

tially identical to the diamond lattice, except that lattice sites are apportioned equally between two different atoms. Ga occupies sites on one of the two interpenetrating fcc sublattices; arsenic (As) populates the other fcc sublattice.

Now that the positioning of atoms within the principal semiconductors has been established, the question may arise as to the practical utilization of such information. Although several applications could be cited, geometrical-type calculations constitute a very common and readily explained use of the unit cell formalism. For example, in Si at room temperature the unit cell side length (a) is 5.43 \AA (where $1 \text{ \AA} = 10^{-8} \text{ cm}$). Since there are eight Si atoms per unit cell and the volume of the unit cell is a^3 , it follows that there are $8/a^3$ or almost exactly $5 \times 10^{22} \text{ atoms/cm}^3$ in the Si lattice. Similar calculations could be performed to determine atomic radii, the distance between atomic planes, and so forth. For the purposes of the development herein, however, a major reason for the discussion of semiconductor lattices was to establish that, as emphasized in Fig. 1.4(c), *atoms in the diamond and zincblende lattices have four nearest neighbors*. The chemical bonding (or crystalline glue) within the major semiconductors is therefore dominated by the attraction between any given atom and its four closest neighbors. This is an important fact that should be filed away for future reference.

Exercise 1.2

P: If the lattice constant or unit cell side-length in Si is $a = 5.43 \times 10^{-8} \text{ cm}$, what is the distance (d) from the center of one Si atom to the center of its nearest neighbor?

S: As noted in the Fig. 1.4 caption, the atom in the upper front corner of the Si unit cell and the atom along the cube diagonal one-fourth of the way down the diagonal are nearest neighbors. Since the diagonal of a cube is equal to $\sqrt{3}$ times a side length, one concludes $d = (1/4)\sqrt{3}a = (\sqrt{3}/4)(5.43 \times 10^{-8}) = 2.35 \times 10^{-8} \text{ cm}$.

(C) Exercise 1.3

P: Construct a MATLAB program that computes the number of atoms/cm³ in cubic crystals. Use the MATLAB `input` function to enter the number of atoms/unit-cell and the unit cell side length (a) for a specific crystal. Make a listing of your program and record the program result when applied to silicon.

S: MATLAB program script . . .

```
%Exercise 1.3
%Computation of the number of atoms/cm3 in a cubic lattice
N=input('input number of atoms/unit cell, N = ');
a=input('lattice constant in angstrom, a = ');
atmden=N*(1.0e24)/(a^3) %number of atoms/cm3
```

```

Program output for Si . . .
input number of atoms/unit cell, N = 8
lattice constant in angstrom, a = 5.43
atmden =
4.9968e+22

```

1.2.4 Miller Indices

Single crystals of silicon used in device processing normally assume the thin, round form exhibited in Fig. 1.5. The pictured plate-like single crystals, better known as Si wafers, are typical of the starting substrates presently employed by major manufacturers. Of particular interest here is the fact that the surface of a wafer is carefully preoriented to lie along a specific crystallographic plane. Moreover, a “flat” or “notch” is ground along the periphery of the wafer to identify a reference direction within the surface plane. Precise surface orientation is critical in certain device processing steps and directly affects the characteristics exhibited by a number of devices. The flat or notch is routinely employed, for example, to orient device arrays on the wafer so as to achieve high yields during device

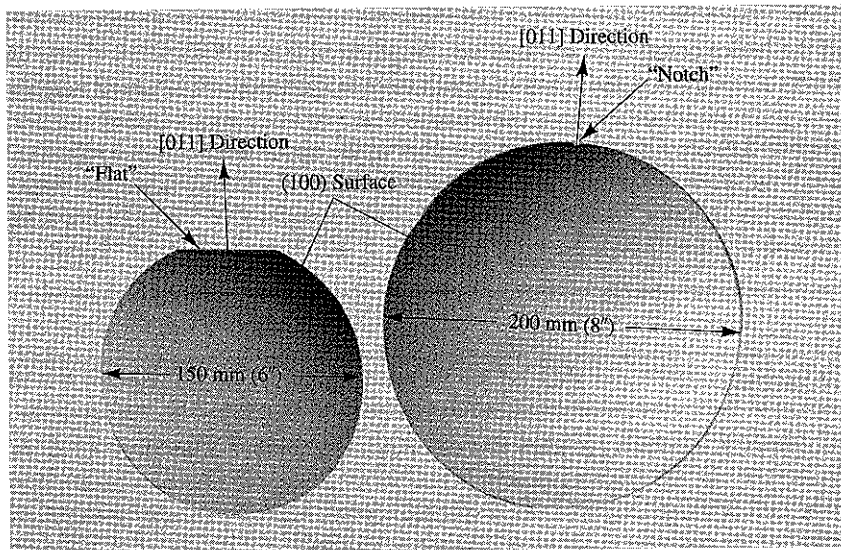


Figure 1.5 Single-crystal silicon wafers typical of the starting substrates presently employed by major device manufacturers. The 150 mm (6 inch) and 200 mm (8 inch) wafers are nominally 0.625 mm and 0.725 mm thick, respectively. The facing surface is polished and etched yielding a damage-free, mirror-like finish. The figure dramatizes the utility of Miller indices exemplified by the (100) plane and [011] direction designations. (Photograph courtesy of Intel Corporation.)

- (e) $1 \text{ \AA} = ? \text{ cm}$.
- (f) In terms of the lattice constant a , what is the distance between nearest-neighbor atoms in a simple cubic lattice?
- (g) How many nearest-neighbor atoms are there in the diamond and the zincblende lattices?
- (h) What is being indicated by the bracket sets $()$, $[\]$, $\{ \}$, and $\langle \rangle$ as employed in the Miller indexing scheme?
- (i) Describe the Czochralski method for obtaining large single crystals of silicon.

1.2 The GaAs unit cell is pictured in Fig. 1.4(b). Describe (or sketch) the unit cell for $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$.

- 1.3** (a) The lattice constant of Ge at room temperature is $a = 5.65 \times 10^{-8} \text{ cm}$. Determine the number of Ge atoms/ cm^3 .
- (b) Copies of computer-required exercises employing MATLAB are included on disk. Run the Exercise 1.3 program to verify your result from part (a).

1.4 In terms of the lattice constant a , what is the distance between nearest-neighbor atoms in

- (a) a bcc lattice?
- (b) an fcc lattice?

1.5 The surface of a Si wafer is a (100) plane.

- (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)/(d) Repeat parts (a) and (b), this time taking the surface of the Si wafer to be a (110) plane.
- (e) Primarily for practice in utilizing MATLAB, construct a MATLAB program that computes the surface density of atoms on (100) planes of cubic crystals. The number of atoms with centers on the (100) face of the unit cell, and the lattice constant in \AA , are to be the input variables. Confirm the result obtained manually in part (b).

1.6 Record all intermediate steps in answering the following questions.

- (a) 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.
 - (i) What is the Miller index notation for the plane?
 - (ii) What is the Miller index notation for the direction normal to the plane?

- (b) Assuming the crystal structure to be cubic, determine the Miller indices for (i) the plane and (ii) the vector pictured in Fig. P1.6(b).

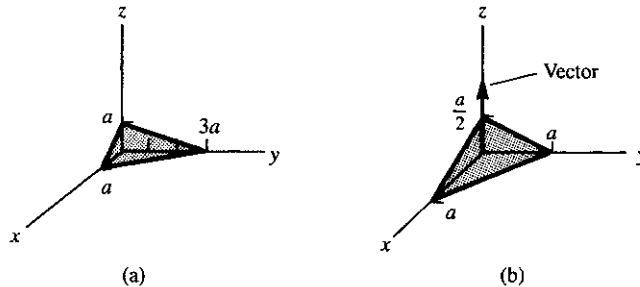


Figure P1.6

1.7 Assuming a cubic crystal system, make a sketch of the following planes.

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

1.8 Assuming a cubic crystal system, use an appropriately directed arrow to identify each of the following directions:

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

1.9 Identify two crystalline directions in a cubic crystal which are perpendicular to

- (a) the [100] direction,
 (b) the [111] direction.

NOTE: 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

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

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

1.10 As pictured in Fig. 1.5, [011] is the direction in the surface plane normal to the major flat when the surface of the Si wafer is a (100) plane. To construct a particular device structure, a parallel set of grooves must be etched in the (100) surface plane along the [010] direction. Make a sketch indicating how the grooves are to be oriented on the wafer's surface. Explain how you arrived at your sketch.