
P A R T I

SEMICONDUCTOR FUNDAMENTALS

1 Semiconductors: A General Introduction

1.1 GENERAL MATERIAL PROPERTIES

The vast majority of all solid state devices on the market today are fabricated from a class of materials known as semiconductors. It is therefore appropriate that we begin the discussion by examining the general nature of semiconducting materials.

1.1.1 Composition

Table 1.1 lists the atomic compositions of semiconductors that are likely to be encountered in the device literature. As noted, the semiconductor family of materials includes the elemental semiconductors Si and Ge, compound semiconductors such as GaAs and ZnSe, and alloys like $\text{Al}_x\text{Ga}_{1-x}\text{As}$.[†] Due in large part to the advanced state of its fabrication technology, Si is far and away the most important of the semiconductors, totally dominating the present commercial market. The vast majority of discrete devices and integrated circuits (ICs), including the central processing unit (CPU) in microcomputers and the ignition module in modern automobiles, are made from this material. GaAs, exhibiting superior electron transport properties and special optical properties, is employed in a significant number of applications ranging from laser diodes to high-speed ICs. The remaining semiconductors are utilized in “niche” applications that are invariably of a high-speed, high-temperature, or optoelectronic nature. Given its present position of dominance, we will tend to focus our attention on Si in the text development. Where feasible, however, GaAs will be given comparable consideration and other semiconductors will be featured as the discussion warrants.

Although the number of semiconducting materials is reasonably large, the list is actually quite limited considering the total number of elements and possible combinations of elements. Note that, referring to the abbreviated periodic chart of the elements in Table 1.2, only a certain group of elements and elemental combinations typically give rise to semiconducting materials. Except for the IV-VI compounds, all of the semiconductors listed in Table 1.1 are composed of elements appearing in Column IV of the Periodic Table or are a combination of elements in Periodic Table columns an equal distance to either side of

[†] The x (or y) in alloy formulas is a fraction lying between 0 and 1. $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ would indicate a material with 3 Al and 7 Ga atoms per every 10 As atoms.

Table 1.1 Semiconductor Materials.

<i>General Classification</i>	<i>Symbol</i>	<i>Semiconductor Name</i>
(1) Elemental	Si Ge	Silicon Germanium
(2) Compounds		
(a) IV-IV	SiC	Silicon carbide
(b) III-V	AlP	Aluminum phosphide
	AlAs	Aluminum arsenide
	AlSb	Aluminum antimonide
	GaN	Gallium nitride
	GaP	Gallium phosphide
	GaAs	Gallium arsenide
	GaSb	Gallium antimonide
	InP	Indium phosphide
	InAs	Indium arsenide
	InSb	Indium antimonide
(c) II-VI	ZnO	Zinc oxide
	ZnS	Zinc sulfide
	ZnSe	Zinc selenide
	ZnTe	Zinc telluride
	CdS	Cadmium sulfide
	CdSe	Cadmium selenide
	CdTe	Cadmium telluride
	HgS	Mercury sulfide
(d) IV-VI	PbS	Lead sulfide
	PbSe	Lead selenide
	PbTe	Lead telluride
(3) Alloys		
(a) Binary	$\text{Si}_{1-x}\text{Ge}_x$	
(b) Ternary	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	(or $\text{Ga}_{1-x}\text{Al}_x\text{As}$)
	$\text{Al}_x\text{In}_{1-x}\text{As}$	(or $\text{In}_{1-x}\text{Al}_x\text{As}$)
	$\text{Cd}_{1-x}\text{Mn}_x\text{Te}$	
	$\text{GaAs}_{1-x}\text{P}_x$	
	$\text{Ga}_x\text{In}_{1-x}\text{As}$	(or $\text{In}_{1-x}\text{Ga}_x\text{As}$)
	$\text{Ga}_x\text{In}_{1-x}\text{P}$	(or $\text{In}_{1-x}\text{Ga}_x\text{P}$)
	$\text{Hg}_{1-x}\text{Cd}_x\text{Te}$	
(c) Quaternary	$\text{Al}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$	
	$\text{Ga}_x\text{In}_{1-x}\text{As}_{1-y}\text{P}_y$	

Table 1.2 Abbreviated Periodic Chart of the Elements.

II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

Column IV. The Column III element Ga plus the Column V element As yields the III-V compound semiconductor GaAs; the Column II element Zn plus the Column VI element Se yields the II-VI compound semiconductor ZnSe; the fractional combination of the Column III elements Al and Ga plus the Column V element As yields the alloy semiconductor $\text{Al}_x\text{Ga}_{1-x}\text{As}$. This very general property is related to the chemical bonding in semiconductors, where, on the average, there are four valence electrons per atom.

1.1.2 Purity

As will be explained in Chapter 2, extremely minute traces of impurity atoms called “dopants” can have a drastic effect on the electrical properties of semiconductors. For this reason, the compositional purity of semiconductors must be very carefully controlled and, in fact, modern semiconductors are some of the purest solid materials in existence. In Si, for example, the unintentional content of dopant atoms is routinely less than one atom per 10^9 Si atoms. To assist the reader in attempting to comprehend this incredible level of purity, let us suppose a forest of maple trees was planted from coast to coast, border to border, at 50-ft centers across the United States (including Alaska). An impurity level of one part per 10^9 would correspond to finding about 25 crabapple trees in the maple tree forest covering the United States! It should be emphasized that the cited material purity refers to *unintentional* undesired impurities. Typically, dopant atoms at levels ranging from one part per 10^8 to one impurity atom per 10^3 semiconductor atoms will be *purposely* added to the semiconductor to control its electrical properties.

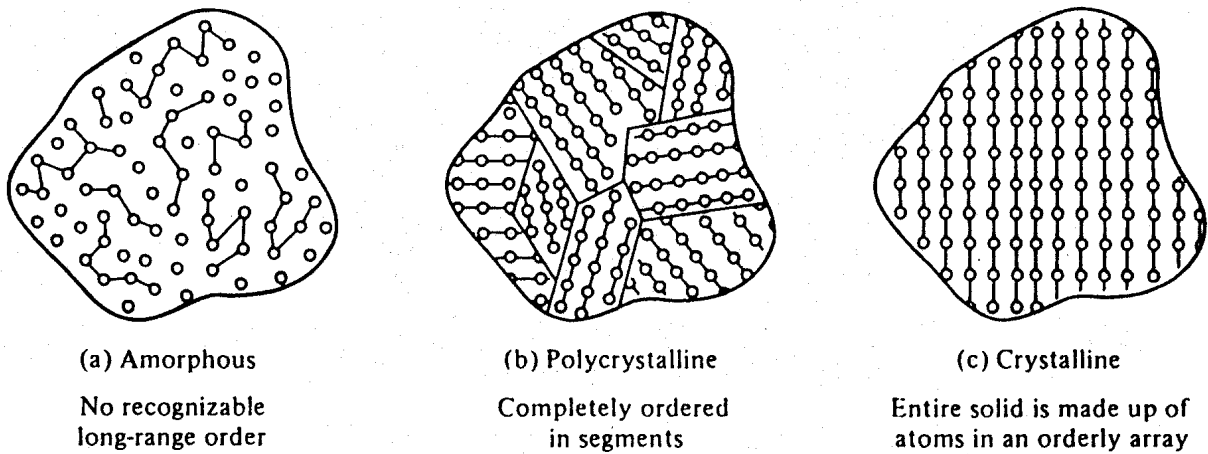


Figure 1.1 General classification of solids based on the degree of atomic order: (a) amorphous, (b) polycrystalline, and (c) crystalline.

1.1.3 Structure

The spatial arrangement of atoms within a material plays an important role in determining the precise properties of the material. As shown schematically in Fig. 1.1, the atomic arrangement within a solid causes it to be placed into one of three broad classifications; namely, amorphous, polycrystalline, or crystalline. An amorphous solid is a material in which there is no recognizable long-range order in the positioning of atoms within the material. The atomic arrangement in any given section of an amorphous material will look different from the atomic arrangement in any other section of the material. Crystalline solids lie at the opposite end of the “order” spectrum; in a crystalline material the atoms are arranged in an orderly three-dimensional array. Given any section of a crystalline material, one can readily reproduce the atomic arrangement in any other section of the material. Polycrystalline solids comprise an intermediate case in which the solid is composed of crystalline subsections that are disjointed or misoriented relative to one another.

Upon examining the many solid state devices in existence, one readily finds examples of all three structural forms. An amorphous-Si thin-film transistor is used as the switching element in liquid crystal displays (LCDs); polycrystalline Si gates are employed in Metal-Oxide-Semiconductor Field-Effect Transistors (MOSFETs). In the vast majority of devices, however, the active region of the device is situated within a *crystalline* semiconductor. The overwhelming number of devices fabricated today employ *crystalline* semiconductors.

1.2 CRYSTAL STRUCTURE

The discussion at the end of the preceding section leads nicely into the topic of this section. Since in-use semiconductors are typically crystalline in form, it seems reasonable to seek out additional information about the crystalline state. Our major goal here is to present a more detailed picture of the atomic arrangement within the principal semiconductors. To

achieve this goal, we first examine how one goes about describing the spatial positioning of atoms within crystals. Next, a bit of "visualization" practice with simple three-dimensional lattices (atomic arrangements) is presented prior to examining semiconductor lattices themselves. The section concludes with an introduction to the related topic of Miller indices. Miller indices are a convenient shorthand notation widely employed for identifying specific planes and directions within crystals.

1.2.1 The Unit Cell Concept

Simply stated, a unit cell is a small portion of any given crystal that could be used to reproduce the crystal. To help establish the unit cell (or building-block) concept, let us consider the two-dimensional lattice shown in Fig. 1.2(a). To describe this lattice or to totally specify the physical characteristics of the lattice, one need only provide the unit cell shown in Fig. 1.2(b). As indicated in Fig. 1.2(c), the original lattice can be readily reproduced by merely duplicating the unit cell and stacking the duplicates next to each other in an orderly fashion.

In dealing with unit cells there often arises a misunderstanding, and hence confusion, relative to two points. First, unit cells are not necessarily unique. The unit cell shown in Fig. 1.2(d) is as acceptable as the Fig. 1.2(b) unit cell for specifying the original lattice of

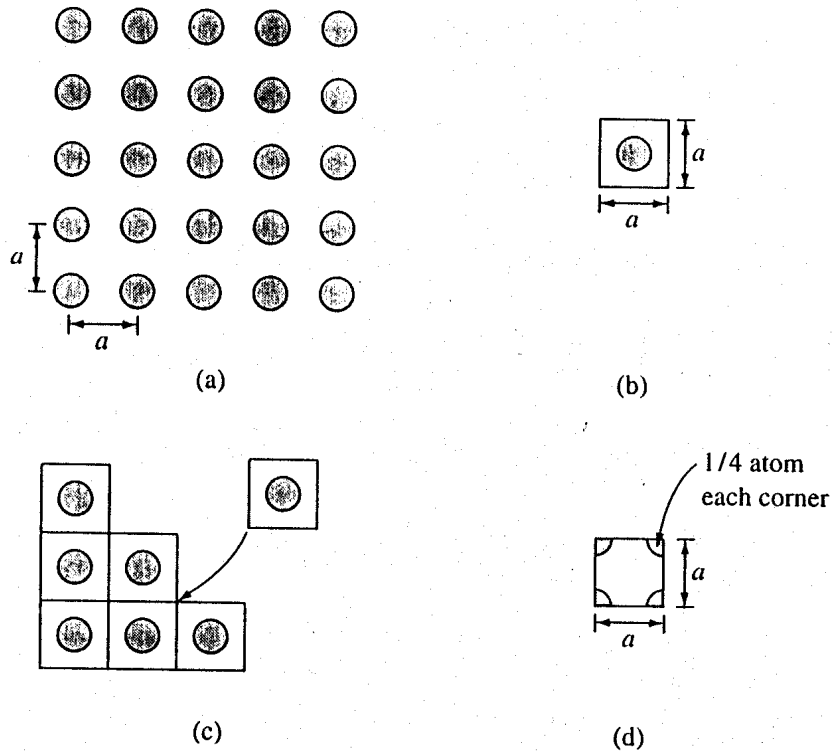
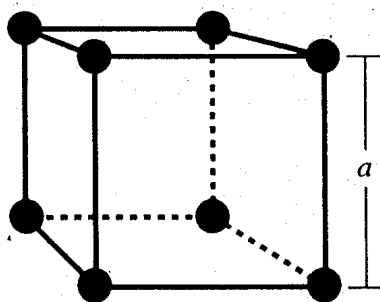


Figure 1.2 Introduction to the unit cell method of describing atomic arrangements within crystals. (a) Sample two-dimensional lattice. (b) Unit cell corresponding to the part (a) lattice. (c) Reproduction of the original lattice. (d) An alternative unit cell.

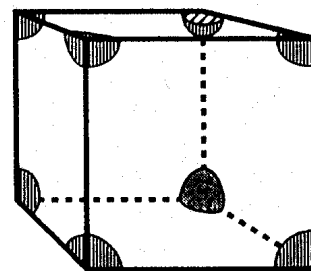
Fig. 1.2(a). Second, a unit cell need not be primitive (the smallest unit cell possible). In fact, it is usually advantageous to employ a slightly larger unit cell with orthogonal sides instead of a primitive cell with nonorthogonal sides. This is especially true in three dimensions where noncubic unit cells are quite difficult to describe and visualize.

1.2.2 Simple 3-D Unit Cells

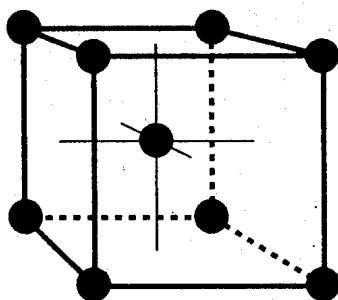
Semiconductor crystals are three-dimensional and are therefore described in terms of three-dimensional (3-D) unit cells. In Fig. 1.3(a) we have pictured the simplest of all three-dimensional unit cells, the simple cubic unit cell. The simple cubic cell is an equal-sided box or cube with an atom positioned at each corner of the cube. The simple cubic lattice associated with this cell is constructed in a manner paralleling the two-dimensional case. In doing so, however, it should be noted that only $1/8$ of each corner atom is actually *inside* the cell, as pictured in Fig. 1.3(b). Duplicating the Fig. 1.3(b) cell and stacking the duplicates like blocks in a nursery yields the simple cubic lattice. Specifically, the procedure generates planes of atoms like that previously shown in Fig. 1.2(a). Planes of atoms parallel to the base plane are separated from one another by a unit cell side length or *lattice con-*



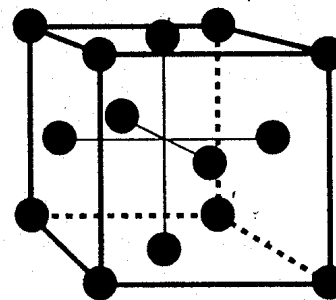
(a) Simple cubic



(b) Pedantically correct simple cubic



(c) bcc



(d) fcc

Figure 1.3 Simple three-dimensional unit cells. (a) Simple cubic unit cell. (b) Pedantically correct simple cubic unit cell including only the fractional portion ($1/8$) of each corner atom actually within the cell cube. (c) Body centered cubic unit cell. (d) Face centered cubic unit cell.

stant, *a*. When viewed normal to the base plane, atoms in a given plane are positioned directly over atoms in a lower-lying plane.

Figures 1.3(c) and 1.3(d) display two common 3-D cells that are somewhat more complex but still closely related to the simple cubic cell. The unit cell of Fig. 1.3(c) has an atom added at the center of the cube; this configuration is appropriately called the body centered cubic (bcc) unit cell. The face centered cubic (fcc) unit cell of Fig. 1.3(d) contains an atom at each face of the cube in addition to the atoms at each corner. (Note, however, that only one-half of each face atom actually lies inside the fcc unit cell.) Whereas the simple cubic cell contains one atom ($1/8$ of an atom at each of the eight cube corners), the somewhat more complex bcc and fcc cells contain two and four atoms, respectively. The reader should verify these facts and visualize the lattices associated with the bcc and fcc cells.

(C) Exercise 1.1

The text-associated software distributed via the Internet or on a floppy disk contains a directory or folder named MacMolecule. Files stored inside this directory or folder are ASCII input files generated by the author for use with a computer program by the same name. The MacMolecule program, copyrighted by the University of Arizona, is distributed free of charge to academic users and is available at many academic sites. As the name implies, the program runs only on Macintosh personal computers. The input files supplied to IBM-compatible users, however, can be readily converted for use on a public-access Macintosh.

MacMolecule generates and displays a "ball-and-stick" 3-D color rendering of molecules, unit cells, and lattices. The input files supplied by the author can be used to help visualize the simple cubic, bcc, and fcc unit cells, plus the diamond and zinc-blende unit cells described in the next subsection. The About-MacMolecule file that is distributed with the MacMolecule program provides detailed information about the use of the program and the generation/modification of input files.

The reader is urged to investigate and play with the MacMolecule software. The initial display is always a *z*-direction view and is typically pseudo-two-dimensional in nature. A more informative view is obtained by rotating the model. Rotation is best accomplished by "grabbing and dragging" the edges of the model. The more adventuresome may wish to try their hand at modifying the existing input files or generating new input files.

1.2.3 Semiconductor Lattices

We are finally in a position to supply details relative to the positioning of atoms within the principal semiconductors. In Si (and Ge) the lattice structure is described by the unit cell pictured in Fig. 1.4(a). The Fig. 1.4(a) arrangement is known as the *diamond lattice* unit cell because it also characterizes diamond, a form of the Column IV element carbon. Examining the diamond lattice unit cell, we note that the cell is cubic, with atoms at each

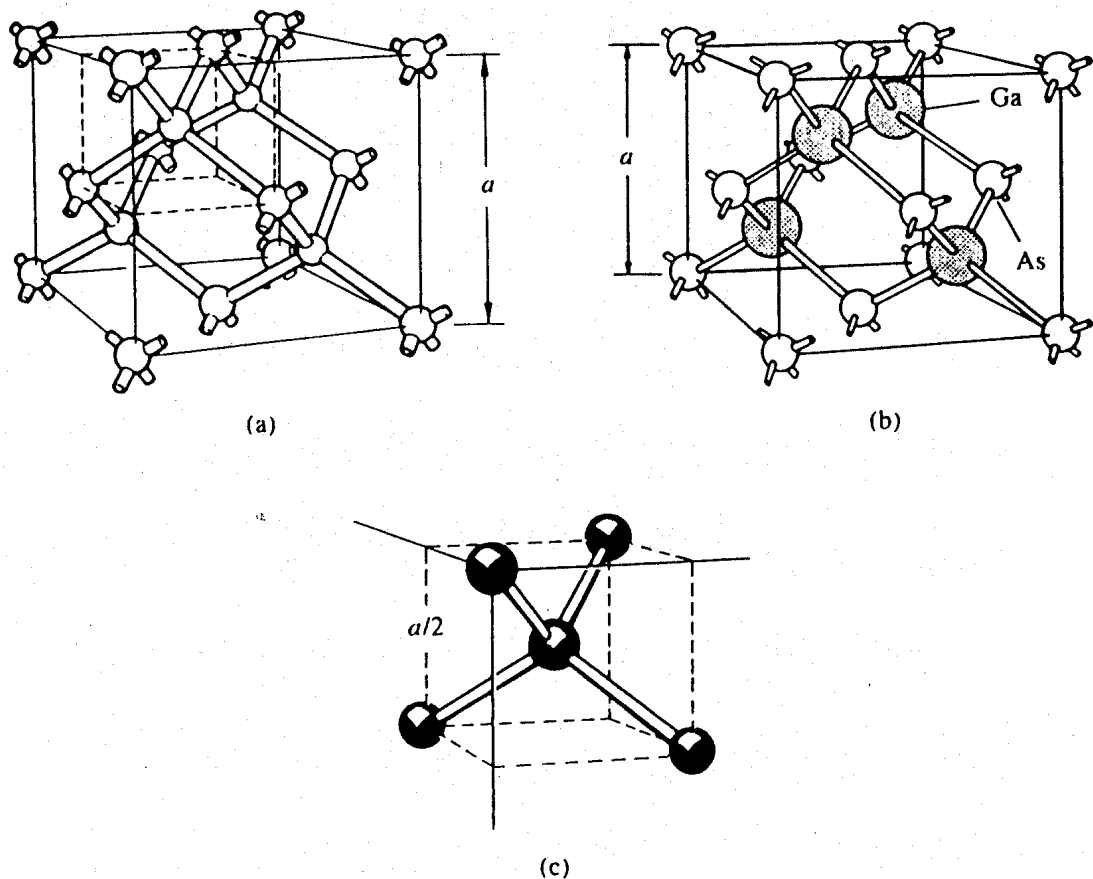


Figure 1.4 (a) Diamond lattice unit cell. (b) Zincblende lattice unit cell (GaAs used for illustration). (c) Enlarged top corner of the part (a) diamond lattice emphasizing the four-nearest-neighbor bonding within the structure. The cube side length, a , is 5.43 \AA and 5.65 \AA at $T = 300 \text{ K}$ for Si and GaAs, respectively. [(a) Adapted from Shockley^[1]. (b) From Sze^[2], ©1981 by John Wiley & Sons, Inc. Reprinted with permission.]

corner and at each face of the cube similar to the fcc-cell. The interior of the Fig. 1.4(a) cell, however, contains four additional atoms. One of the interior atoms is located along a cube body diagonal exactly one-quarter of the way down the diagonal from the top front left-hand corner of the cube. The other three interior atoms are displaced one-quarter of the body diagonal length along the previously noted body diagonal direction from the front, top, and left-side face atoms, respectively. Although it may be difficult to visualize from Fig. 1.4(a), the diamond lattice can also be described as nothing more than two interpenetrating fcc lattices. The corner and face atoms of the unit cell can be viewed as belonging to one fcc lattice, while the atoms totally contained within the cell belong to the second fcc lattice. The second lattice is displaced one-quarter of a body diagonal along a body diagonal direction relative to the first fcc lattice.

Most of the III-V semiconductors, including GaAs, crystallize in the *zincblende* structure. The zincblende lattice, typified by the GaAs unit cell shown in Fig. 1.4(b), is essen-

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 $d = (1/4)\sqrt{3}a = (\sqrt{3}/4)(5.43 \times 10^{-8}) = \boxed{2.35 \times 10^{-8} \text{ cm}}$.

(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

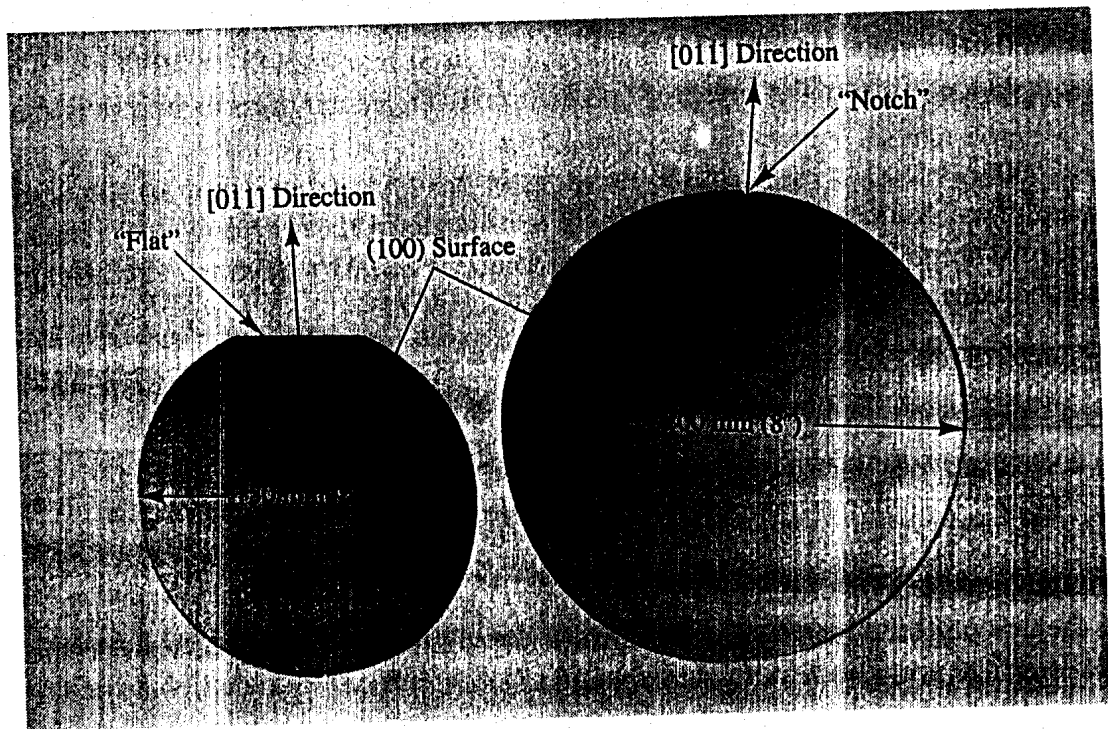


Figure 1.5 Single-crystal silicon wafers typical of the starting substrates presently employed by major device manufacturers. The 150 mm (6 inch) and 200 mm (8 inch) wafers are nominally 0.625 mm and 0.725 mm thick, respectively. The facing surface is polished and etched yielding a damage-free, mirror-like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

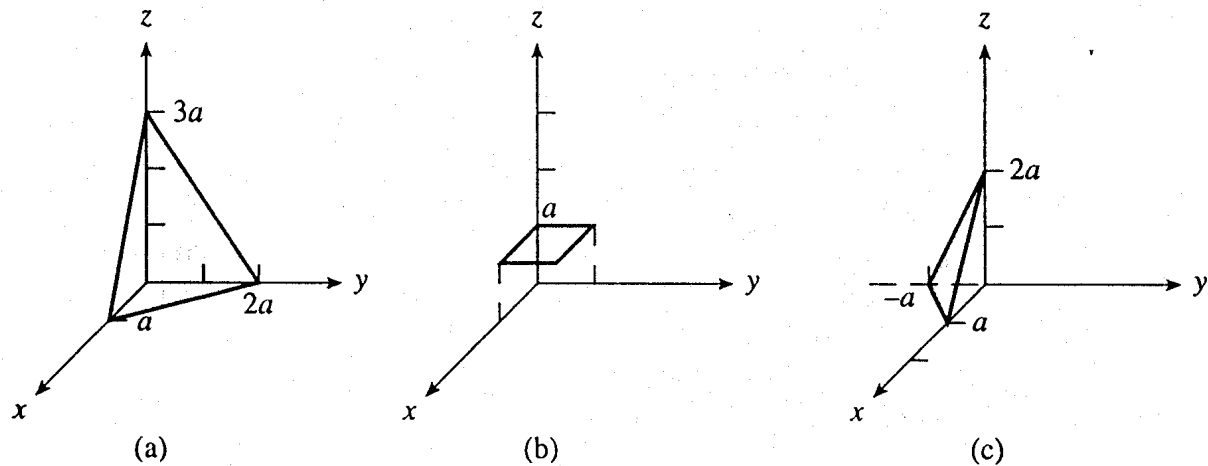


Figure 1.6 Sample cubic crystal planes. (a) The (632) plane used in explaining the Miller indexing procedure. (b) The (001) plane. (c) The ($2\bar{2}1$) plane.

separation. The point we wish to make is that the specification of crystallographic planes and directions is of practical importance. Miller indices, exemplified by the (100) plane and [011] direction designations used in Fig. 1.5, constitute the conventional means of identifying planes and directions within a crystal.

The Miller indices for any given plane of atoms within a crystal are obtained by following a straightforward four-step procedure. The procedure is detailed below, along with the simultaneous sample indexing of the plane shown in Fig. 1.6(a).

Indexing Procedure	Sample Implementation
After setting up coordinate axes along the edges of the unit cell, note where the plane to be indexed intercepts the axes. Divide each intercept value by the unit cell length along the respective coordinate axis. Record the resulting normalized (pure-number) intercept set in the order x, y, z .	1, 2, 3
Invert the intercept values; that is, form $[1/\text{intercept}]$ s.	1, $\frac{1}{2}$, $\frac{1}{3}$
Using an appropriate multiplier, convert the $1/\text{intercept}$ set to the smallest possible set of whole numbers.	6, 3, 2
Enclose the whole-number set in curvilinear brackets.	(632)

To complete the description of the plane-indexing procedure, the user should also be aware of the following special facts:

- (i) If the plane to be indexed is parallel to a coordinate axis, the “intercept” along the axis is taken to be at infinity. Thus, for example, the plane shown in Fig. 1.6(b) intercepts the coordinate axes at $\infty, \infty, 1$, and is therefore a (001) plane.

- (ii) If the plane to be indexed has an intercept along the negative portion of a coordinate axis, a minus sign is placed *over* the corresponding index number. Thus the Fig. 1.6(c) plane is designated a $(2\bar{2}1)$ plane.
- (iii) Referring to the diamond lattice of Fig. 1.4(a), note that the six planes passing through the cube faces contain identical atom arrangements; that is, because of crystal symmetry, it is impossible to distinguish between the “equivalent” (100) , (010) , (001) , $(\bar{1}00)$, $(0\bar{1}0)$, and $(00\bar{1})$ planes; or, it is impossible to distinguish between $\{100\}$ planes. A group of equivalent planes is concisely referenced in the Miller notation through the use of $\{ \}$ braces.
- (iv) Miller indices cannot be established for a plane passing through the origin of coordinates. The origin of coordinates must be moved to a lattice point not on the plane to be indexed. This procedure is acceptable because of the equivalent nature of parallel planes.

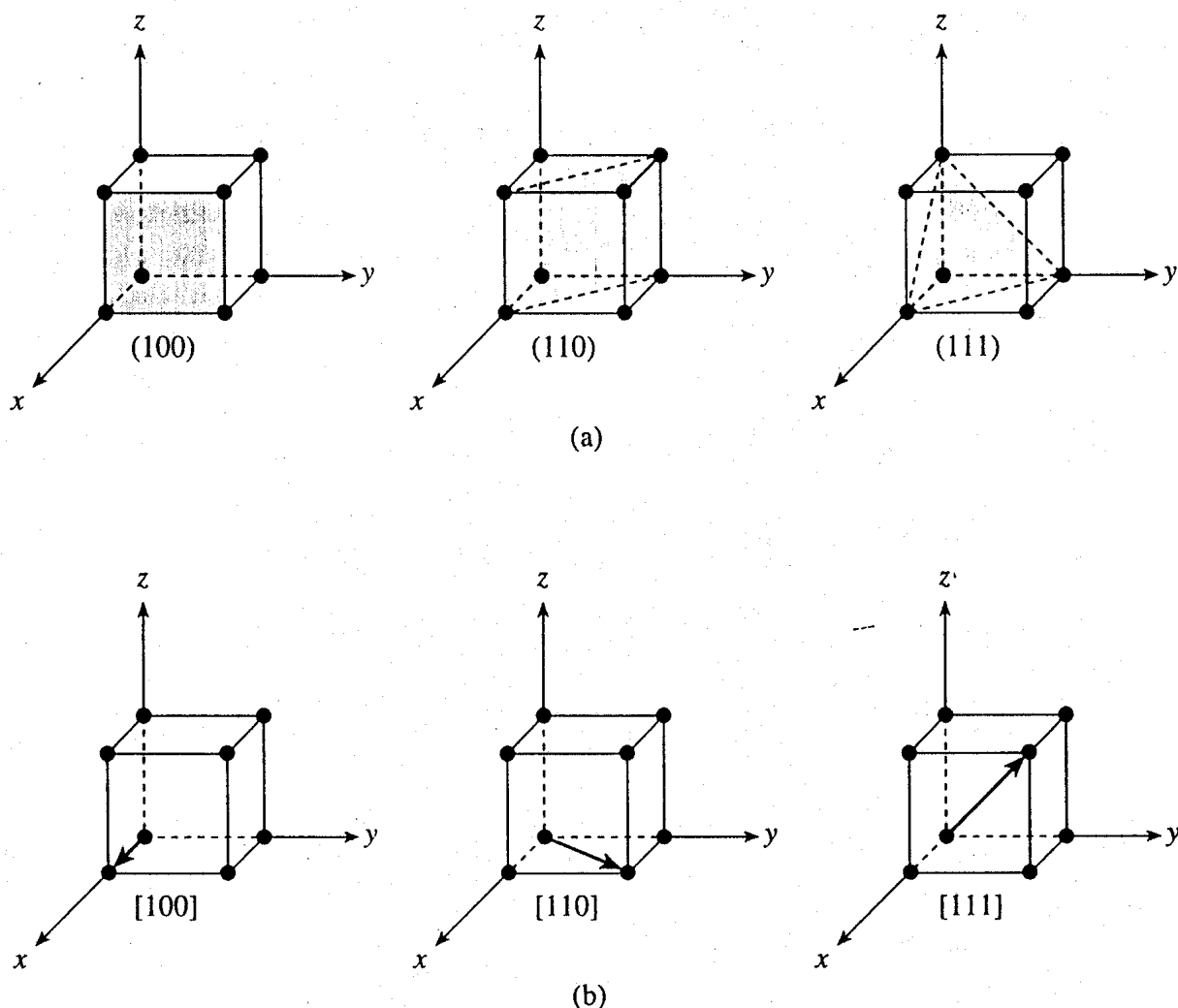


Figure 1.7 Visualization and Miller indices of commonly encountered (a) crystalline planes and (b) direction vectors.

Table 1.3 Miller Convention Summary.

<i>Convention</i>	<i>Interpretation</i>
(hkl)	Crystal plane
$\{hkl\}$	Equivalent planes
$[hkl]$	Crystal direction
$\langle hkl \rangle$	Equivalent directions

Using the simple cubic cell as a reference, the three most commonly encountered crystal-line planes are visualized in Fig. 1.7(a).

The Miller indices for *directions* are established in a manner analogous to the well-known procedure for finding the components of a vector. First, set up a vector of arbitrary length in the direction of interest. Next, decompose the vector into its components by noting the projections of the vector along the coordinate axes. Using an appropriate multiplier, convert the component values into the smallest possible whole-number set. This of course changes the length of the original vector but not its direction. Finally, enclose the whole-number set in brackets. Square brackets, $[\]$, are used to designate specific directions within a crystal; triangular brackets, $\langle \rangle$, designate an equivalent set of directions. Common direction vectors and their corresponding Miller indices are displayed in Fig. 1.7(b). A summary of the Miller bracketing convention for planes and directions is given in Table 1.3.

In the foregoing discussion we presented the procedure for progressing from a given plane or direction in a crystal to the corresponding Miller indices. More often than not, one is faced with the inverse process—visualizing the crystalline plane or direction corresponding to a given set of indices. Fortunately, one seldom encounters other than low-index planes and directions such as (111) , (110) , $[001]$. Thus it is possible to become fairly adept at the inverse process by simply memorizing the orientations for planes and directions associated with small-number indices. It is also helpful to note that, *for cubic crystals, a plane and the direction normal to the plane have precisely the same indices*—e.g., the $[110]$ direction is normal to the (110) plane. Of course, any plane or direction can always be deduced by reversing the indexing procedure.

Exercise 1.4

P: For a cubic crystal lattice:

- Determine the Miller indices for the plane and direction vector shown in Fig. E1.4(a).
- Sketch the plane and direction vector characterized by (011) and $[011]$, respectively.

S: (a) The intercepts of the plane are -1 , 1 , and 2 along the x , y , and z coordinate axes, respectively. Taking $[1/\text{intercept}]$ s yields -1 , 1 , $1/2$. Multiplying by 2 to obtain the lowest whole-number set, and enclosing in parentheses, gives $(\bar{2}21)$ for the Miller indices of the plane. The direction vector has projections of $2a$, a , and 0 along the x , y , and z coordinate axes, respectively. The Miller indices for the direction are then $[210]$.

(b) For the (011) plane, $[1/\text{intercept}]$ s = 0 , 1 , 1 . The normalized x , y , z intercepts of the plane are therefore ∞ , 1 , 1 ; the plane intersects the y -axis at a , intersects the z -axis at a , and is parallel to the x -axis. In a cubic crystal the $[011]$ direction is normal to the (011) plane. The deduced plane and direction are as sketched in Fig. E1.4(b).

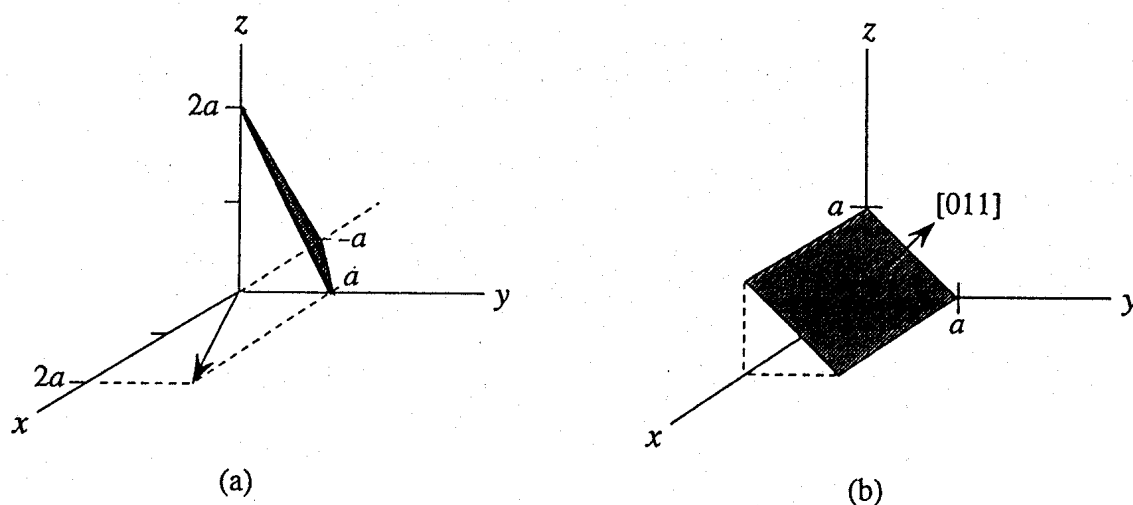


Figure E1.4

1.3 CRYSTAL GROWTH

1.3.1 Obtaining Ultrapure Si

Given the obvious general availability and widespread use of semiconductor materials, particularly Si, it is reasonable to wonder about the origin of the single-crystal Si used in modern-day device production. Could it be that Si is readily available in sandstone deposits?—No. Perhaps, as a sort of by-product, Si single crystals come from South African diamond mines?—Wrong again. As suggested recently in a low-budget science fiction movie, maybe Si is scooped from the ocean bottom by special submarines?—Sorry, no. Although Si is the second most abundant element in the earth's crust and a component in numerous compounds, chief of which are silica (impure SiO_2) and the silicates ($\text{Si} + \text{O} + \text{another element}$), silicon never occurs alone in nature as an element. Single-crystal Si used in device production, it turns out, is a man-made material.

Given the preceding introduction, it should be clear that the initial step in producing device-quality silicon must involve separating Si from its compounds and purifying the

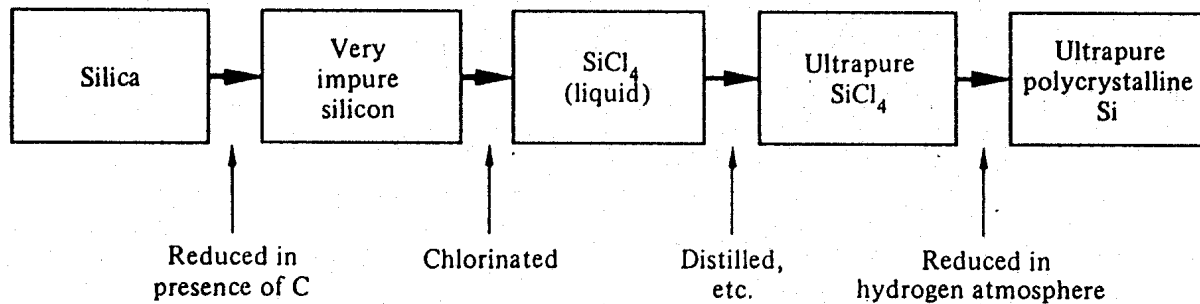
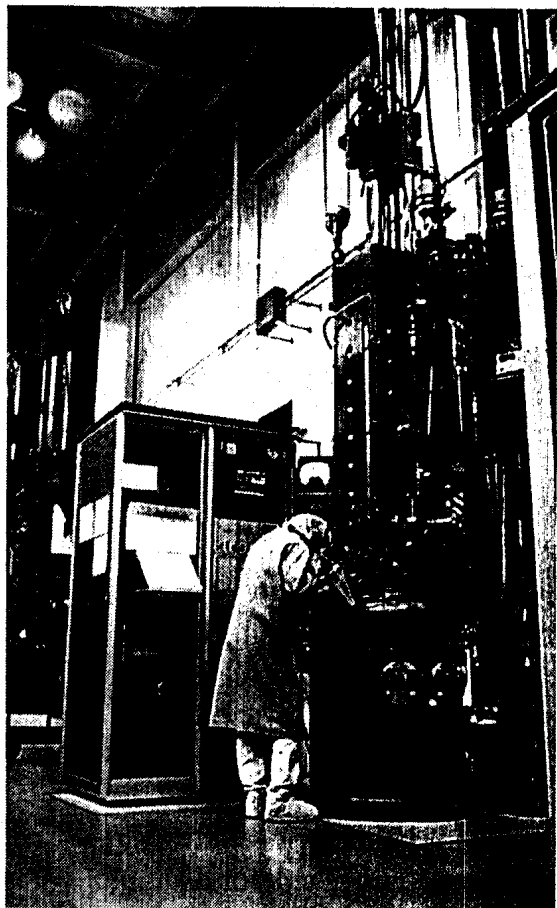


Figure 1.8 Summary of the process employed to produce ultrapure silicon.

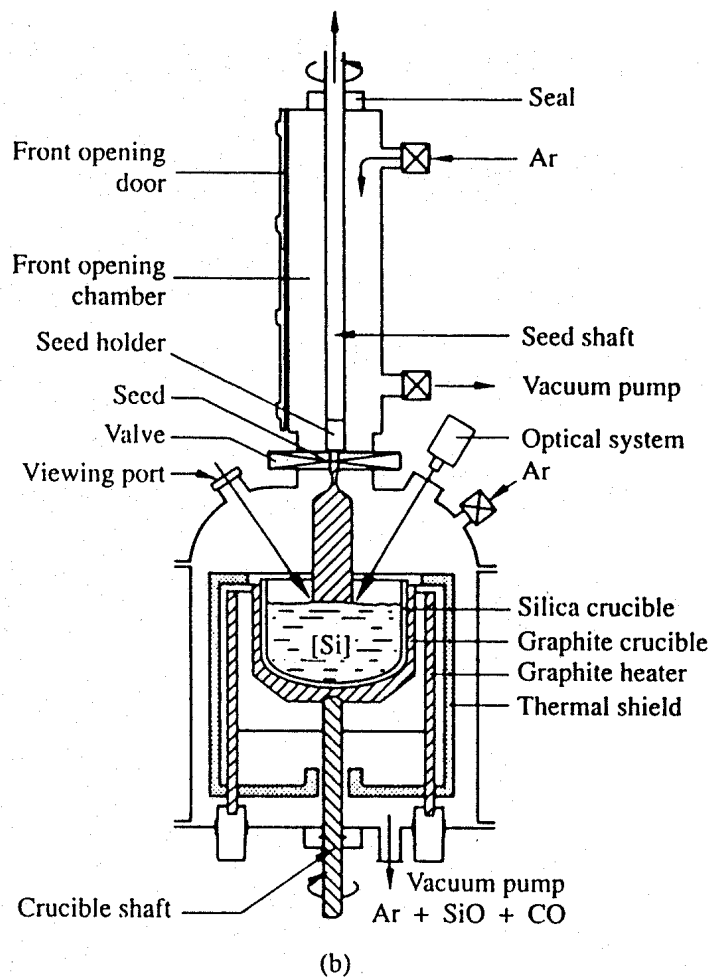
separated material. The ingenious separation and purification process that has evolved is summarized in Fig. 1.8. Low-grade silicon or ferrosilicon is first produced by heating silica with carbon in an electric furnace. The carbon essentially pulls the oxygen away from the impure SiO_2 (i.e., *reduces* the SiO_2), leaving behind impure Si. Next, the ferrosilicon is chlorinated to yield SiCl_4 or SiHCl_3 , both of which are liquids at room temperature. Although appearing odd at first glance, the liquefaction process is actually a clever maneuver. Whereas solids are very difficult to purify, a number of standard procedures are available for purifying liquids. An ultrapure SiCl_4 (or SiHCl_3) is the result after multiple distillation and other liquid purification procedures. Lastly, the high-purity halide is chemically reduced, yielding the desired ultrapure elemental silicon. This is accomplished, for example, by heating SiCl_4 in a hydrogen atmosphere [$\text{SiCl}_4 + 2\text{H}_2 \rightarrow 4\text{HCl} + \text{Si}$].

1.3.2 Single-Crystal Formation

Although ultrapure, the silicon derived from the separation and purification process as just described is not a single crystal, but is instead polycrystalline. Additional processing is therefore required to form the large single crystals used in device fabrication. The most commonly employed method yielding large single crystals of Si is known as the Czochralski method. In this method the ultrapure polycrystalline silicon is placed in a quartz crucible and heated in an inert atmosphere to form a melt, as shown in Fig. 1.9. A small single crystal, or Si “seed” crystal, with the normal to its bottom face carefully aligned along a predetermined direction (typically a $\langle 111 \rangle$ or $\langle 100 \rangle$ direction), is then clamped to a metal rod and dipped into the melt. Once thermal equilibrium is established, the temperature of the melt in the vicinity of the seed crystal is reduced, and silicon from the melt begins to freeze out onto the seed crystal, the added material being a structurally perfect extension of the seed crystal. Subsequently, the seed crystal is slowly rotated and withdrawn from the melt; this permits more and more silicon to freeze out on the bottom of the growing crystal. A photograph showing a crystal after being pulled from the melt is displayed in Fig. 1.9(c). The large, cylindrically shaped single crystal of silicon, also known as an ingot, is routinely up to 200 mm (8 inches) in diameter and 1 to 2 meters in length. The Si wafers used in device processing, such as those previously pictured in Fig. 1.5, are ultimately produced by cutting the ingot into thin sections using a diamond-edged saw.



(a)



(b)



(c)

Figure 1.9 Silicon crystal-pulling apparatus and resulting single crystal. (a) Photograph of a computer-controlled Czochralski crystal puller. (b) Simplified schematic drawing of the puller. (c) Silicon ingot. [(a) and (c) Photographs courtesy of Wacker Siltronic. (b) From Zuhlířner and Huber^[3]; reprinted with permission.]

1.4 SUMMARY

This chapter provides basic information about semiconductors in general and silicon in particular. Examining the elemental compositions of semiconductors, one finds that there are, on average, four valence electrons per atom. Moreover, device-quality semiconductors are typically single crystals of high compositional purity. Si crystallizes in the diamond lattice, GaAs crystallizes in the zincblende lattice, and the lattice atoms in both cases have four nearest neighbors. Miller indices, introduced herein as an adjunct to the crystal structure discussion, are the accepted means for identifying planes and directions within a crystal. Finally, large single crystals of device-grade Si are commonly produced by the Czochralski method.

PROBLEMS

CHAPTER 1 PROBLEM INFORMATION TABLE				
<i>Problem</i>	<i>Complete After</i>	<i>Difficulty Level</i>	<i>Suggested Point Weighting</i>	<i>Short Description</i>
1.1	1.4	1	10 (a::h-1, i-2)	Short answer review
1.2	1.2.3	1	8	Unit cell for alloy
● 1.3	"	1	10 (5 each part)	Ge atomic density
1.4	"	1	8 (4 each part)	Nearest-neighbor distances
● 1.5	1.2.4	2-3	15 (a-2, b-2, c-3, d-3, e-5)	Atoms/cm ² on planes
1.6	"	1	8 (2 each subpart)	Determine Miller indices
1.7	"	1	16 (2 each part)	Given (<i>hkl</i>), sketch plane
1.8	"	1	16 (2 each part)	Given [<i>hkl</i>], sketch direction
1.9	"	1	8 (4 each part)	Perpendicular directions
1.10	"	2	10	Direction on wafer surface
1.11	"	2	10 (a-3, b-2, c-3, d-2)	Combination question
1.12	"	2	12 (2 each part)	Equivalent planes/directions
1.13	1.2.3	3	20 (5 each part)	% of volume occupied

1.1 Quick Quiz. Answer the following questions as concisely as possible.

- Name (i) one elemental semiconductor and (ii) one III-V compound semiconductor.
- What is the difference between a crystalline and a polycrystalline material?
- Give a word definition of *unit cell*.
- How many atoms are there in a simple cubic unit cell? in a bcc unit cell? in a fcc unit cell? in the unit cell characterizing the diamond lattice?

- (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).

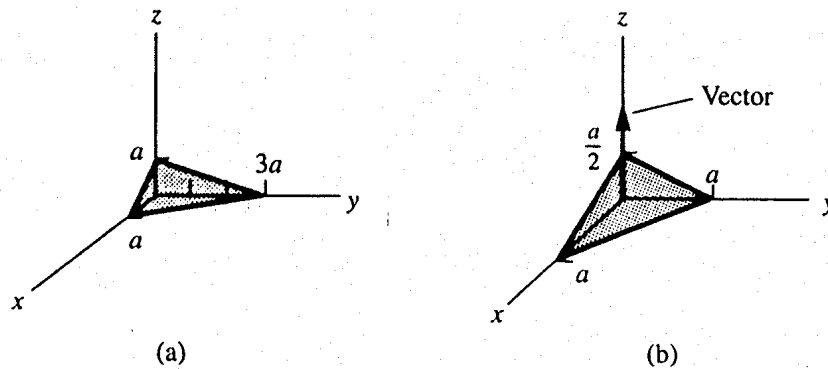


Figure P1.6

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) [001], (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.

1.11 A crystalline lattice is characterized by the cubic unit cell pictured in Fig. P1.11. The cell has a single atom positioned at the center of the cube.

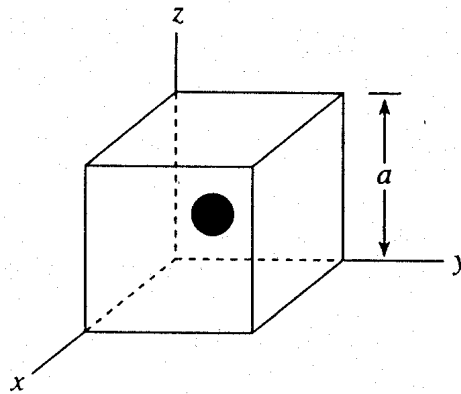


Figure P1.11

- (a) What is the name of the lattice generated by the given unit cell?
- (b) Determine the number of atoms per unit volume in the crystal. (Your answer should be in terms of the lattice constant, a .)
- (c) Suppose the crystal has a (110) surface plane. Determine the number of atoms per unit area whose centers lie on the (110) plane.
- (d) A direction vector is drawn through the center of the atom in the unit cell. Specify the Miller indices of the direction vector.

1.12 Given a cubic lattice, indicate how many equivalent planes [parts (a) to (c)] or equivalent directions [parts (d) to (f)] are associated with each of the following designations:

- (a) $\{100\}$, (b) $\{110\}$, (c) $\{111\}$,
- (d) $\langle 100 \rangle$, (e) $\langle 110 \rangle$, (f) $\langle 111 \rangle$.

1.13 Treating atoms as rigid spheres with radii equal to one-half the distance between nearest neighbors, show that the ratio of the volume occupied by the atoms to the total available volume in the various crystal structures is

- (a) $\pi/6$ or 52% for the simple cubic lattice.
- (b) $\sqrt{3}\pi/8$ or 68% for the body centered cubic lattice.
- (c) $\sqrt{2}\pi/6$ or 74% for the face centered cubic lattice.
- (d) $\sqrt{3}\pi/16$ or 34% for the diamond lattice.