

Homework 1

1. Given the ternary compound semiconductor $\text{In}_x\text{Ga}_{1-x}\text{As}$,
 - 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,

$$E_g = 0.85 \text{ eV}, E_g^{\text{InAs}} = 0.36 \text{ eV}, E_g^{\text{GaAs}} = 1.43 \text{ eV}$$

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 $\text{In}_{0.54}\text{Ga}_{0.46}\text{As}$.

Calculating lattice constant a_{InGaAs} ,

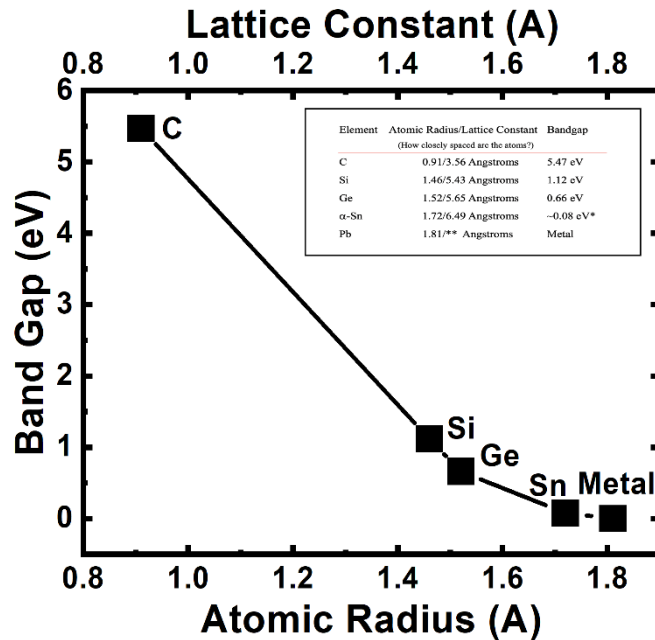
Given that, $a_{\text{InAs}} = 6.06 \text{ angstrom}$, $a_{\text{GaAs}} = 5.65 \text{ angstrom}$

$$a_{\text{InGaAs}} = 6.06 + (5.65 - 6.06)(1 - 0.54)$$

$$\Rightarrow a_{\text{InGaAs}} = 5.87 \text{ angstrom}$$

- (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.
- 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?
 - 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,

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

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

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

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

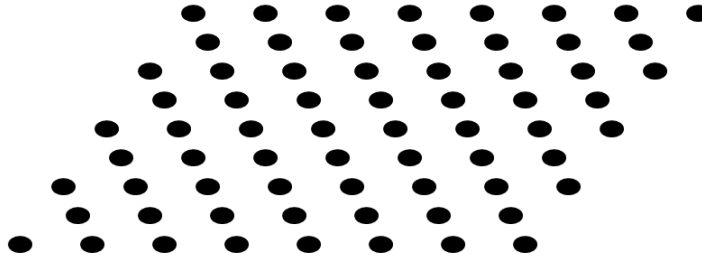
Considering GaP as a metal, we can safely assume that each atom will give one electron. Therefore, this atomic density will be the electron concentration in the crystal.

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.

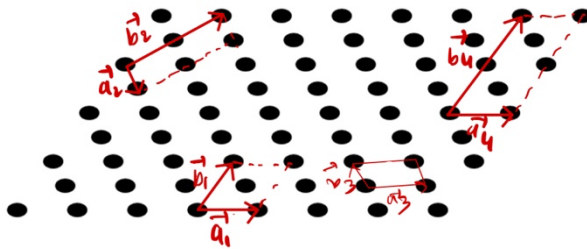
- Assuming one-trillionth (10^{12}) of the atoms in the crystal gave up an electron,

Therefore, the electron concentration = $\frac{4.97 \cdot 10^{22}}{10^{12}} \approx 4.97 \cdot 10^{10} \text{ cm}^{-3}$

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.

Periodic Table of the Elements

| 1 IA 1A | 2 IIA 2A | | | | | | | | | | | | 13 IIIA 3A | 14 IVA 4A | 15 VA 5A | 16 VIA 6A | 17 VIIA 7A | 18 VIIIA 8A | | | | | | | |
|--------------------------------|--------------------------------|--------------------------------|-----------------------------------|---------------------------------|---------------------------------|----------------------------------|---------------------------------|--------------------------------|----------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|----------------------------------|---------------------------------|----------------------------------|---------------------------------|---------------------------------|-----------------------------|--|--|--|--|--------------------------------|-----------------------------|
| 1 H Hydrogen 1.008 | | | | | | | | | | | | | 5 B Boron 10.811 | 6 C Carbon 12.011 | 7 N Nitrogen 14.007 | 8 O Oxygen 15.999 | 9 F Fluorine 18.998 | 10 Ne Neon 20.180 | | | | | | | |
| 3 Li Lithium 6.941 | 4 Be Beryllium 9.012 | | | | | | | | | | | 11 Na Sodium 22.990 | 12 Mg Magnesium 24.305 | | | | | | | | | | | 17 Cl Chlorine 35.453 | 18 Ar Argon 39.948 |
| 19 K Potassium 39.098 | 20 Ca Calcium 40.078 | 21 Sc Scandium 44.956 | 22 Ti Titanium 47.88 | 23 V Vanadium 50.942 | 24 Cr Chromium 51.996 | 25 Mn Manganese 54.938 | 26 Fe Iron 55.833 | 27 Co Cobalt 58.933 | 28 Ni Nickel 58.693 | 29 Cu Copper 63.546 | 30 Zn Zinc 65.39 | 31 Ga Gallium 69.723 | 32 Ge Germanium 72.61 | 33 As Arsenic 74.922 | 34 Se Selenium 78.972 | 35 Br Bromine 79.904 | 36 Kr Krypton 84.40 | | | | | | | | |
| 37 Rb Rubidium 84.464 | 38 Sr Strontium 87.62 | 39 Y Yttrium 88.906 | 40 Zr Zirconium 91.224 | 41 Nb Niobium 92.906 | 42 Mo Molybdenum 95.95 | 43 Tc Technetium 98.907 | 44 Ru Ruthenium 101.07 | 45 Rh Rhodium 102.906 | 46 Pd Palladium 106.42 | 47 Ag Silver 107.868 | 48 Cd Cadmium 112.411 | 49 In Indium 114.818 | 50 Sn Tin 118.71 | 51 Sb Antimony 121.760 | 52 Te Tellurium 127.6 | 53 I Iodine 126.905 | 54 Xe Xenon 131.29 | | | | | | | | |
| 55 Cs Cesium 132.905 | 56 Ba Barium 137.327 | 57-71 Lanthanide Series | 72 Hf Hafnium 178.49 | 73 Ta Tantalum 180.948 | 74 W Tungsten 183.85 | 75 Re Rhenium 186.207 | 76 Os Osmium 190.23 | 77 Ir Iridium 192.22 | 78 Pt Platinum 195.08 | 79 Au Gold 196.967 | 80 Hg Mercury 200.59 | 81 Tl Thallium 204.383 | 82 Pb Lead 207.2 | 83 Bi Bismuth 208.980 | 84 Po Polonium 209 | 85 At Astatine 209 | 86 Rn Radon 222.018 | | | | | | | | |
| 87 Fr Francium 223 | 88 Ra Radium 226 | 89-103 Actinide Series | 104 Rf Rutherfordium 261 | 105 Db Dubnium 262 | 106 Sg Seaborgium 263 | 107 Bh Bohrium 264 | 108 Hs Hassium 265 | 109 Mt Meitnerium 266 | 110 Ds Darmstadtium 269 | 111 Rg Roentgenium 271 | 112 Cn Copernicium 277 | 113 Uut Ununtrium 288 | 114 Fl Flerovium 289 | 115 Uup Ununpentium 288 | 116 Lv Livermorium 293 | 117 Uus Ununseptium 289 | 118 Uuo Ununoctium 289 | | | | | | | | |
| | | | | | | | | | | | | | | | | | | 119 Uue Ununennium 289 | 120 Uub Unbium 289 | | | | | | |