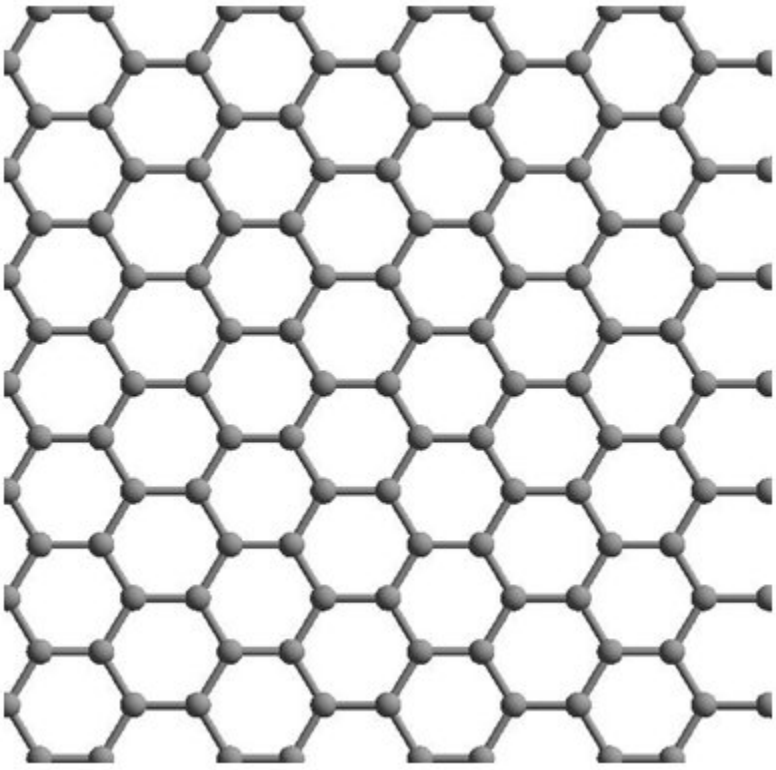
Solid State Devices I - Purdue ECE-606

Homework No. 1

Student name: _____
Student ID: _____

I solved the homework assignment myself without copying a solution from someone else or from the web. Student Initials here: _____

Problem 1.
Graphene is a 2D crystal with carbon atoms arranged in a honeycomb structure as shown below.



Using the above information and picture, answer the following questions

a. Assuming that the unit cell is a hexagon of carbon atoms, how many atoms of carbon are there in each unit cell?
(2 points)

b. What are the basis vectors needed to reproduce the whole crystal in 2D space?
(4 Points)

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Problem 1a Solution (2 points)

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Problem 1b Solution (4 points)

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Problem 2.
Find the number and relative positions of all nearest and second-nearest neighbors of a lattice point in a simple cubic Bravais lattice.
(8 points)
Problem 2 Solution (8 points):

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Problem 3.

(a) Packing fraction in two dimensions: A two-dimensional crystal is constructed by packing circles. The ratio between the area occupied by the circles and the total area is referred as the packing fraction in two dimensions. Find the packing fraction for a two-dimensional square Bravais lattice.
(4 points)

(b) Repeat the same calculation for a two-dimensional triangular lattice.
(4 points)

(c) Which one of the two is more closely packed?
(2 points)

Problem 3a Solution (4 points)

Problem 3b Solution (4 points)

Problem 3c Solution (2 points)

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Problem 4. (10 points)
Show that the angle between two planes (or two directions) is

$$\cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^{\,2} + k_1^{\,2} + l_1^{\,2}}\sqrt{h_2^{\,2} + k_2^{\,2} + l_2^{\,2}}}$$

[h_i , k_i , l_i] are the miller indices of the two planes, where i = 1 , 2

Problem 4 Solution (10 points):

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Problem 5. For silicon (Fig. 1.5a in ASF), answer the following questions:

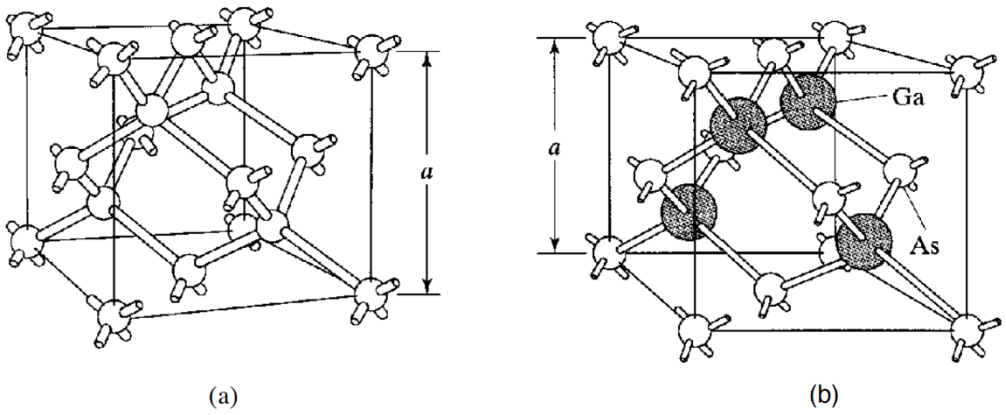

Figure 1.5 (a) Diamond lattice unit cell. (b) Zincblende lattice unit cell (GaAs used for illustration). [Cal After Shocklcy;[5] (b) after Sze.[16]] Reprinted with permission.]

a. How many Si atoms per sq. cm are there on a (100) plane?
(4 points)

b. How many on a (110) and (111) plane?
(4 points)

Problem 5a Solution (4 points)

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Problem 5b Solution (4 points)

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Problem 6.
The density of BCC iron is 8,000 kg/m^3. Determine the lattice constant of the cubic unit cell. (4 points)

Problem 6 Solution (4 points)

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Problem 7.
Above, you worked out the nearest, second nearest neighbors and their coordinate positions for a simple cubic lattice. Repeat the same exercise for a bcc and fcc lattice and work out the following related sub-parts.

a) Find the number and relative positions of all nearest and second-nearest neighbors of a lattice point in a bcc Bravais lattice.
(8 points)
b) Find the number and relative positions of all nearest and second-nearest neighbors of a lattice point in a fcc Bravais lattice.
(8 points)
c) What type of lattice is the silicon crystal?
(2 points)
d) How many silicon atoms we have in each unit cell?
(2 points)
e) What are the fractional coordinates for each silicon atom in the unit cell?
(2 points)

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Problem 1a Solution (8 points)

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Problem 1b Solution (8 points)

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Problem 1c Solution (2 points)

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Problem 1d Solution (2 points)

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Problem 1e Solution (2 points)

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Problem 8.
Visualize a zinc blende crystal system from three different directions [100], [110], [111] taken from three different crystal cuts.
Utilize the Crystal Viewer Tool in ABACUS on nanoHUB. The tool can be found at:
https://nanohub.org/tools/abacus (you will need a free nanoHUB login)
(4 points each – 12 points total)

Problem 8a Solution [100] (4 points)

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Problem 8b Solution [110] (4 points)

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Problem 8c Solution [111] (4 points)