

Ch/ChE 140a
Problem Set #1
Due: Thurs. Jan.31st 2008
SHOW ALL OF YOUR WORK!
160 points total

Please read chapters 1-3 (pp. 1-86) of Advanced Semiconductor Fundamentals by Pierret.

(50 points)

1. The purpose of this question is to help you gain an understanding of some of the numbers relevant to semiconductors. The calculations in this section are not difficult but the answers will hopefully be illuminating.

Table 1: Lattice Constant, a_0 , values for Si, Ge and GaAs.

Semiconductor	Lattice Constant (Å)
Si	5.43095
Ge	5.646
GaAs	5.6533

First let's examine the different crystallographic faces and see how they differ.

- a. Calculate the number of silicon atoms per square centimeter (# Si atoms/cm²) on the (111), (100) and (110) faces. Which face has the most Si atoms/cm²? It might be helpful to either build a model or look at the one on my desk. HINT: first use basic trigonometry to calculate the area of the crystallographic face in terms of a_0 , then divide the number of atoms on this face by the area you just calculated, plugging in the a_0 value for Si from Table 1.

(20 points)

- b. Most surface modification techniques done in our lab are performed using Si sample sizes on the order of 1 cm² or less. Given your answer in part a comment on the experimental sensitivity required to observe a monolayer of surface-bound species. (*i.e.* compare the number of Si surface atoms/cm² to the number of molecules in 1 mL of a 1 mM solution of analyte. This is just to give you a numerical idea of the sensitivity required for surface science over conventional solution based techniques.)

(5 points)

Now let's look at some of the bulk properties.

- c. Calculate the volume of the Si unit cell in cm³. (5 points)
- d. Calculate the number of Si atoms per cubic centimeter, $\rho_a(\text{Si})$ (# Si atoms/cm³). How does this value compare to Avogadro's number (or the number of molecules in a mol)? (5 points)
- e. Compare the density of Si atoms to typical dopant densities ranging from $N_D = 10^{13} - 10^{16} \text{ cm}^{-3}$. Is $N_D/\rho_a(\text{Si})$ in the range of ppt, ppm, ppb? In terms of a reference, experimentalists are happy if they can get the concentration of oxygen

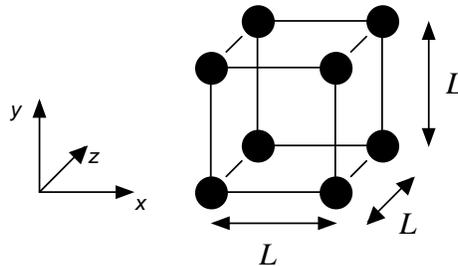
in a glove box to less than a ppm for oxygen sensitive experiments, and they consider such experiments essentially “oxygen-free.” What does this tell you about doping in general and the device control performed by semiconductor manufacturing companies? (15 points)

(85 points)

2. In class it was presented that the wavefunction:

$$\Psi_{3D}(x, y, z) = A \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$$

is a solution to the particle in a three dimensional cubic box of dimension, L , as shown below. Outside the box the potential energy is infinitely high. For this reason the wavefunction is forced to be zero at any point on the cube surface, in other words, the boundary conditions are $\Psi_{3D}(x,y,z=0) = 0$ and $\Psi_{3D}(x,y,z=L) = 0$.



a. Plug this wavefunction into the Schrödinger equation and show that this is in fact a solution. (5 points)

The potential, $U(x,y,z)$, everywhere inside the box is zero and infinite outside the box. Since we're looking at a wavefunction inside the box, $U(x,y,z)=0$ so the Hamiltonian is shortened to only account for the kinetic energy.

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + U(x, y, z) \Psi = \epsilon \Psi \quad \text{-----} \rightarrow \quad -\frac{\hbar^2}{2m} \nabla^2 \Psi = \epsilon \Psi$$

All we have to do is derive $\Psi_{3D}(x,y,z)$ twice and multiply by $-\hbar/2m$.

$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

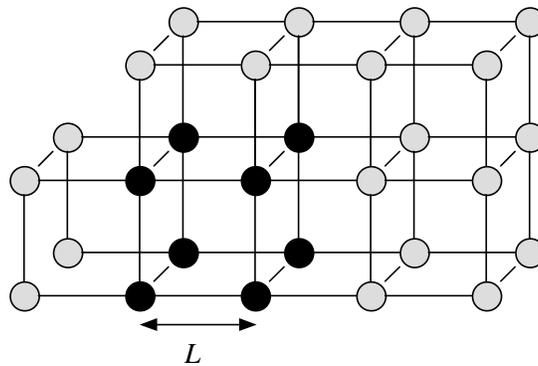
$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) A \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) =$$

$$A \left(\frac{n_x \pi}{L}\right) \cos\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) + A \left(\frac{n_y \pi}{L}\right) \sin\left(\frac{n_x \pi x}{L}\right) \cos\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) + A \left(\frac{n_z \pi}{L}\right) \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \cos\left(\frac{n_z \pi z}{L}\right)$$

It's important to note that even though we've placed atoms at distances, L , apart in this 3D space and invoked a periodicity requirement of period, L , on the wavefunction

b. What is the energy? (5 points)

When the cubic 3D box (or unit cell) is repeated infinitely in all directions as (partially depicted) below, Ψ_{3D} is no longer a valid solution for this repeated network.



Instead, the function (described in class):

$$\Psi_{rep}(r) = \exp(ik \cdot r)$$

is a correct solution to the periodic repetition of the 3D box. To answer the next set of questions, just examine one dimension; the trends can be extended to 3 dimensions. For example, use:

$$\Psi_{3D}(x) = A \sin\left(\frac{n_x \pi x}{L}\right)$$

$$\Psi_{rep}(x) = \exp(ikx)$$

c. Why is $\Psi_{3D}(x)$ no longer a valid solution for the periodic repetition along the x -axis? (Hint: one boundary condition is relaxed while a new boundary condition is required once periodicity is required.) Comment on the difference in boundary

conditions for the 3D box and the repeated 3D box. Show how $\Psi_{3D}(x)$ fails one of these conditions. (10 points)

d. Show that $\Psi_{rep}(x)$ satisfies all the boundary conditions. (5 points)

e. Show that $\Psi_{rep}(x)$ is also a solution to the Schrödinger equation. What is the energy? (10 points)

f. The probability density, $p(x)$ of finding an electron at a given position, x , (within this infinitely repeated 3D box) is given by

$$p(x) = \Psi^*(x)\Psi(x)$$

where $\Psi^*(x)$ is the complex conjugate of $\Psi(x)$. Calculate $p(x)$ for $\Psi_{rep}(x)$. Does the probability density, $p(x)$ show any effect from the crystal lattice? (10 points)

g. A good model should describe a periodic probability density in registry with the crystal lattice atoms. Consider the following standing waves:

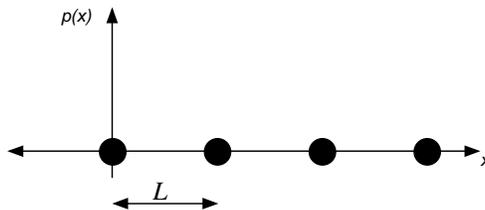
$$\psi(+)=\exp\left(\frac{i\pi x}{L}\right)+\exp\left(\frac{-i\pi x}{L}\right)=2\cos\left(\frac{\pi x}{L}\right)$$

$$\psi(-)=\exp\left(\frac{i\pi x}{L}\right)-\exp\left(\frac{-i\pi x}{L}\right)=2i\sin\left(\frac{\pi x}{L}\right)$$

g1. Are these wavefunctions periodic in L ; do they adhere to the same boundary conditions imposed above for the infinitely-repeated 3D cell? (10 points)

g2. Is the probability density periodic in L ? Does the probability density adhere to the boundary conditions imposed above? (10 points)

g3. Draw a picture of the probability densities for each wavefunction on an x -axis with atoms placed at length L apart as below. (10 points)



g4. Which wavefunction, $\psi(+)$ or $\psi(-)$, would you think is lower in energy and why? (Consider the atoms to be slightly positively charged.) (10 points)

A good model would show that the electron has slightly lower potential energy near the positively charged lattice atoms as indicated above. This is done more rigorously by adding a potential energy term, $U(x)$ (where $U(x)$ is periodic with the crystal lattice), to the Hamiltonian we used before, so that the total Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + U(x)\Psi = \epsilon\Psi$$

The Kronig-Penney model uses a square-well periodic potential and the derivation is given in the text. The derivation is beyond the scope of this class but the conceptual basis should be understood.

- (25 points)
3. Attached is an E vs. k diagram. Zero on the energy scale indicates the top of the valence band edge. (At zero temperature, all states below zero energy would be filled with electrons and all states above zero energy would be empty.)
- Is this a direct gap or indirect gap semiconductor? (5 points)
 - Approximate the band gap energy? (It's hard to get a precise number from the diagram) (5 points)
 - If this semiconductor were a solar cell, comment on the current and voltage output you would expect. Would you want to use this semiconductor as a solar cell? What would be a good application for this semiconductor? (15 points)