume of all the unit cells is simply a^3, so the structures with the highest number of atoms per unit cell will have the highest atomic density, which the structures with the least number of atoms per unit cell will have the lowest atomic density. The highest would be diamond and zinc blende while the smallest atomic density is the simple cubic lattice .

3. TERNARY ALLOYS

To do this problem you must first look up the lattice constants of the constituent binary semiconductors that form the ternary alloy (that would be AlP and InP), which you can find in Appendix III of your Streetman book.

(A). So:

Lattice constant of AlP = 5.46 Å
Lattice constant of InP = 5.87 Å

Lattice constant of $Al_xIn_{1-x}P = x a_{AlP} + (1\text{-}x)a_{InP}$

$$a_{Al_{0.15}In_{0.85}P} = (0.15) \cdot 5.46 \text{ Å} + (0.85) \cdot 5.87 \text{ Å} = \boxed{5.81 \text{ Å}} \tag{3.1}$$

(B). In the zinc blende unit cell (this is a III-V semiconductor so we can safely assume it is zinc blende, though this is not always the case), there are 4 atoms of each type assuming a binary alloy such as AlP. For a ternary, this must be modified by the mole fraction. So, in AlP there are 4 Al atoms per unit cell and 4 P atoms per unit cell. However, in $Al_{0.15}In_{0.85}P$ there are $4 \cdot 0.15 = 0.6$ Al atoms per unit cell (on average). Given our calculated lattice constant from part (a), we can calculate the unit cell volume and the atomic density of Al atoms in this ternary

alloy:

$$\text{atomic density of Al} = \frac{0.6 \text{ Al atoms}}{(5.81 \times 10^{-8} \text{ cm})^3} = 3.06 \times 10^{21} \frac{\text{Al atoms}}{\text{cm}^3} \tag{3.2}$$

4. MASS DENSITY

To calculate the mass density of Si and AlAs you will need the atomic weights of Si, Al, and As, as well as the lattice constants of Si and AlAs. Finally you, will need the Avogadro constant (6.02×10^{23}) and the following equation:

$$\text{mass density} = \frac{\text{m}}{\text{V}} = \frac{\text{atomic mass} \cdot \text{atoms in unit cell}}{\text{unit cell volume}} \tag{4.1}$$

Si mass density:

$$
\begin{aligned}
a_{\text{Si}} &= 5.43 \text{ Å} = 5.43 \times 10^{-8} \text{ cm} \\
m_{\text{Si}} &= 28.09 \text{ u} = 28.09 \cdot \frac{1}{6.02 \times 10^{23}} = 4.67 \times 10^{-23} \text{ g} \\
V_{\text{Si}} &= (5.43 \text{ Å})^3 = 1.60 \times 10^{-22} \text{ cm}^3 \\
\text{atoms per unit cell} &= 8
\end{aligned}
\tag{4.2}
$$

$$\text{mass density} = \frac{4.67 \times 10^{-23} \text{ g} \cdot 8}{1.60 \times 10^{-22} \text{ cm}^3} = 2.33 \frac{\text{g}}{\text{cm}^3} \tag{4.3}$$

Notice that this calculated value is the same as the value given for Si in Appendix III.

AlAs mass density:

$$
\begin{aligned}
a_{\text{AlAs}} &= 5.66 \text{ Å} = 5.66 \times 10^{-8} \text{ cm} \\
m_{\text{Al}} &= 26.98 \text{ u} = 26.98 \cdot \frac{1}{6.02 \times 10^{23}} = 4.48 \times 10^{-23} \text{ g} \\
m_{\text{As}} &= 74.92 \text{ u} = 74.92 \cdot \frac{1}{6.02 \times 10^{23}} = 1.25 \times 10^{-22} \text{ g} \\
V_{\text{AlAs}} &= (5.66 \text{ Å})^3 = 1.81 \times 10^{-22} \text{ cm}^3 \\
\text{atoms per unit cell} &= 8
\end{aligned}
\tag{4.4}
$$

$$\text{mass density} = \frac{4.48 \times 10^{-23} \text{ g} \cdot 4 + 1.25 \times 10^{-22} \text{ g} \cdot 4}{1.81 \times 10^{-22} \text{ cm}^3} = 3.75 \frac{\text{g}}{\text{cm}^3} \tag{4.5}$$

The value given in Appendix III is 3.60 g/cm³, making our calculated value 4% higher. The key thing to recognize when calculating the mass density of a binary alloy as opposed to a semiconductor such as Si or Ge is that the different atoms contribute different values of mass to the total system. In this case, the binary zinc blende unit cell has 4 Al atoms and 4 As atoms, which is why the calculation of mass in the mass density equation above differs from Si, in which the crystal structure is diamond and all 8 atoms in the unit cell are Si.

5. WAVELENGTH AND ENERGY OF PHOTONS

The lattice constant of GaAs is 5.65 Å, or 5.65x10^{-8} cm, meaning our first photon will have a wavelength of 5.65x10^{-8} cm. The wave number, which can be viewed as the number of waves that exist over a specified distance, is calculated using the following equation:

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{5.65 \times 10^{-8} \text{ cm}} = \boxed{1.11 \times 10^8 \text{ cm}^{-1}} \tag{5.1}$$

The energy of a photon with this wavelength can be calculated the following way:

$$\text{E} = h\nu = \frac{hc}{\lambda} = \frac{6.63 \times 10^{-34} \text{ Js} \cdot 3 \times 10^8 \text{ m/s}}{5.65 \times 10^{-10} \text{ m}} = 3.52 \times 10^{-16} \text{ J} \cdot \frac{1 \text{ eV}}{1.602 \times 10^{-19} \text{ J}} = \boxed{2.20 \times 10^3 \text{ eV}} \tag{5.2}$$

If the energy of the photon is equal to the band gap of GaAs, which is equal to 1.43 eV at room temperature (300 K), then we have:

$$\lambda = \frac{hc}{\text{E}} = \frac{6.63 \times 10^{-34} \text{ Js} \cdot 3 \times 10^8 \text{ m/s}}{1.43 \text{ eV} \cdot 1.602 \times 10^{-19} \text{ J}} = 8.69 \times 10^{-7} \text{ m} = 0.869 \, \mu\text{m} = \boxed{869 \text{ nm}} \tag{5.3}$$

Given the GaAs lattice constant above, this means that a photon with an energy equal to the band gap of GaAs spans 1538 lattice constants .

Note: Since wavelengths of photons in semiconductor physics are typically given in the nm to micrometer range and energies are typically given in eV, it is very helpful to have a quick and easy formula to convert between the two.

$$hc = 6.63 \times 10^{-34} \text{ Js} \cdot 3 \times 10^8 \text{ m/s} = 1.24 \times 10^{-6} \text{ eV} \cdot \text{m} = 1.24 \text{ eV} \cdot \mu\text{m} \tag{5.4}$$

So:

$$\text{E (eV)} \approx \frac{1.24 \text{ eV} \cdot \mu\text{m}}{\lambda(\mu\text{m})}$$
$$\lambda(\mu\text{m}) \approx \frac{1.24 \text{ eV} \cdot \mu\text{m}}{\text{E (eV)}} \tag{5.5}$$

This is a very useful formula so it is highly recommended that you memorize it!