Columbia University
Department of Electrical Engineering
Solid State Devices and Materials
ELEN E3106/4106
Homework #1

Due: Friday, September 12th by 5pm
Goal: Practice simple calculations on crystals and understand the notation system for planes and directions.
Instructions: Show your work and include units in answers for full credit. For the multiple-choice questions, please clearly mark your selection. No credits will be given for answers without supporting work or explanation, even if the final value is correct.
Points: 110 pts for 3106. 130 pts for 4106.

- **Problem 1 (30 pts)**
  (a) Sketch a bcc unit cell with a monoatomic basis. Label the (110) plane and both side lengths of the plane in terms of the lattice constant, a. (6 pts)
  (b) If the atomic density is $1.6 \times 10^{22} cm^{-3}$, calculate the lattice constant and choose the correct answer. (8 pts)
  (1)3.96 Å (2)5 Å (3)6.29 Å (4)7.93 Å
  (c) What is the atomic density per unit area on the (110) plane? Choose the correct answer. [Hint: Refer to your diagram in (a) to find the # of atoms in the plane and the area of the plane, and use your lattice constant value from (b)] (8 pts)
  (1)$5.65 \times 10^{14}\ cm^{-2}$ (2)$2.82 \times 10^{14}\ cm^{-2}$ (3)$1.13 \times 10^{14}\ cm^{-2}$ (4)$5.65 \times 10^{15} cm^{-2}$
  (d) What is the radius of each atom? Choose the correct answer. (8 pts)
  (1)1.08 Å (2)2.16 Å (3)4.33 Å (4)8.66 Å

- **Problem 2 (30 pts)**

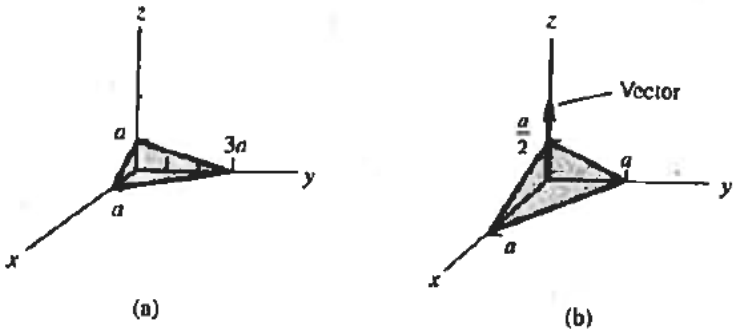

Figure P1.6

As shown in Fig. P1.6(a), a crystalline plane has intercepts of $1a$, $3a$, and $1a$ on the x, y, and z axes, respectively. a is the cubic cell side length.
(a) What is the Miller index notation for the plane? Choose the correct answer. (10 pts)
(1) **(101)** (2) **(131)** (3) **(313)** (4) **(010)**

(b) What is the Miller index notation for the direction normal to the plane? Choose the correct answer. (5 pts)
(1) **[101]** (2) **[131]** (3) **[313]** (4) **[010]**

As shown in Fig. P1.6(b), a crystalline plane has intercepts of $1a$, $1a$, and $1/2a$ on the x, y, and z axes, respectively, with a vector pictures in the z direction. a is the cubic cell side length. Assuming the crystal structure to be cubic,

(c) Determine the Miller indices for the plane in Fig. P1.6(b) and choose the correct answer. (10 pts)
(1) **(211)** (2) **(121)** (3) **(112)**

(d) Determine the Miller indices for the vector pictured in Fig. P1.6(b) and choose the correct answer. (5 pts)
(1) **[010]** (2) **[001]** (3) **[100]**

- **Problem 3 (18 pts)**
  Identify two crystalline directions in a cubic crystal which are perpendicular to
  (a) the $[100]$ direction (9 pts)
  (b) the $[111]$ direction (9 pts)

[Hint: The cosine of the angle θ between two arbitrary directions, $[h_1 k_1 l_1]$ and $[h_2 k_2 l_2]$, in a cubic crystal is

$$cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\left[\left(h_1^2 + k_1^2 + l_1^2\right)\left(h_2^2 + k_2^2 + l_2^2\right)\right]^{\frac{1}{2}}}$$

Consequently, for two directions to be perpendicular, $cos(\theta) = 0$ and one must have $h_1 h_2 + k_1 k_2 + l_1 l_2 = 0$]

- **Problem 4 (22 pts)**
  Review questions.
  (a) What is the difference between a diamond structure and a Zincblende structure? (3 pt)
  (b) List the three cubic bravais lattices (don't use abbreviations). (2 pt)
  (c) What type of crystal lattice structure does silicon have? (2 pt)
  (d) What sort of bonds exist in silicon? (3 pt)
  (e) Explain the concept of unit cell. What is a primitive unit cell? (4 pts)
  (f) Is silicon a compound semiconductor? Why or not? (4 pts)
  (g) Differentiate in words between crystalline, polycrystalline, and amorphous semiconductors and draw suitable diagrams. (4 pts)

- **Problem 5 (10 pts)**

For this problem, you will need to run the simulation program, Crystal Viewer (new interactive front end), which is part of the ABACUS Tool Suite on nanoHUB.org. The Assembly of Basic

Applications for Coordinated Understanding of Semiconductors (ABACUS) suite of simulation tools and supporting educational content will serve as an aid to our course. Be sure you have an account through your Columbia credentials, then proceed with the exercises below. .

(a) How many atoms form the basis of the following materials? Verify using the Crystal Viewer minimal basis. (1 pt each)
- Silicon (Si)
- Gallium Nitride (GaN)
- Molybdenum Disulfide (MoS_2)

(b) What are the crystals for the following materials? Verify using the Crystal Viewer. (1 pt each)
- Silicon
- Gallium Arsenide (GaAs)
- Gold (Au)

(c) Examine the textbook basis using the Bravais Viewer for the following crystals. Include screenshots of your findings. (1 pt each)
- Simple Cubic
- Body-centered cubic
- Face-centered cubic
- Simple trigonal

- **Problem 6 (Required for 4106 students ONLY, 20 pts)**

The lattice constant of a single crystal is 4.5Å. Calculate the surface density of atoms on the following planes for a face-centered cubic lattice structure and choose the correct answers.

(a) Plane (100)

(1)$1.97 \times 10^{15}\ cm^{-2}$ (2)$9.87 \times 10^{14}\ cm^{-2}$ (3)$4.93 \times 10^{14}\ cm^{-2}$

(b) Plane (110)

(1)$6.98 \times 10^{14}\ cm^{-2}$ (2)$9.87 \times 10^{14}\ cm^{-2}$ (3)$1.39 \times 10^{15}\ cm^{-2}$

(c) Plane (111)

(1)$2.85 \times 10^{14}\ cm^{-2}$ (2)$5.7 \times 10^{14}\ cm^{-2}$ (3)$1.14 \times 10^{15}\ cm^{-2}$