Solutions

Homework #1

Crystal Structure of Solids – *100 points*

DUE @ Beginning of Class: Thursday, September 7

1) Consider the surface of a Si wafer that has a (100) plane: (12 points)
   - a. Sketch the placement of Si atoms on the surface of the wafer.
   - b. Determine the number of atoms per cm^2 at the surface of the wafer.
   - c. Repeat part a., this time taking the surface of the Si wafer to be (110).
   - d. Repeat part b., this time taking the surface of the Si wafer to be (110).

2) Assuming a cubic crystal system with lattice constant a_0, make a sketch of the following planes being sure to label your axis and intersections: (16 points)

a. (001)	b. (111)	c. (123)	d. $(\bar{1}10)$
e. (010)	f. $(\bar{1}\bar{1}\bar{1})$	g. (221)	h. $(0\bar{1}0)$

3) Assuming a cubic crystal system, use an appropriately directed arrow to identify each of the following directions: (16 points)

a. [010]	b. [101]	c. $[00\bar{1}]$	d. [111]
e. [001]	f. [110]	g. $[0\bar{1}0]$	h. [123]

4) E-Book, problem 1.5 (15 points)

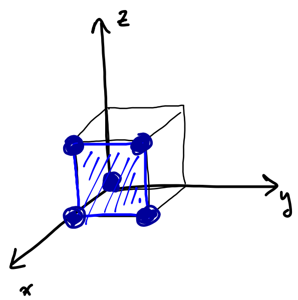
5) E-Book, problem 1.16 – show your steps clearly! (14 points)

6) E-Book, problem 1.20 (15 points)

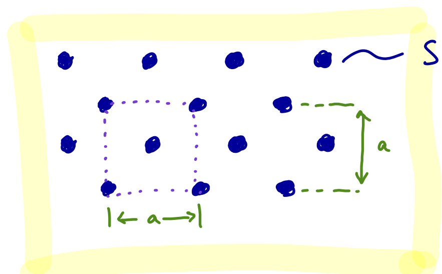
7) E-Book, problem 1.24 (12 points)

1) Consider the surface of a Si wafer that has a (100) plane: (12 points)
   a. Sketch the placement of Si atoms on the surface of the wafer.
   b. Determine the number of atoms per cm^2 at the surface of the wafer.
   c. Repeat part a., this time taking the surface of the Si wafer to be (110).
   d. Repeat part b., this time taking the surface of the Si wafer to be (110).

a) Looking at Fig. 1.11 in the E-book for the diamond lattice of Si, the (100) plane would be:



Si atoms on the surface:



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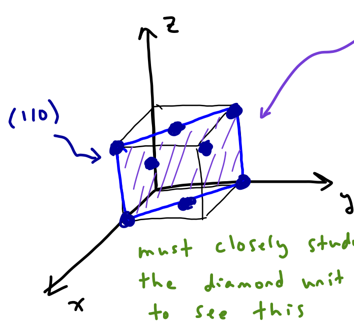
b) For Si at room temperature, $a = 5.43 \times 10^{-8}$ cm

From part a), there are : $\underbrace{4\left(\tfrac{1}{4}\right)}_{\text{corner atom}} + \underbrace{1}_{\text{center atom}} = 2$ atoms per a^2

$$\therefore \frac{2}{a^2} = \frac{2}{(5.43 \times 10^{-8}\ cm)^2} = \boxed{6.78 \times 10^{14}\ \text{Si atoms}/cm^2}$$ 3

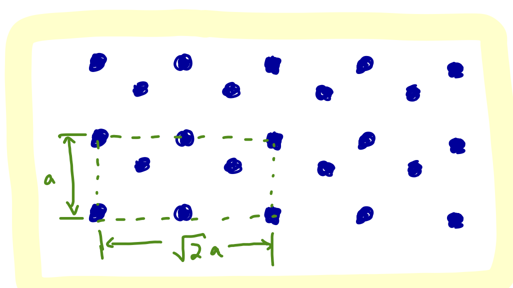
c) For a (110) plane :



must closely study the diamond unit cell to see this

The two atoms in middle could be closer to top (as shown) or bottom depending on orientation of unit cell used.

Si atoms on surface:



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d) $\underbrace{4\left(\tfrac{1}{4}\right)}_{\text{corner}} + \underbrace{2\left(\tfrac{1}{2}\right)}_{\text{middle}} + \underbrace{2}_{\text{center}} = 4$ atoms

$$\therefore \frac{4}{\sqrt{2}a^2} = \frac{4}{\sqrt{2}\,(5.43 \times 10^{-8}\ cm)^2} = \boxed{9.59 \times 10^{14}\ \text{Si atoms}/cm^2}$$ 3

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Fall 2017

2) Assuming a cubic crystal system with lattice constant a_0, make a sketch of the following planes being sure to label your axis and intersections: (16 points)

a. (001) b. (111) c. (123) d. $(\bar{1}10)$
e. (010) f. $(\bar{1}\bar{1}\bar{1})$ g. (221) h. $(0\bar{1}0)$

2 each

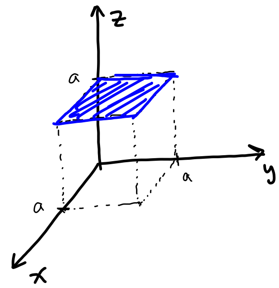
Must reverse the Miller indices procedure to find intercepts of the plane.

a) (0 0 1) reciprocate

$\frac{1}{0}, \frac{1}{0}, \frac{1}{1}$ x lattice constant

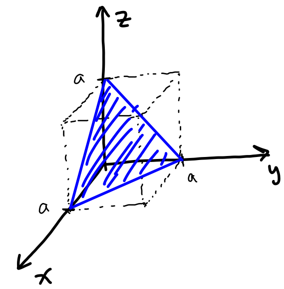
∞, ∞, a

$= A, = B, = C$ — intercepts



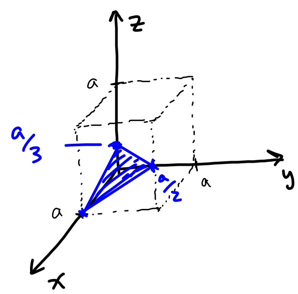
b) (1 1 1)

a, a, a



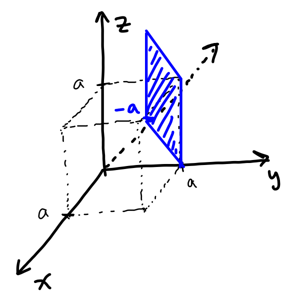
c) (1 2 3)

a, a/2, a/3



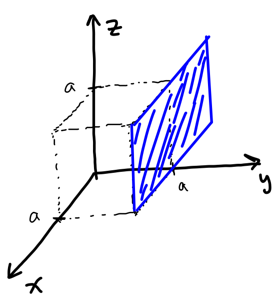
d) $(\bar{1}\, 1\, 0)$

−a, a, ∞



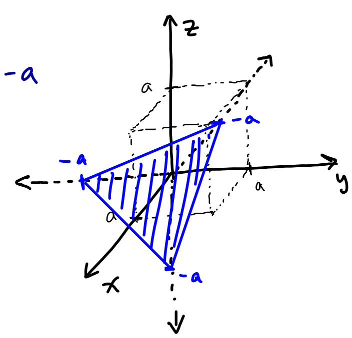
e) (0 1 0)

∞, a, ∞



f) $(\bar{1}\,\bar{1}\,\bar{1})$

−a, −a, −a

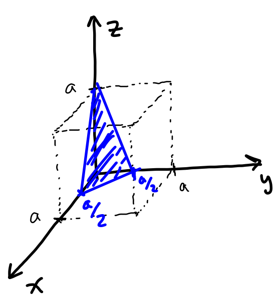


g) (2 2 1)

a/2, a/2, a

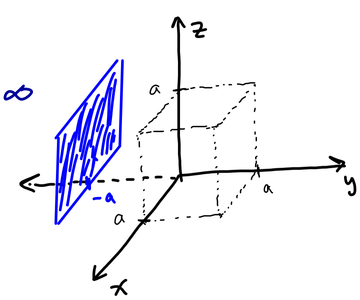
OR

×2 ⇒ a, a, 2a



h) $(0\,\bar{1}\,0)$

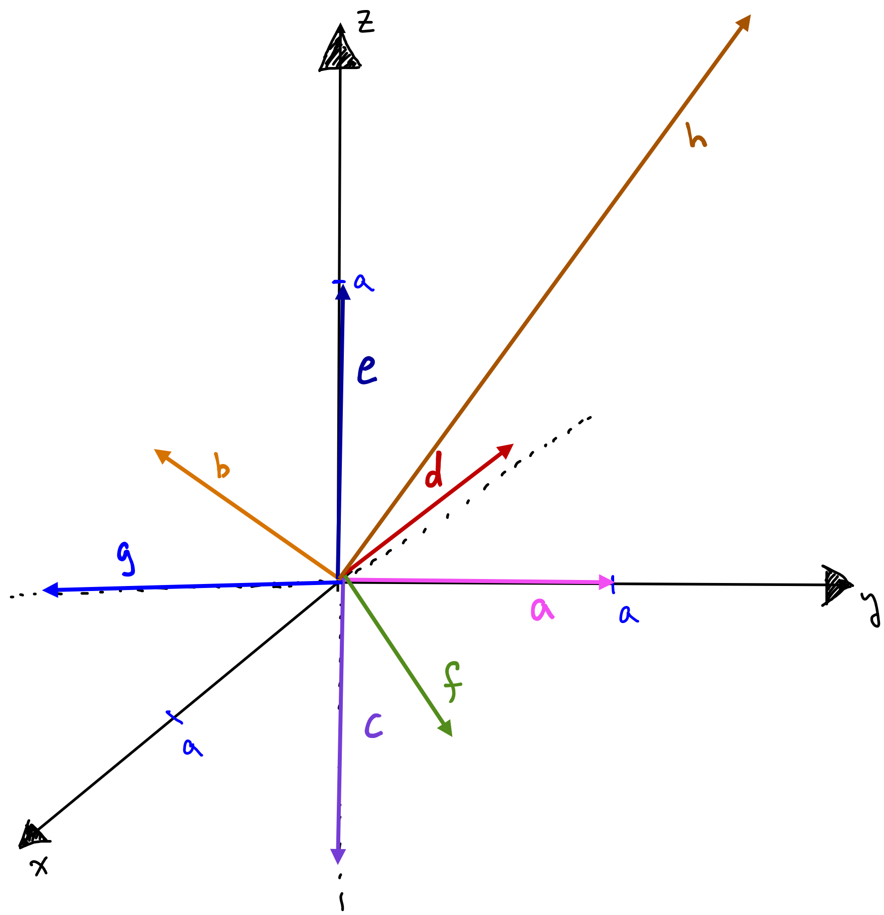
∞, −a, ∞



3) Assuming a cubic crystal system, use an appropriately directed arrow to identify each of the following directions: (16 points)

a. [010]	b. [101]	c. $[00\bar{1}]$	d. [111]
e. [001]	f. [110]	g. $[0\bar{1}0]$	h. [123]

2 each



4) E-Book, problem 1.5 (15 points)

1.5 The lattice constant of GaAs is $a = 5.65$ Å. Calculate (*a*) the distance between the centers of the nearest Ga and As atoms, and (*b*) the distance between the centers of the nearest As atoms.

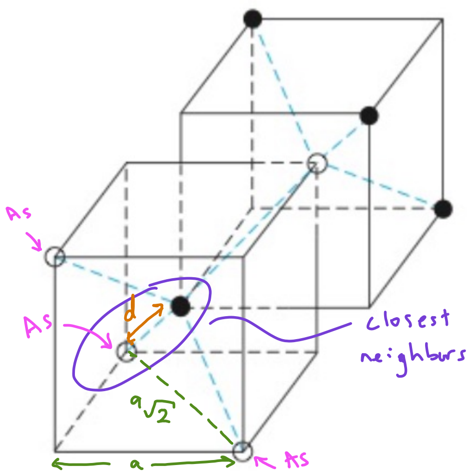


Figure 1.15 | The tetrahedral structure of closest neighbors in the zincblende lattice.

a) this is a tetrahedron, so apply geometrical principles of this shape gives:

$$d = \left(\frac{a}{2}\right)\left(\frac{\sqrt{3}}{2}\right) = 0.433\,a$$

$$= 0.433(5.65\text{ Å}) = \boxed{2.45\text{ Å}}$$

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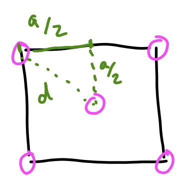
b) As atoms are in FCC config, so:



$$d = \sqrt{\frac{a^2}{4} + \frac{a^2}{4}} = \sqrt{\frac{2a^2}{4}} = \frac{\sqrt{2}}{2}a$$

$$= \frac{\sqrt{2}}{2}(5.65\text{ Å}) = \boxed{3.995\text{ Å}}$$

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5) E-Book, problem 1.16 – show your steps clearly! (14 points)

1.16 For a simple cubic lattice, determine the Miller indices for the planes shown in Figure P1.16.

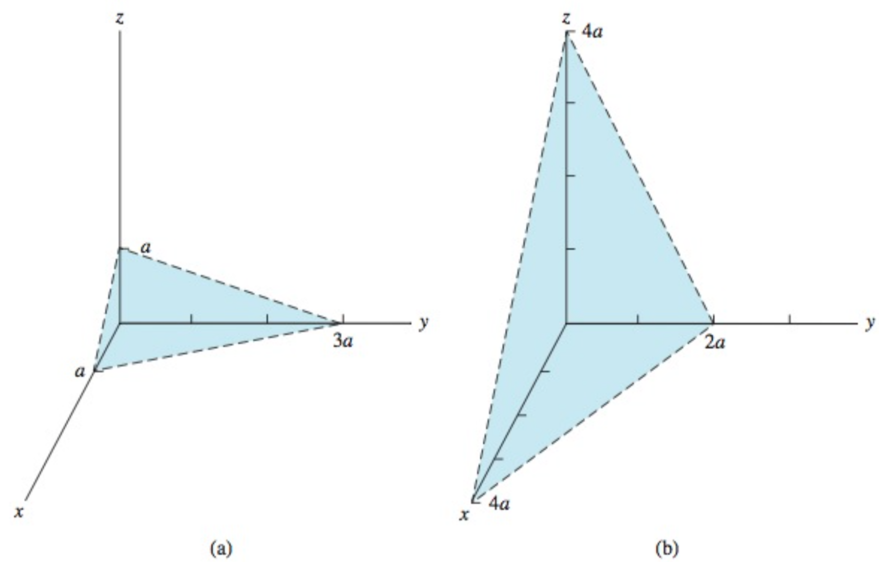


Figure P1.16 | Figure for Problem 1.16.

a) Intercepts: $A = a$, $B = 3a$, $C = a$

Reciprocal × a : $\frac{1}{\cancel{a}} \cdot \cancel{a}$ $\quad$ $\frac{1}{3\cancel{a}} \cdot \cancel{a}$ $\quad$ $\frac{1}{\cancel{a}} \cdot \cancel{a}$

× Integer n = 3 : 1 $\quad$ $1/3$ $\quad$ 1 $\quad$ $\times 3$

$h = 3$ $\quad$ $k = 1$ $\quad$ $l = 3$

$\therefore$ $\boxed{(3\ 1\ 3)}$ $\quad$ 7

☆ (h k l) answers must have NO commas and use parentheses.

b) Intercepts: $A = 4a$, $B = 2a$, $C = 4a$

Reciprocal × a : $1/4$ $\quad$ $1/2$ $\quad$ $1/4$ $\quad$ $\times 4$

× Integer n = 4 : $h = 1$ $\quad$ $k = 2$ $\quad$ $l = 1$

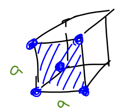
$\therefore$ $\boxed{(1\ 2\ 1)}$ $\quad$ 7

6) E-Book, problem 1.20 (15 points)

1.20 Determine the surface density of atoms for silicon on the (*a*) (100) plane, (*b*) (110) plane, and (*c*) (111) plane.

Lattice constant for Si: $a = 5.43\ \text{Å}$

a) (100) plane



corners center

$$\text{Surface density} = \frac{\#\ \text{atoms}}{\text{area}} = \frac{\frac{1}{4}(4) + 1}{a^2} = \frac{2}{(5.43\times10^{-8}\ \text{cm})^2} = \boxed{6.78\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$$

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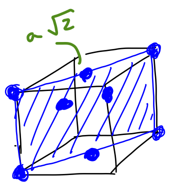
b) (110) plane (see problem 1c from this HW)

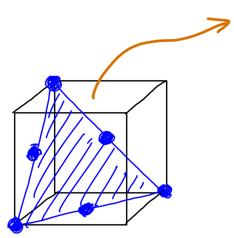


$$\text{Surface density} = \frac{\frac{1}{4}(4) + \frac{1}{2}(2) + 2}{a(a\sqrt{2})} = \frac{4}{a^2\sqrt{2}}$$

$$= \frac{4}{(5.43\times10^{-8}\ \text{cm})^2\sqrt{2}} = \boxed{9.59\times10^{14}\ \text{atoms/cm}^2}$$

4

c) (111) plane



area of plane $= \frac{1}{2}$ base × height , base $= a\sqrt{2} = 7.679\ \text{Å}$

use triangle to find height: $h^2 = (a\sqrt{2})^2 - \left(\frac{a\sqrt{2}}{2}\right)^2$

.... $h = 6.65\ \text{Å}$

$$\text{Surface density} = \frac{\frac{1}{6}(3) + \frac{1}{2}(3)}{\frac{1}{2}\,b\cdot h} = \frac{2}{\frac{1}{2}(7.679\times10^{-8}\ \text{cm})(6.65\times10^{-8}\ \text{cm})}$$

$$= \boxed{7.83\times10^{14}\ \frac{\text{atoms}}{\text{cm}^2}}$$

8

7) E-Book, problem 1.24 (12 points)

1.24 (*a*) If 5×10^{17} phosphorus atoms per cm^3 are add to silicon as a substitutional impurity, determine the percentage of silicon atoms per unit volume that are displaced in the single crystal lattice. (*b*) Repeat part (a) for 2×10^{15} boron atoms per cm^3 added to silicon.

a) Density of Si atoms:

$$N = \frac{\text{atoms / unit cell}}{\text{volume unit cell}} = \frac{8}{a^3} = \frac{8}{(5.43\times10^{-8}\ cm)^3} = 5\times10^{22}\ \text{atoms}/cm^3$$ 5

$$\therefore \frac{5\times10^{17}\ \text{P atoms}/cm^3}{5\times10^{22}\ \text{Si atoms}/cm^3}\times 100\% = \boxed{10^{-3}\ \%}$$ 3

b) $$\therefore \frac{2\times10^{15}\ \text{B atoms}/cm^3}{5\times10^{22}\ \text{Si atoms}/cm^3}\times 100\% = \boxed{4\times10^{-6}\ \%}$$ 4