ECE 3040
Dr. Doolittle

Homework 1

1. Given the ternary compound semiconductor $In_xGa_{1-x}As$,
   a) What is the lattice constant and composition that would result in a 0.85 eV semiconductor?
   b) What is the relationship between lattice constant and chemical bond strength and how does that translate into energy bandgap? You can use the data from Lecture 1.

   Hints:
   Assume that the bonds are covalent in nature.
   Assume that energy bandgaps and lattice constants of compound semiconductors scale linearly (which is a good first-order approximation).
   InAs has a bandgap of 0.36 eV, while GaAs has a bandgap of 1.43 eV.
   InAs has a lattice constant *a* = 6.06 angstroms, while GaAs has a lattice constant *a* = 5.65 angstroms.

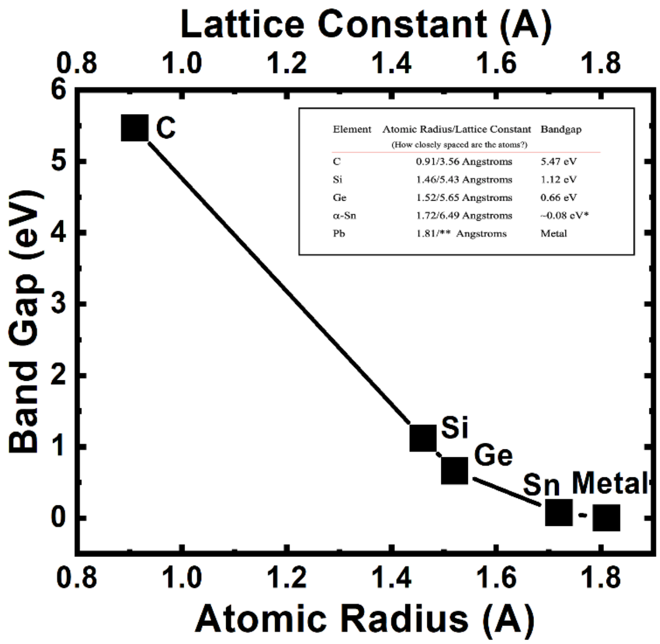
   Ans:
   (a) Given that,
   $E_g = 0.85\ ev$, $E_g^{InAs} = 0.36\ ev$, $E_g^{GaAs} = 1.43\ ev$

   Let x be the fraction of given ternary compound semiconductor.
   Equation to find the x value,
   $0.85 = 0.36 + (1.43 - 0.36) * (1 - x)$
   $\Rightarrow 1.07 * x = 0.58$
   $\Rightarrow x = 0.54$
   Therefore, the composition of InGaAs would be $In_{0.54}Ga_{0.46}As$.

   Calculating lattice constant a_{InGaAs} ,
   Given that, $a_{InAs} = 6.06\ angstrom$, $a_{GaAs} = 5.65\ angstrom$

   $a_{InGaAs} = 6.06 + (5.65 - 6.06)(1 - 0.54)$
   $\Rightarrow a_{InGaAs} = 5.87\ angstrom$

   (b) A shorter lattice constant indicates that the atoms are closer together in the crystal lattice. When atoms are closer, the overlap of their electron clouds (where they share electrons) is greater. This increased overlap leads to stronger covalent bonds because the shared electrons are held more tightly between the nuclei of the atoms, resulting in a stronger attraction.
   The bandgap in a semiconductor decreases with increasing lattice constant because the larger atomic spacing leads to weaker electron-electron interactions, greater electron wave function overlap, and changes in effective mass, all of which reduce the energy separation between the valence and conduction bands, resulting in a smaller bandgap.



2. GaP is a III-V compound semiconductor with a zincblende crystal structure and lattice constant a = 5.45 angstroms.
   a) Suppose that instead of the semiconductor it is (Eg=2.24 eV), GaP was a metal and as such, each atom in GaP gave up exactly one electron. What would the electron concentration in the crystal be?
   b) Alternatively, suppose only one-trillionth of the atoms in the crystal gave up an electron. What would the electron concentration be?

   Note: It may be helpful to use the visualization aids on the web page or the images in your text or 3D images online.

   Ans:

   (a) Finding the atomic density for GaP,

   $a_{GaP} = 5.45\ angstrom = 5.45 * \ 10^{-8}\ cm$

   Volume = $(a_{GaP})^3 = (5.45 * 10^{-8})^3 \approx 1.61 * 10^{-22}\ cm^3$

   Zincblende can be seen as two interpenetrating FCC structures. So, the no. of atoms per unit cell = 8

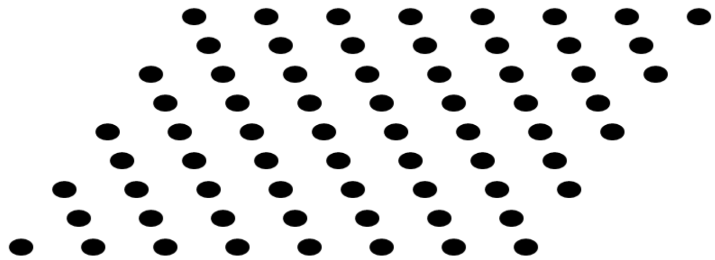
   Therefore, atomic density = $\frac{8}{1.61*10^{-22}} \approx 4.97 * 10^{22}\ cm^{-3}$

   Considering GaP as a metal, we can safely assume that each atom will give one electron. Therefore, this atomic density will be the electron concentration in the crystal.

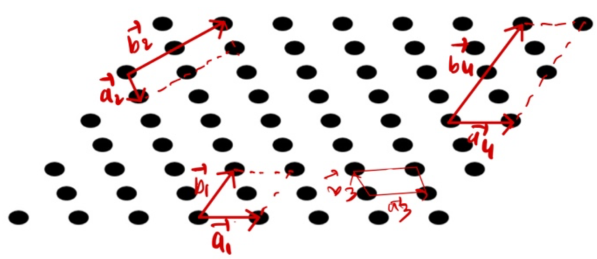
   Note: This sets the maximum electron density achievable within a specific crystal structure. If the substance is a semiconductor or insulator (with a relatively large bandgap), the actual electron concentration will be considerably less than this upper limit.

   (b) Assuming one-trillionth (10^{12}) of the atoms in the crystal gave up an electron, Therefore, the electron concentration $= \frac{4.97*10^{22}}{10^{12}} \approx 4.97 * 10^{10} cm^{-3}$

3. Using the two-dimensional lattice below, draw and label four different unit cells and identify which one(s) is/are primitive.



Ans: 4 unit cells are shown as below,



4. Describe in three sentences or less how an acceptor atom in silicon can have a stationary (fixed) negative charge and where that negative charge is located at in the region around the acceptor atom.
   Ans:
   An acceptor atom in silicon, such as boron, creates a stationary negative charge through a process called doping. When boron is introduced into the silicon lattice, it leaves behind a vacancy or "hole" in the crystal structure, which is effectively a positive charge. Electrons from nearby silicon atoms occupy this hole, forming a stationary negative charge localized at the position of the missing electron. This negative charge effectively neutralizes the positive charge of the boron atom, maintaining overall electrical balance within the silicon crystal.

5. In GaAs (a III-V compound) what is the role (donor or acceptor) and why of:
   a) Oxygen substituting for As? b) Si substituting for Ga? c) Si substituting for As? d) Mg substituting for Ga? Note you may need to reference a periodic table.
   Ans:
   (a)Refer to the periodic table,
   Oxygen(Grp VI) substituting for arsenic(Grp V) in GaAs introduces extra energy levels near the conduction band, creating donor levels. Due to its electron configuration, oxygen

brings an extra electron into the crystal. Therefore, in GaAs, oxygen serves as a shallow donor.

(b)When silicon (Si) (Grp IV) is substituted for gallium (Ga) in GaAs, it typically acts as a donor impurity. Si introduces extra electrons into the crystal lattice. This additional electron is loosely bound and can easily become mobile within the crystal.

(c)When silicon (Si) (Grp IV) is substituted for As (Grp V) silicon acts as a deep acceptor. According to the electron configuration, Si has four valence electrons, while As has five valence electrons. When silicon replaces arsenic in the GaAs lattice, it introduces fewer electrons into the crystal structure. These electrons create holes in the valence band, as there is an electron deficiency.

(d) Mg introduces an extra positive charge (holes) into the crystal lattice, making it p-type (positively doped). Because Mg has two fewer electrons in its outermost shell compared to gallium. When it replaces a gallium atom in the GaAs lattice, it introduces a deficiency of electrons, creating holes in the valence band.