

## Homework #1: Crystal Structure and Intro to Quantum Mechanics

### Problem 1:

Objective: Exposure to crystal structure.

- (a) Do problem 1.9 **part (a)**. Don't forget that surface atoms are also shared with adjacent unit cells.
- (b) Do problem 1.10 **part (b)**. The sketch of the atomic arrangement on the  $\{110\}$  plane given in class will help.
- (c) InP has the same crystal structure as GaAs. Sketch the atomic arrangement of In and P in the (100) plane. Be sure to label which atoms are In and which are P.
- (d) Based on the graph on slide 33 from section 1 of the notes, what four ternary (3-element) compounds could one grow on InP while remaining "lattice matched"? There is no need to give the exact alloy compositions, just give the three elements for each.
- (e) Determine the Miller indices for a plan that intersects x-, y-, and z-axes at  $1a$ ,  $2a$ , and  $3a$ , respectively ( $a$  is the crystal-lattice constant).
- (f) Determine the Miller indices for a plan that intersects x-, y-, and z-axes at  $2a$ ,  $2a$ , and  $2a$ , respectively.

Here are the problems from the book in case you don't have it yet:

**1.9** What is the density of atoms at the surface of a simple cubic crystal, if the crystal is terminated at

- (a)  $\{100\}$  plane
- (b)  $\{110\}$  plane
- (c)  $\{111\}$  plane **A**

The crystal-lattice constant is  $a = 0.5$  nm.

**1.10** How many silicon atoms per unit area are found in

- (a)  $\{110\}$  plane **A**
- (b)  $\{111\}$  plane

### Problem 2:

Objective: Exposure to crystal structure.

Go to Virginia Semiconductors' website (<https://www.virginiasemi.com>) and browse their selection of in stock wafers. There are LOTS of wafer vendors, but Virginia Semiconductor has a few unusual wafers that make this question a bit more interesting.

- (a) What range of wafer diameters is available?

For 100 mm diameter, single side polished (SSP) wafers,

- (b) What crystal orientations are available?
- (c) What dopants are available? For each dopant indicate whether it would make the material n-type or p-type.
- (d) What range of wafer thicknesses are available?
- (e) What is a typical price for one wafer?

**Problem 3:**

Objective: Exposure to crystal structure.

Copper has the same FCC crystal structure as gold (see slide 27 from section 1). Assume one electron from each copper atom is free to conduct electricity (it is shared by all the atoms in the crystal). Estimate the concentration of free electrons (per  $\text{cm}^3$ ), knowing that the lattice constant of copper is  $3.62\text{\AA} = 3.62 \times 10^{-8}\text{cm}$ .

**Problem 4:**

Objective: 1. Understanding of ... basic quantum mechanics.

Calculate the wavelength and wavenumber for the following free electrons:

(a) An electron with velocity  $1 \times 10^5 \text{ m/s}$  (this is roughly the thermal velocity of an electron at room temperature). How does this compare to typical lattice constants of the materials we have seen?

(b) An electron with kinetic energy of  $1.6 \times 10^{-19} \text{ J}$  (this is 1 eV).

(c) An electron with kinetic energy of 1000 eV (this is a reasonable energy in an electron microscope; although, it is on the low end of what is typically used).

**Problem 5:**

Objective: 1. Understanding of ... basic quantum mechanics.

(a) Show that a simply travelling wave described by  $\psi(x) = A_+ e^{jkx}$  satisfies the time independent Schrodinger equation if  $k \equiv \sqrt{2mE / \hbar^2}$ .

(b) In class we discussed the energy momentum (or  $E$ - $k$ ) relationship for a free particle.  $E$ - $k$  relationships prove to be important for understanding the energy-band theory of semiconductors. To become more familiar with this concept, plot or sketch  $E$  vs.  $\hbar k$  for the free electron ( $m_e = 9.11 \times 10^{-31} \text{ kg}$ ) and  $E$  vs.  $\hbar k$  for a particle with half the electron mass ( $m = 4.56 \times 10^{-31} \text{ kg}$ ) on the same graph. Which particle yields an  $E$ - $k$  relationship with larger curvature (or, equivalently, the larger second derivative)? A reasonable energy range to plot might be  $0 < E < 1.6 \times 10^{-17} \text{ joules}$  ( $E < 100 \text{ eV}$ ).

The key insight to take away from this problem is the dependence of shape of the curve on mass. We will see this type of plot again when we study the effective mass of electrons and holes in a semiconductor.

**Problem 6:**

Objective: 1. Understanding of ... basic quantum mechanics.

Consider a Gaussian wave packet described by  $\psi(x) = A e^{-(\sigma_k^2 x^2 / 2)} e^{-jk_0 x}$  where we have neglected the time dependence.

- What is the probability distribution,  $|\psi(x)|^2 = \psi^* \psi$ , associated with this wave packet?
- At what value of  $x$  does  $|\psi(x)|^2$  drop to  $1/e$  of its maximum value? (This is one way to define the width of the probability distribution).
- If the probability distribution changes so that its spatial extent is reduced by half, how would the value of  $\sigma_k$  change?