## ICE 3040 Homework 1

1) Given the IV-IV compound semiconductor $\mathrm{Si}_{\mathrm{x}} \mathrm{Ge}_{1-\mathrm{x}}$ (assume that covalent bonds exist although strictly speaking this is not entirely true) and that energy bandgaps and lattice constants scale linearly, a) What is the lattice constant and composition that would result in a 1.0 eV semiconductor? b) What is the relationship between lattice constant, chemical bond strength, and lattice constant? You can use the data from lecture 1.
From lecture 1, Eg of $\mathrm{Si}=1.1 \mathrm{eV}$ and Eg of $\mathrm{Ge}=0.66 \mathrm{eV}$. Thus, a linear extrapolation of bandgaps to composition and composition to lattice constant would result in:

$$
S_{i x} G e_{1-x}
$$

$$
\begin{aligned}
\text { Lattice constant } \\
\begin{aligned}
L C & =5.65 \AA+(5.43-5.65) x \\
& =5.65-0.22 x \\
L C & =5.65-0.22(0.773) \\
L C & =5.48 \AA
\end{aligned}
\end{aligned}
$$

Note: many real semicunductor alloys have close to linear relationships of bandgaps vs composition and almost always have linear relationships of composition and lattice constant. However, is some cases, the Eg vs X relationship is HIGHLY bowed (i.e. curved not linear). One interesting example is the GaAsN system which has for $N \sim 3-6 \%$ a bandgap, $\sim 1 \mathrm{eV}$, which is substantially lower than either BaAs ( $\sim 1.4 \mathrm{eV}$ ) or $\mathrm{GaN}(\sim 3.4 \mathrm{eV})$.
2) Given the direction defined below, what is the plane normal to that direction?


Divide (normalize) each axis by it's lattice constant (a, b and c) => 2 , 4, 1
Invert: $1 / 2,1 / 4,1$
Multiply by lowest common denominator, 4: result= $(2,1,4)$. The plane is pictured below:

3) What is the Miller index of the $x$-y plane of a cubic crystal?

Since the plane intersects the x and y axes at multiple points, move the coordinate system any value away from original origin keeping the new coordinate system parallel with the old one. Example New plane defined by plane intersecting the z axis at $\mathrm{z}=212 \mathrm{c}$ (arbitrary choice emphasized by large z selection).
New Miller index: $(0,0,1)$
4) If GaAs, Zinceblende crystal with a lattice constant of 5.65 angstroms were not a semiconductor but instead was a metal where each atom can easily give up one electron, what would the electron concentration in the crystal be? Note, it may be helpful to use the visualization aids on the web page or the images in your text.
8 atoms per unit cell, volume $=(5.65 \mathrm{e}-8 \mathrm{~cm})^{3}=1.8 \mathrm{e}-22 \mathrm{~cm}^{3}$ Results in a atomic density $(\# / \mathrm{Vol})=4.43 \mathrm{e} 22 \mathrm{~cm}^{-3}$. Since in a metal, each atom can easily give up one electron, this atomic density is also the electron density. NOTE: as discussed in class, this represents the upper limit on the electron density of a given crystal structure. If the material is a semiconductor or insulator (possesses a reasonably large bandgap) the actual electron concentration will be substantially lower than this upper limit.
5) Given the 2-demensional lattice shown below with unit cell vectors $a_{1}$ and $b_{1}$, draw and show 4 different unit cells labeling which one/ones are the primitive unit cells.



Note: these solutions (number 5 and 6) are not unique.
6) Extend ONE unit cell into the $3^{\text {rd }}$ dimension to give one possible 3D unit cell (draw your
unit cell answer).

7) Identify 2 crystalline directions in a cubic system which are perpendicular to the [111] direction. Note that the cosine of the angle $T$ between two arbitrary directions [ $\left.h_{1} k_{1} l_{1}\right]$ and $\left[\mathrm{h}_{2} \mathrm{k}_{2} \mathrm{l}_{2}\right.$ ] in a cubic crystal is:
$\cos (\theta)=\frac{h_{1} h_{2}+k_{1} k_{2}+l_{1} l_{2}}{\sqrt{\left(h_{1}^{2}+k_{1}^{2}+l_{1}^{2}\right)\left(h_{2}^{2}+k_{2}^{2}+l_{2}^{2}\right)}}$
Resulting in the condition for two directions to be perpendicular $(\cos (T)=0)$ being: $\mathrm{h}_{1} \mathrm{~h}_{2}+$ $\mathrm{k}_{1} \mathrm{k}_{2}+\mathrm{l}_{1} \mathrm{l}_{2}=0$

Given direction $\left[h_{1} k_{1} l_{1}\right]=[111]$ the numerator $h_{1} h_{2}+k_{1} k_{2}+l_{1} l_{2}=0$ reduces to $h_{2}+k_{2}+l_{2}$ $=0$. There are an infinite number of choices to satisfy this. Two specific ones are: $[1,0, \overline{1}]$ and $[1,1, \overline{2}]$

