Properties of Group-IV, III–V and II–VI Semiconductors

Sadao Adachi
Department of Electronic Engineering
Gunma University
Japan

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Series Preface

WILEY SERIES IN MATERIALS FOR ELECTRONIC AND OPTOELECTRONIC APPLICATIONS

This book series is devoted to the rapidly developing class of materials used for electronic and optoelectronic applications. It is designed to provide much-needed information on the fundamental scientific principles of these materials, together with how these are employed in technological applications. The books are aimed at postgraduate students, researchers and technologists, engaged in research, development and the study of materials in electronics and photonics, and industrial scientists developing new materials, devices and circuits for the electronic, optoelectronic and communications industries.

The development of new electronic and optoelectronic materials depends not only on materials engineering at a practical level, but also on a clear understanding of the properties of materials, and the fundamental science behind these properties. It is the properties of a material that eventually determine its usefulness in an application. The series therefore also includes such topics as electrical conduction in solids, optical properties, thermal properties, etc., all with applications and examples of materials in electronics and optoelectronics. The characterization of materials is also covered within the series in as much as it is impossible to develop new materials without the proper characterization of their structure and properties. Structure–property relationships have always been fundamentally and intrinsically important to materials science and engineering.

Materials science is well known for being one of the most interdisciplinary sciences. It is the interdisciplinary aspect of materials science that has led to many exciting discoveries, new materials and new applications. It is not unusual to find scientists with a chemical engineering background working on materials projects with applications in electronics. In selecting titles for the series, we have tried to maintain the interdisciplinary aspect of the field, and hence its excitement to researchers in this field.

Peter Capper
Safa Kasap
Arthur Willoughby

Preface

Almost all the semiconductors of practical interest are the group-IV, III–V and II–VI semiconductors and the range of technical applications of such semiconductors is extremely wide. All such semiconductor devices can be characterized to a greater or lesser degree. Many scientific papers, review papers, book chapters and specialized books exist that discuss the various semiconductor properties, but no one has integrated such topics on the group-IV, III–V and II–VI semiconductors into one volume.

The purpose of this book is twofold: (i) to discuss key properties of the group-IV, III–V and II–VI semiconductors; and (ii) to systemize these properties from a solid-state physics aspect. The bulk of the text is devoted to the comprehensive description of the lattice structural, thermal, elastic, lattice dynamic, electronic energy-band structural, optical and carrier transport properties of these semiconductors. Some corrective effects and related properties, such as piezoelectric, elasto-optic and electro-optic properties, have also been discussed.

The book contains convenient tables summarizing the various material parameters and the definitions of important semiconductor properties. The book also contains graphs in order to make the information more quantitative and intuitive. I felt that these have not been adequately covered in existing books.

The book is intended not only for semiconductor device engineers, but also physicists and physical chemists, and particularly students specializing in the fields of semiconductor synthesis, crystal growth, semiconductor device physics and technology.

SADAO ADACHI
Gunma, Japan

Acknowledgements/Dedication

The author wishes to thank the editors and authors of the following journals and symposium papers for permission to reproduce previously published figures: *Appl. Phys. Lett.* for Figs. 6.19, 10.37, 12.10, 12.13, 12.14 and 12.24; *IEEE Proc.-J* for Fig. 11.7; *IEEE Proc. Int. Electron. Dev. Meeting* for Figs. 6.18 and 6.20; *J. Appl. Phys.* for Figs. 4.4, 7.7, 10.25 and 12.26; *J. Cryst. Growth* for Fig. 10.36; *J. Phys. Chem. Solids* for Figs. 10.40 and 12.5; *Jpn. J. Appl. Phys.* for Figs. 6.14 and 12.32; *Kluwer Academic Publishers* for Figs. 2.7, 2.10, 2.11, 3.5, 4.9, 6.12, 6.25, 6.27, 9.4–9.8, 10.4, 10.15, 12.6–12.8, 12.15–12.17, 12.30, 12.33–12.38, 12.41–12.43; *Phys. Rev.* for Figs. 1.3, 2.1, 4.10, 6.1, 6.3, 6.5, 6.7, 8.6, 10.5(a), 10.11, 10.17, 10.21, 10.23, 10.24, 10.34, 10.38, 11.4, 11.9, 12.9, 12.19, 12.21, 12.22, 12.27–12.29; *Proc. Phys. Soc.* for Fig. 4.6; *Semicond. Sci. Technol.* for Fig. 10.5(b); *Solid State Commun.* for Figs. 4.5, 10.22 and 11.10; and *Solid-State Electron.* for Fig. 9.10.

1 Structural Properties

1.1 IONICITY

1.1.1 Definition

All tetrahedrally coordinated $A^N B^{8\text{-}N}$ semiconductors can be treated within the framework of a simple model. The success of this approach requires a careful choice of parameters entering in the model. The most important of these is the ionicity of the bond [1.1].

The ionicity of a bond can be defined as the fraction f_i^α of ionic or heteropolar character in the bond compared with the fraction f_h^α of covalent or homopolar character. By definition, these fractions satisfy the relation

$$f_i^\alpha + f_h^\alpha = 1 \tag{1.1}$$

In an elemental semiconductor such as Si, we must have $f_h^\alpha = 1$ and $f_i^\alpha = 0$. In contrast, we shall find that some alkali halides (NaCl, KCl, etc.) are more than 90% ionic.

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(a) Phillips ionicity

Phillips studied the connection between the chemical bonding properties of the $A^NB^{8\text{-}N}$ family of crystals and their electronic energy-band structures [1.1]. His concept evolves from a molecular picture in terms of bonding and antibonding states separated by an energy gap E_g. His ionicity scale f_i is defined in terms of average quantities such as the homopolar E_h and heteropolar parts C of the complex energy gap E_g associated with the A–B bond in the crystal

$$E_g = E_h + iC \tag{1.2}$$

Ionicity is then introduced via the relation

$$f_i = \frac{C^2}{E_g^2} = \frac{C^2}{E_h^2 + C^2} \tag{1.3}$$

Some numerical examples of E_g (f_i) are: $E_g = 4.70 + i0$ ($f_i = 0$) for Si; $E_g = 4.32 + i2.90$ ($f_i = 0.310$) for GaAs; $E_g = 4.29 + i5.60$ ($f_i = 0.630$) for ZnSe, where E_g are in eV.

(b) Pauling ionicity

Pauling based his definition of ionicity scale f_i^P not on the total energy of the bond, but on empirical heats of formation [1.2]. Denote the power of an atom A to attract electrons to itself by a dimensionless number called its electronegativity X_A. The Coulomb interaction between the ionic charge left behind and the valence charge transferred is proportional to $(X_A - X_B)^2$, and this is the origin of the extra ionic energy (i.e., f_i^P). By definition f_i^P never exceeds one, and as $X_A - X_B$ becomes large f_i^P tends to one. Moreover, the ionicity of an A–B bond should be the same as ionicity of a B–A bond. Pauling then defined ionicity of a single bond

$$f_i^P = 1 - \exp\left(-\frac{(X_A - X_B)^2}{4}\right) \tag{1.4}$$

(c) Harrison ionicity

In Harrison's model [1.3], the ionicity parameter f_i^H can be given in terms of two of the parameters of the electronic structure, by

$$f_i^H = \frac{V_3}{\sqrt{V_2^2 + V_3^2}} \tag{1.5}$$

Here, V_2 is half the splitting between bonding and antibonding states; V_3 is half the energy change in transferring an electron from anion to cation. This parameter f_i^H can be defined as the excess number of electrons placed on the anion from each bond, called the polarity. Thus, each anion in a tetrahedral structure contains a charge of $Z^* = 4f_i^H - \Delta Z$,

Table 1.1 Phillips (f_i), Pauling (f_i^P) and Harrison ionicities (f_i^H) for a number of group-IV, III–V and II–VI semiconductors

System	Material	f_i	f_i^P	f_i^H	System	Material	f_i	f_i^P	f_i^H
IV	Diamond	0	0	0	II–VI	MgO	0.841	0.88	
	Si	0	0	0		MgS	0.786		
	Ge	0	0	0		MgSe	0.790		
	Sn	0	0	0		MgTe	0.554		
	SiC	0.177	0.11	0.35		ZnO	0.616	0.80	0.69
						ZnS	0.623	0.59	0.69
III–V	BN	0.221	0.42	0.43		ZnSe	0.630	0.57	0.70
	BP	0.032				ZnTe	0.609	0.53	0.68
	BAs	0.044				CdS	0.685	0.59	0.74
	AlN	0.449	0.56	0.57		CdSe	0.699	0.58	0.74
	AlP	0.307	0.25	0.47		CdTe	0.717	0.52	0.76
	AlAs	0.274	0.27	0.44		HgS	0.790		
	AlSb	0.250	0.26	0.56		HgSe	0.680		
	GaN	0.500	0.55	0.61		HgTe	0.650		0.78
	GaP	0.327	0.27	0.48					
	GaAs	0.310	0.26	0.47					
	GaSb	0.261	0.26	0.43					
	InN	0.578							
	InP	0.421	0.26	0.55					
	InAs	0.357	0.26	0.51					
	InSb	0.321	0.25	0.48					

where ΔZ is the difference in valence from 4 ($\Delta Z = 1$ for nitrogen, 2 for oxygen, etc.). Similarly, then, each bond provides an electronic dipole moment of $\boldsymbol{P} = \gamma f_i^H\ (-e\boldsymbol{d})$, where $\boldsymbol{d}$ is vector distance from cation to anion and γ is a scale parameter to take into account local fields and charge symmetries; a value of $\sqrt{2}$ gave a good fit to experiment.

1.1.2 Ionicity value

Table 1.1 summarizes the values of Phillips (f_i) [1.1], Pauling (f_i^P) [1.2] and Harrison ionicities (f_i^H) [1.3] for a number of group-IV, III–V and II–VI semiconductors. We also show in Figure 1.1 Phillips ionicity f_i versus (a) Pauling (f_i^P) and (b) Harrison ionicities (f_i^H) for these semiconductors.

1.2 ELEMENTAL ISOTOPIC ABUNDANCE AND MOLECULAR WEIGHT

1.2.1 Elemental isotopic abundance

There are a great many semiconductor materials. We list in Table 1.2 the elements which form at least one tetrahedrally coordinated $A^N B^{8\text{-}N}$ semiconductor, together with their

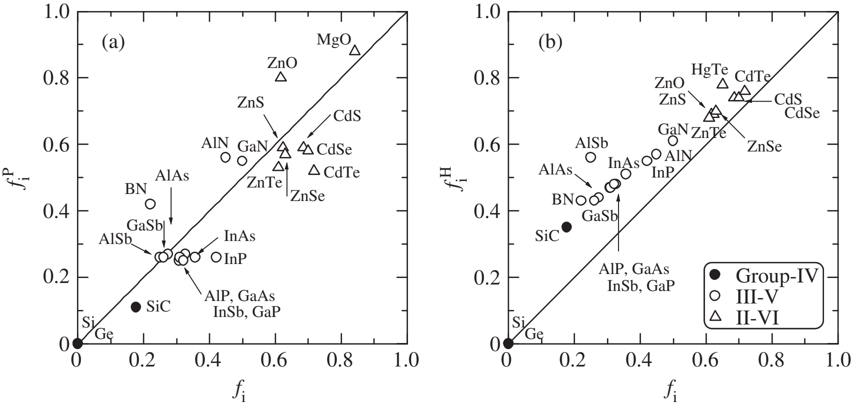

Figure 1.1 Phillips ionicity f_i versus (a) Pauling (f_i^P) and (b) Harrison ionicities (f_i^H) for some group-IV, III–V and II–VI semiconductors. The solid lines in (a) and (b) indicate the relations of $f_i = f_i^P$ and $f_i = f_i^H$, respectively

natural isotopic abundance in percent [1.4]. Table 1.3 also lists the standard atomic weight for some group IV, III, V, II and VI elements [1.4].

1.2.2 Molecular weight

The molecular weight M for an $A^N B^{8\text{-}N}$ semiconductor ($N \neq 4$) can be simply given by the sum of the atomic weights of atoms A and B. For an elemental semiconductor ($N = 4$), it is given by the atomic weight of the element atom A = B. Tables 1.4 and 1.5 list the values of M for a number of group-IV, III–V and II–VI semiconductors with cubic and hexagonal (rhombohedral) structures, respectively.

1.3 CRYSTAL STRUCTURE AND SPACE GROUP

1.3.1 Crystal structure

(a) Diamond, zinc-blende and wurtzite structures

The atoms of certain elements are held together in the solid by strongly covalent bonds at tetrahedral angles of 109.5°. Each atom has four nearest neighbors and twelve next nearest neighbors, which is a consequence of each atom sharing one of its outer electrons with each of four neighbors. The typical structure so formed is that of *diamond*, as shown in Figure 1.2(a). The space lattice is face-centered cubic with pairs of atoms at (0, 0, 0) and (1/4, 1/4, 1/4) forming a pattern unit.

The atomic orbitals that are used to form hybridized bonding orbitals are usually not the same ones that are occupied in the ground state of the atom. For example, in silicon the ground valence configuration of the atom is $3s^2 3p^2$, whereas the hybridized configuration appropriate for the diamond-type crystal structure is $3s^1 3p^3$ (tetrahedral coordination).

Table 1.2 Natural isotopic abundance in percent for some group IV, III, V, II and VI elements

Group	Isotope	Natural abundance (%)	Group	Isotope	Natural abundance (%)
IV	^{12}C	98.90	IV	^{112}Sn	0.97
	^{13}C	1.10		^{114}Sn	0.65
	^{28}Si	92.23		^{115}Sn	0.34
	^{29}Si	4.67		^{116}Sn	14.53
	^{30}Si	3.10		^{117}Sn	7.68
	^{70}Ge	21.23		^{118}Sn	24.23
	^{72}Ge	27.66		^{119}Sn	8.59
	^{73}Ge	7.73		^{120}Sn	32.59
	^{74}Ge	35.94		^{122}Sn	4.63
	^{76}Ge	7.44		^{124}Sn	5.79
III	^{10}B	19.9	V	^{14}N	99.634
	^{11}B	80.1		^{15}N	0.366
	^{27}Al	100		^{31}P	100
	^{69}Ga	60.108		^{75}As	100
	^{71}Ga	39.892		^{121}Sb	57.36
	^{113}In	4.3		^{123}Sb	42.64
	^{115}In	95.7			
II	^{24}Mg	78.99	VI	^{16}O	99.762
	^{25}Mg	10.00		^{17}O	0.038
	^{26}Mg	11.01		^{32}S	95.02
	^{64}Zn	48.6		^{33}S	0.75
	^{66}Zn	27.9		^{34}S	4.21
	^{67}Zn	4.1		^{36}S	0.02
	^{68}Zn	18.8		^{74}Se	0.89
	^{70}Zn	0.6		^{76}Se	9.36
	^{106}Cd	1.25		^{77}Se	7.63
	^{108}Cd	0.89		^{78}Se	23.78
	^{110}Cd	12.49		^{80}Se	49.61
	^{111}Cd	12.80		^{82}Se	8.73
	^{112}Cd	24.13		^{120}Te	0.096
	^{113}Cd	12.22		^{122}Te	2.603
	^{114}Cd	28.73		^{123}Te	0.908
	^{116}Cd	7.49		^{124}Te	4.816
	^{196}Hg	0.15		^{125}Te	7.139
	^{198}Hg	9.97		^{126}Te	18.95
	^{199}Hg	16.87		^{128}Te	31.69
	^{200}Hg	23.10		^{130}Te	33.80
	^{201}Hg	13.18			
	^{202}Hg	29.86			
	^{204}Hg	6.87			

Table 1.3 Standard atomic weight for some group IV, III, V, II and VI elements. Numbers in parentheses give the uncertainty in the last digit of the stated values

Group	Symbol	Atomic weight	Group	Symbol	Atomic weight
IV	C	12.0107(8)			
	Si	28.0855(3)			
	Ge	72.61(2)			
	Sn	118.710(7)			
III	B	10.811(7)	V	N	14.00674(7)
	Al	26.981538(2)		P	30.973761(2)
	Ga	69.723(1)		As	74.921560(2)
	In	114.818(3)		Sb	121.760(1)
II	Mg	24.3050(6)	VI	O	15.9994(3)
	Zn	65.39(2)		S	32.066(6)
	Cd	112.411(8)		Se	78.96(3)
	Hg	200.59(2)		Te	127.60(3)

The diamond cubic lattice is a consequence of the carbon valency of four. We can expect to find the same structure in compounds where one atom has more than four electrons and the other the same number less than four, so that a total of four valency electrons to each atom is maintained. If the compound is of the form of AB, this structure can be produced in two ways. The first is the cubic, *zinc-blende* structure as shown in Figure 1.2(b), with four A (Ga) and four B (As) atoms per conventional unit cell.

The second method by which a structure is formed where each atom of one kind is surrounded by four of another is shown in Figure 1.2(c). This is the hexagonal CdS (w-CdS or β-CdS) or *wurtzite* lattice, which differs only from the zinc-blende structure in the stacking sequence of the sulfur layers. Ideally, the wurtzite structure has the axial ratio $c/a = (8/3)^{1/2} = 1.633$ (hexagonal close-packed structure). Most III–V semiconductors crystallize in the zinc-blende structure, however, many II–VI and some III–V semiconductors crystallize in the wurtzite structure.

In III–V compounds, group III atoms have three electrons with an s^2p^1-configuration outside a core of closed shells and group V atoms five electrons in a s^2p^3-configuration. The III and V atoms have, therefore, an average of four valence electrons per atom available for bonding. We might then expect that the covalent bonds are formed between tetrahedral s^1p^3-hybrid orbitals, e.g., for GaAs:

$$\mathrm{Ga}(4s^24p^1) + \mathrm{As}(4s^24p^3) \rightarrow \mathrm{Ga}(4s^14p^3)^- + \mathrm{As}(4s^14p^3)^+ \qquad (1.6)$$

For such a covalent bonding each V atom donates an electron to a III atom, so that V^+ and III^- ions are formed, each with four valence electrons.

An ionic bond is due to Coulomb attraction between the excess positive and negative charges on ions formed by transfer of electrons from the metallic to the nonmetallic atom in the scheme:

$$\mathrm{Ga}(4s^24p^1) + \mathrm{As}(4s^24p^3) \rightarrow \mathrm{Ga}(4s^04p^0)^{+3} + \mathrm{As}(4s^24p^6)^{-3} \qquad (1.7)$$

Table 1.4 Molecular weight M, lattice constant a and crystal density g for a number of cubic group-IV, III–V and II–VI semiconductors at 300 K

System	Material	M (amu)	a (Å)	g (g/cm^3)
IV	Diamond	12.0107	3.5670	3.5156
	Si	28.0855	5.4310	2.3291
	Ge	72.61	5.6579	5.3256
	α-Sn	118.710	6.4892	5.7710
	3C-SiC	40.0962	4.3596	3.2142
III–V	c-BN	24.818	3.6155	3.4880
	BP	41.785	4.5383	2.9693
	BAs	85.733	4.777	5.224
	c-AlN	40.98828	4.38	3.24
	AlP	57.955299	5.4635	2.3604
	AlAs	101.903098	5.66139	3.73016
	AlSb	148.742	6.1355	4.2775
	β-GaN	83.730	4.52	6.02
	GaP	100.696	5.4508	4.1299
	GaAs	144.645	5.65330	5.31749
	GaSb	191.483	6.09593	5.61461
	InP	145.792	5.8690	4.7902
	InAs	189.740	6.0583	5.6678
	InSb	236.578	6.47937	5.77677
II–VI	MgO	40.3044	4.203	3.606
	β-MgS	56.371	5.62	2.11
	β-MgSe	103.27	5.91	3.32
	β-MgTe	151.91	6.42	3.81
	β-ZnS	97.46	5.4102	4.0879
	ZnSe	144.35	5.6692	5.2621
	ZnTe	192.99	6.009	5.908
	c-CdS	144.477	5.825	4.855
	c-CdSe	191.37	6.077	5.664
	CdTe	240.01	6.481	5.856
	β-HgS	232.66	5.8514	7.7135
	HgSe	279.55	6.084	8.245
	HgTe	328.19	6.4603	8.0849

The bonds in most III–V or II–VI semiconductors are not adequately described by any of these extreme types, but have characteristics intermediate to those usually associated with the terms covalent (Equation (1.6)) and ionic (Equation (1.7)).

(b) Hexagonal and rhombohedral structures

It is well known that silicon carbide (SiC) is a semiconductor crystallizing in a large number of polytypes [1.5]. The various types of SiC differ one from another only by the

Table 1.5 Molecular weight M, lattice constants a and c and crystal density g for a number of hexagonal and rhombohedral group-IV, III–V and II–VI semiconductors at 300 K

System	Material	M (amu)	Lattice constant (Å)		g (g/cm^3)
			a	c	
IV	6H-SiC	40.0962	3.0806	15.1173	3.2153
	15R-SiC	40.0962	3.079	37.78	
			($\alpha = 13°54.5'$)		
III–V	h-BN	24.818	2.5040	6.6612	2.2787
	w-AlN	40.98828	3.112	4.982	3.258
	α-GaN	83.730	3.1896	5.1855	6.0865
	InN	128.825	3.548	5.760	6.813
II–VI	ZnO	81.39	3.2495	5.2069	5.6768
	α-ZnS	97.46	3.8226	6.2605	4.0855
	w-CdS	144.477	4.1367	6.7161	4.8208
	w-CdSe	191.37	4.2999	7.0109	5.6615

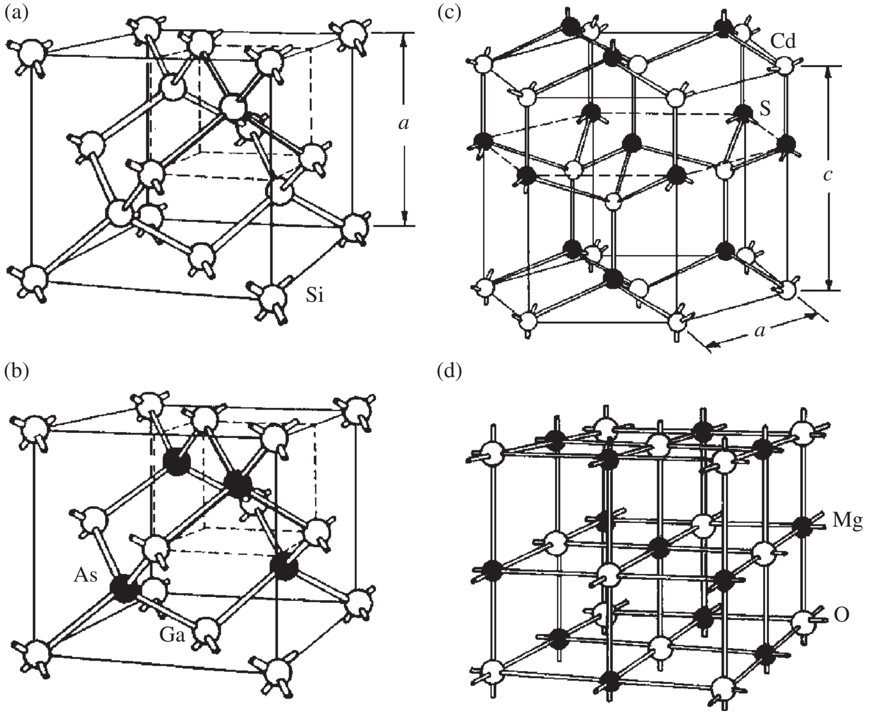

Figure 1.2 Some important crystal lattice structures. (a) diamond lattice (Si); (b) zinc-blende lattice (GaAs); (c) wurtzite lattice (w-CdS); and (d) rocksalt lattice (MgO)

order in which successive planes of Si (or C) atoms are stacked along the *c* axis; one polytype is cubic (3C-SiC) while the remainder, including two of the more frequently occurring forms, 6H and 15R, possess uniaxial symmetry. Note that in the polytype name, the integer refers to the number of Si (C) layers in the unit cell, and C, H and R indicate cubic, hexagonal and rhombohedral (trigonal) symmetry, respectively. Of all the polytypes, 6H is by far the most commonly occurring modification in commercial SiC. The next most common types are 15R and 4H, respectively. Silicon carbide can also crystallize in the wurtzite structure (2H-SiC).

Figure 1.3 shows the stacking sequences in 3C-SiC, 2H-SiC and 6H-SiC [1.6]. In the zinc-blende (3C) structure, the sequence involves three layers which are repeated periodically (ABC ABC ...). All the Si–C bond lengths are the same, and the angles are exactly tetrahedral (109.5°). In the wurtzite (2H) structure, only two layers are repeated (AB AB ...). The Si–C bond length along the stacking direction is not equal to that which is approximately perpendicular to it, and the angles are not exactly tetrahedral. In the 6H polytype, the basic sequence involves six layers (ABCACB ABCACB ...). Similarly, in the 15R polytype the basic sequence involves fifteen layers (ABCACBCABACABCB ...). The II–VI semiconductor, α-HgS, can also crystallize in the rhombohedral (red cinnabar) structure.

(c) Rocksalt structure

The II–VI compound MgO crystallizes in the rocksalt (NaCl) structure. The rocksalt structure shown in Figure 1.2(d) is typical of ionic bonding. The Bravais lattice is face-centered

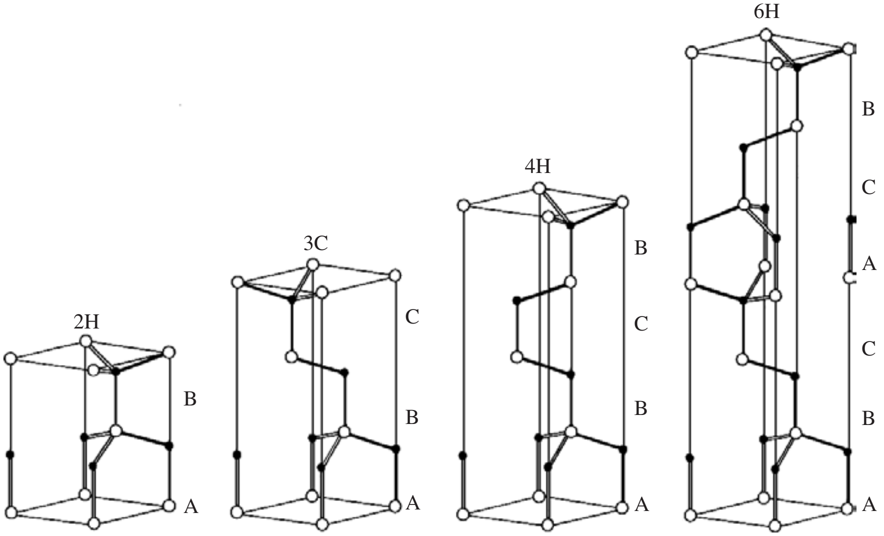

Figure 1.3 Three-dimensional perspective view of the 2H-SiC, 3C-SiC, 4H-SiC and 6H-SiC polytypes. The characteristic chain structures are represented by the heavy solid lines in the $(11\bar{2}0)$ plane. The stacking sequences AB (2H), ABC (3C), ABCB (4H) and ABCACB (6H) are also indicated. [From P. Käckell, B. Wenzien, and F. Bechstedt, *Phys. Rev. B* **50**, 17037 (1994), reproduced by permission from the American Physical Society]

cubic with the unit cell of atomic pattern consisting of one Mg and one O ion separated by one-half the body diagonal of the cube. Since each ion has six nearest neighbors of the opposite kind, the coordination number is six.

We summarize in Table 1.6 the crystal classes for easily or normally grown: (a) group-IV, (b) III–V and (c) II–VI binaries. Table 1.7 also lists the crystal structure for a number of group-IV, III–V and II–VI semiconductors.

1.3.2 Space group

A self-consistent arrangement of symmetry elements in a crystal lattice is known as a space group. The operation of any element of the group must have the pattern of symmetry elements unaltered. By inspection of the 230 space groups, or from first principles, there are just 32 different point groups. Crystals are, therefore, divided into 32 crystal classes according to the point-group symmetry they possess. In Table 1.7, we list the space (point) group for a number of group-IV, III–V and II–VI semiconductors.

Table 1.6 Summary of easily or normally grown crystal structure for: (a) group-IV; (b) III–V and; (c) II–VI semiconductors. d = diamond; zb = zinc-blende; h = hexagonal (wurtzite); rh = rhombohedral (trigonal); rs = rocksalt; or = orthorhombic

(a)

IV/IV	Si	C
Si	d	zb, h, rh
C	zb, h, rh	d

(b)

III/V	N	P	As	Sb
B	zb, h	zb	zb	
Al	h	zb	zb	zb
Ga	h	zb	zb	zb
In	h	zb	zb	zb

(c)

II/VI	O	S	Se	Te
Mg	rs	rs	zb	h
Zn	h	zb, h	zb	zb
Cd	rs	h	h	zb
Hg	rh, or	rh, zb	zb	zb