CHAPTER 1

1.1

(a) From Table 1.1...
(i) Si or Ge
(ii) AlP, AlAs, AlSb, GaN, GaP, GaAs, GaSb, InP, InAs, or InSb

(b) Crystalline material has the same atomic pattern or order throughout the material, while polycrystalline material has crystalline subsections that are misaligned with respect to each other.

(c) A *unit cell* is a small portion of a crystal that could be used to reproduce the crystal. (The preceding is from the first sentence of Subsection 1.2.1.)

(d)

Unit cell	Atoms/unit cell
simple cubic.....	1
bcc.....	2
fcc.....	4
diamond.....	8

(e) $1\text{Å} = 10^{-8}$ cm

(f) a (one lattice constant)

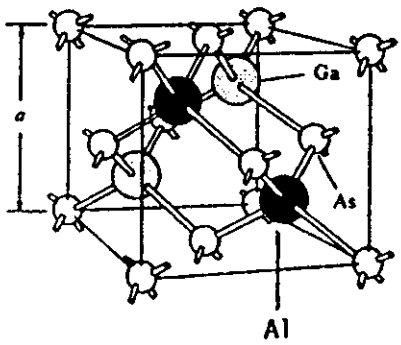
(g) 4

(h) As summarized in Table 1.3: ( )--crystal plane, { }--equivalent planes, [ ]--crystal direction, and < >--equivalent directions.

(i) See Subsection 1.3.2.

1.2

In the $Al_{0.5}Ga_{0.5}As$ unit cell, pictured below, fcc sublattice sites containing the Column III elements are equally occupied by Al and Ga atoms.



1.3

(a) Ge crystallizes in the diamond lattice where there are 8 atoms per unit cell (see Subsection 1.2.3). Thus

$$\text{DENSITY} = \frac{8}{a^3} = \frac{8}{(5.65 \times 10^{-8})^3} = \mathbf{4.44 \times 10^{22}\ atoms/cm^3}$$

1.4

(a) From Fig. 1.3(c), we conclude nearest-neighbors in the bcc lattice lie along the unit cell body diagonal. Since the body diagonal of a cube is equal to $\sqrt{3}$ times a cube side length (the lattice constant a),

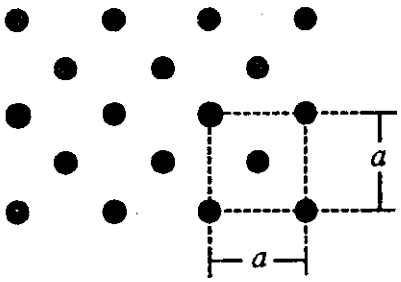
$$\left(\frac{\text{Nearest-Neighbor}}{\text{Distance}}\right) = \frac{\sqrt{3}}{2}a$$

(b) From Fig. 1.3(d), nearest-neighbors in the fcc lattice are concluded to lie along a *cube-face* diagonal. The diagonal of a cube face is equal to $\sqrt{2}$ times a cube side length. Thus

$$\left(\frac{\text{Nearest-Neighbor}}{\text{Distance}}\right) = \frac{\sqrt{2}}{2}a$$

1.5

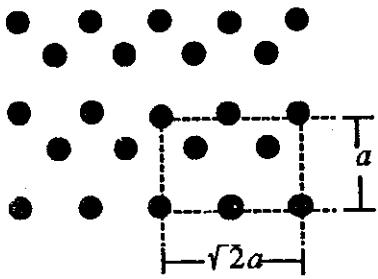
(a) Looking at Fig. 1.4(a) one concludes



(b) For Si at room temperature $a = 5.43 \times 10^{-8}$ cm. From the above figure one concludes that there are (1/4 × 4 corner atoms) + 1 body atom = 2 atoms per an area of a^2 on the (100) surface. Thus one has

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

(c) For a (110) plane one has the atom placement pictured below



(d) On the (110) plane in the area $a \times \sqrt{2}a$ one has (1/4 × 4 corner atoms) + (1/2 × 2 edg atoms) + 2 body atoms = 4 atoms. Thus one has

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

(e) MATLAB program script (paralleling Exercise 1.3)...

```
%Solution to Problem 1.5(e)
N=input('input number of atoms on (100) face of unit cell, N = ');
a=input('lattice constant in angstrom, a = ');
surfaceden=N*(1.0e16)/(a^2)      %number of atoms/cm^2
```

(Note: This and all other problem solutions are available on disk.)

1.6

(a) (i) Following the procedure outlined in the text

1, 3, 1	...intercepts (normalized)
1, 1/3, 1	...[1/intercept]s
3, 1, 3	...reduction to lowest whole-number set
(313)	...Miller index notation for plane

(ii) As noted in the text near the end of Subsection 1.2.4, the normal to a plane in the cubic crystal system has the same Miller indices as the plane.

[313]	...Miller index notation for normal to plane

(b) (i) Again following the Miller indexing procedure,

1, 1, 1/2	...normalized intercepts
1, 1, 2	...[1/intercept]s
1, 1, 2	...lowest whole-number set
(112)	...Miller indices of plane

(ii) Assume the vector has a length d. Its projections along the x, y, and z axes are then 0, 0, and d, respectively. Reducing to the lowest possible whole-number set and enclosing in square brackets, then yields

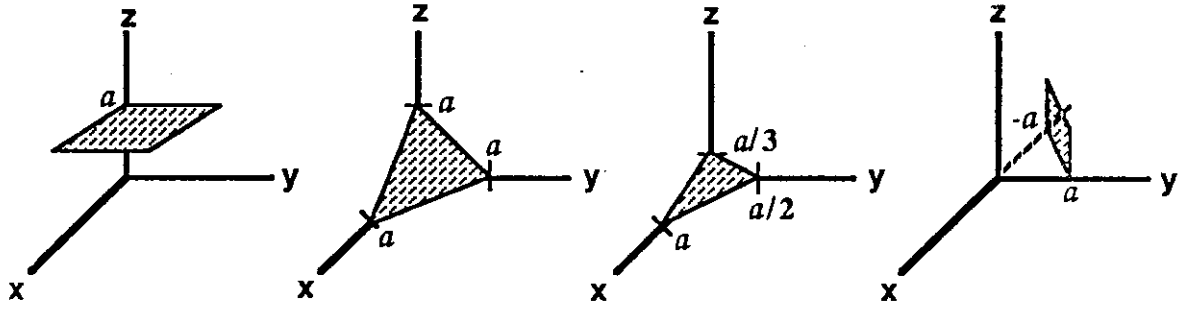
[001] ...Miller indices of direction vector

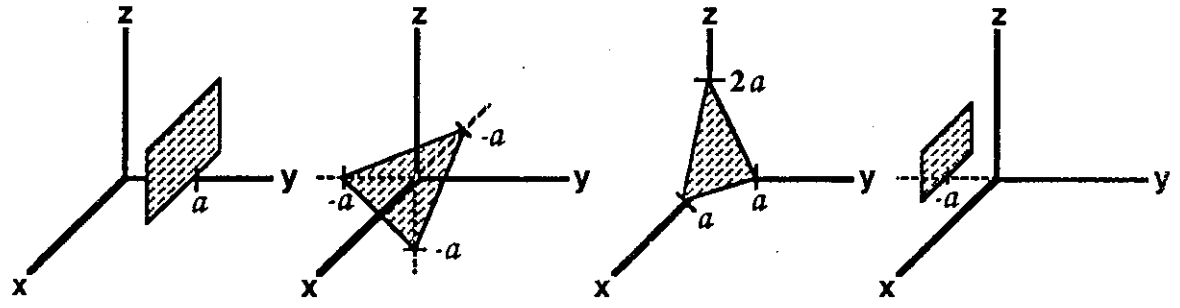
1.7

For each of the given planes, the Miller indexing procedure must be reversed to determine the intercepts of the given plane on the coordinate axes. Using part (c) as an example, one proceeds as follows:

(123) ...Miller indices
1, 2, 3 ...[1/intercept]s
1,1/2,1/3 ...intercepts

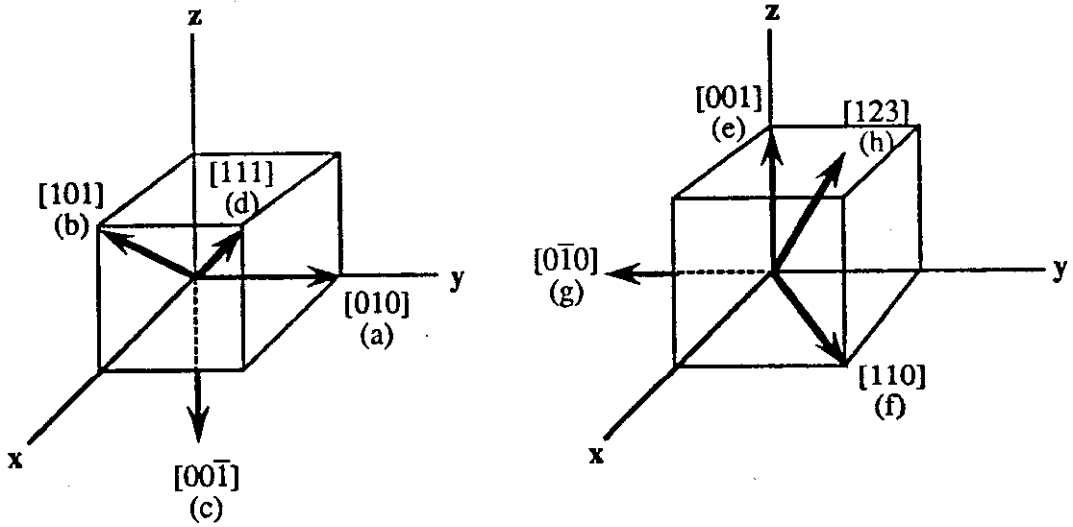
The plane in question intercepts the x, y, z coordinate axes at a, $a/2$, and $a/3$, respectively. Note that any multiple of the cited intercept set – such as $3a$, $2a$, a – would also be correct. All such planes are parallel equivalent planes.





1.8

Miller indices may be viewed as specifying the projection (in arbitrary units) of the to-be-pictured vectors along the coordinate axes. For example, [010] corresponds to a vector with a unit projection along the y-axis and no projection along the x- or z-axes. In other words, [010] is coincident with the $+y$ coordinate axis. The other required direction vectors are deduced in a similar manner and are as pictured below.



1.9

As noted in the problem statement, two directions $[h_1k_1l_1]$ and $[h_2k_2l_2]$ will be mutually perpendicular if

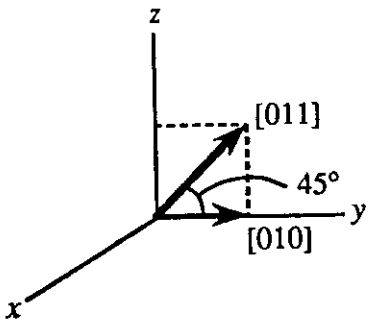
$$h_1h_2 + k_1k_2 + l_1l_2 = 0$$

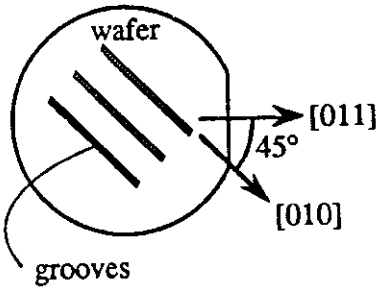
(a) Here $[h_1k_1l_1] = [100]$, requiring $h_2 = 0$. *All directions* $[0k_2l_2]$ *are perpendicular t* [100]. Two specific simple examples are [001] and [011].

(b) Given $[h_1k_1l_1] = [111]$, one requires the Miller indices of the perpendicular direction t be such that $h_2 + k_2 + l_2 = 0$. Two specific examples are [01$\bar{1}$] and [11$\bar{2}$].

1.10

As shown in the following left-hand figure, when the [011] and [010] directions are pictured simultaneously, it becomes obvious that the angle between the two directions is 45°. Alternatively, the angle between the two directions can be computed using the $\cos(\theta)$ relationship in Problem 1.9. Specifically, given $[h_1k_1l_1] = [011]$ and $[h_2k_2l_2] = [010]$, $\cos(\theta) = 1/\sqrt{2}$ and $\theta = 45°$. The required positioning of the "grooves" on the wafer's surface is pictured in the following right-hand figure.



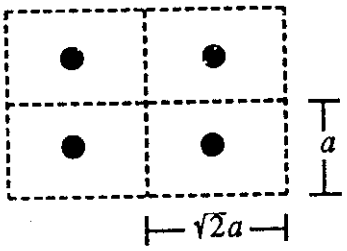


1.11

(a) If the Fig. P1.11 unit cell is conceptually copied and the cells stacked like blocks in a nursery, one concludes the resulting latttice is a simple cubic lattice.

(b) There is one atom inside the unit cell and the unit cell volume is a^3. Thus atoms/unit volume = $1/a^3$.

(c) For a (110) surface plane the atom positioning would be as pictured below.



$$\frac{\text{atoms}}{\text{unit area}} = \frac{1 \text{ atom}}{(a)(\sqrt{2}a)} = \frac{1}{\sqrt{2}a^2}$$

(d) [111] ... The specified vector has equal projections on the three coordinate axes.

1.12

Equivalent planes: (a) 6, (b) 12, (c) 8.

Equivalent directions: (d) 6, (e) 12, (f) 8.

NOTE: The answers may be deduced from geometrical considerations – or – by noting the total number of possible combinations of the given, and negatives of the given, Miller indices.

1.13

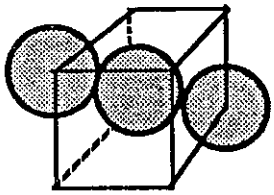
(a) In the simple cubic lattice the nearest-neighbor distance is a, where a is the side length of the cube, and the atomic radius r is therefore $a/2$. Moreover, there is one atom per unit cell. Thus

$$\text{Occupied volume} = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi (a/2)^3 = \pi a^3/6$$

$$\text{Total cell volume} = a^3$$

$$\text{Ratio} = \frac{\text{Occupied volume}}{\text{Total volume}} = \frac{\pi}{6}$$

(b) In the body centered cubic lattice the atom in the center and any one of the cube corner atoms are nearest neighbors. Thus 1/2 the nearest neighbor distance is $r = \sqrt{3}\, a/4$. Also, there are two atoms per unit cell.



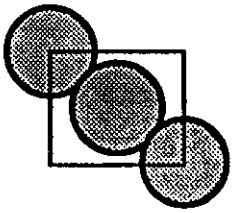
$$\text{diagonal} = 4r = \sqrt{3}\, a$$

$$\text{Occupied volume} = 2(\frac{4}{3}\pi r^3) = \frac{8}{3}\pi (\sqrt{3}\, a/4)^3 = \frac{\sqrt{3}}{8}\pi a^3$$

$$\text{Total cell volume} = a^3$$

$$\text{Ratio} = \frac{\text{Occupied volume}}{\text{Total volume}} = \frac{\sqrt{3}\pi}{8}$$

(c) For a face centered cubic lattice, the closest atoms lie in a cube face. Also, there are four atoms per unit cell in the fcc lattice.



face diagonal $= 4r = \sqrt{2}\,a$; $r = \sqrt{2}\,a/4$

Occupied volume $= 4(\frac{4}{3}\pi r^3) = \frac{16}{3}\pi(\sqrt{2}\,a/4)^3 = \frac{\sqrt{2}}{6}\pi a^3$

Total volume $= a^3$

Ratio $= \frac{\sqrt{2}\pi}{6}$

(d) As emphasized in Fig. 1.4(c), the atom in the upper front corner of the unit cell and the atom along the cube diagonal 1/4 of the way down the diagonal are nearest neighbors. Since the diagonal of the cube is equal to $\sqrt{3}$ times a cube side length, the center-to-center distance between nearest-neighbor atoms in the diamond lattice is $\sqrt{3}\,a/4$, and the atomic radius $r = \sqrt{3}\,a/8$. Moreover, there are eight atoms per unit cell in the diamond lattice. Thus

Occupied volume $= 8(\frac{4}{3}\pi r^3) = \frac{32}{3}\pi(\sqrt{3}\,a/8)^3 = \frac{\sqrt{3}}{16}\pi a^3$

Total volume $= a^3$

Ratio $= \frac{\sqrt{3}\pi}{16}$