



Springer 手册精选原版系列

k_z

半导体数据手册 (上册)

Semiconductors: Data Handbook

3rd Edition

Otfried Madelung

K

W

X

k_y



哈尔滨工业大学出版社
HARBIN INSTITUTE OF TECHNOLOGY PRESS

 Springer 手册精选原版系列

半导体数据手册 (上册)

Semiconductors: Data Handbook

3rd Edition

Otfried Madelung



哈尔滨工业大学出版社
HARBIN INSTITUTE OF TECHNOLOGY PRESS

黑版贸审字08-2014-011号

Reprint from English language edition:

Semiconductors: Data Handbook

by Otfried Madelung

Copyright © 2004 Springer Berlin Heidelberg

Springer Berlin Heidelberg is a part of Springer Science+Business Media

All Rights Reserved

This reprint has been authorized by Springer Science & Business Media for distribution in China

Mainland only and not for export therefrom.

图书在版编目 (CIP) 数据

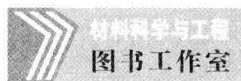
半导体数据手册. 上册: 英文/ (德) 马德朗 (Madelung, O.) 主编. —哈尔滨: 哈尔滨工业大学出版社, 2014.3

(Springer手册精选原版系列)

ISBN 978-7-5603-4514-7

I. ①半… II. ①马… III. ①半导体材料—手册—英文 IV. ①TN304-62

中国版本图书馆CIP数据核字 (2013) 第297008号



责任编辑 张秀华 杨 桦 许雅莹

出版发行 哈尔滨工业大学出版社

社 址 哈尔滨市南岗区复华四道街10号 邮编 150006

传 真 0451—86414749

网 址 <http://hitpress.hit.edu.cn>

印 刷 哈尔滨市石桥印务有限公司

开 本 787mm × 960mm 1/16 印张 25.5

版 次 2014年3月第1版 2014年3月第1次印刷

书 号 ISBN 978-7-5603-4514-7

定 价 158.00元

(如因印刷质量问题影响阅读, 我社负责调换)

Otfried Madelung

Semiconductors: Data Handbook

3rd edition



Springer

Preface

"The frequent use of well known critical data handbooks like Beilstein, Gmelin and Landolt -Börnstein is impeded by the fact that only larger libraries - often far away from the scientist's working place - can afford such precious collections. To satisfy an urgent need of many scientists working in the field of semiconductor physics for having at their working place a comprehensive, high quality, but inexpensive collection of at least the basic data of their field of interest this volume contains the most important data of semiconductors. All data were compiled from information on semiconductors presented on more than 6 000 pages in various volumes of the New Series of Landolt - Börnstein."

With these words the aim of the volume "Semiconductors – Basic Data", published by the present author – was defined in the preface to its first Edition. This edition – published in two volumes in the Series "Data in Science and Technology" – appeared in 1991/92. The 2nd Edition was published in one volume five years later.

While preparing the third edition, it became clear that a complete revision was necessary for several reasons:

- To the eleven subvolumes of volumes III/17 and III/22 of the New Series of Landolt-Börnstein – published between 1982 and 1988 – eight new supplementary subvolumes (III/41) appeared in the meantime. The 19 volumes now available comprise about 10 000 pages with more than 13 000 figures. Thus, much new data had to be included in this collection of basic data.
- The Landolt -Börnstein series is now available on the Internet. So easy access to the data via Internet had to be considered in the structure of this volume.
- Last but not least the possibility to *combine a printed medium with an enclosed CD-ROM* gives the opportunity to improve the value of a data collection by shifting parts of the information onto the CD-ROM, thereby increasing the amount of information substantially without an undue increase of the number of pages.

By this opportunity, a drawback of earlier editions could be eliminated: To limit the number of pages, a comprehensive presentation of the most important data was only possible for the group IV and III-V semiconductors. All other groups of semiconductors could only be handled very briefly in tabular form with a restricted number of figures and without references. This drawback is now eliminated. The (printed) volume contains the basic data for all known groups of semiconductors in suitable length. Figures on crystal structures and band structures supplement the tables.

Further information was shifted to the CD-ROM:

- *Figures.* A user of this book usually first looks for *data collected in tables*. Figures can supply deeper information by presenting functional dependences, such as temperature dependence, pressure dependence, and by presenting dispersion curves, optical spectra etc. Such additional information is now provided in about 1000 additional figures on the CD-ROM. Presenting these figures in the printed version had required several hundred pages.
- *References.* The knowledge of the origin of data is necessary for the user to find the context in which the data were measured. Thus, data presented in this volume should also contain more than 100 pages of references. These references were shifted to the enclosed CD-ROM.
- *Additional information useful for the reader but too spacious to be presented in the printed version.* There are a large number of substances (e.g. boron compounds, transition metal and rare earths compounds) exhibiting "semiconducting properties". A presentation of data referring to such substances in the printed text seemed to be too extensive and was therefore left to the CD-ROM

Thus, the present edition differs substantially from the former editions in the amount of information and the manner of presentation (and unavoidable also in the number of pages). To emphasize this change the title of the third edition has been changed from "*Semiconductors: Basic Data*" to "*Semiconductors: Data Handbook*".

I do hope the users of the volume will profit from these innovations.

Marburg, August 2003

Otfried Madelung

Detailed table of contents

A	Introduction		
1	General remarks to the structure of this volume.....	1	
2	Physical quantities tabulated in this volume....	2	
B	Tetrahedrally bonded elements and compounds		
1	Elements of the IVth group and IV-IV compounds		
1.0	Crystal structure and electronic structure.....	7	
1.1	Diamond (C).....	11	
1.2	Silicon (Si).....	16	
1.3	Germanium (Ge)	45	
1.4	Grey tin (α -Sn)	57	
1.5	Silicon carbide (SiC)	60	
1.6	Silicon germanium mixed crystals ($\text{Si}_x\text{Ge}_{1-x}$)	70	
2	III-V compounds		
2.0	Crystal structure and electronic structure.....	71	
2.1	Boron nitride (BN)	79	
2.2	Boron phosphide (BP)	84	
2.3	Boron arsenide (BAs)	87	
2.4	Boron antimonide (BSb).....	88	
2.5	Aluminum nitride (AlN).....	88	
2.6	Aluminum phosphide (AlP)	91	
2.7	Aluminum arsenide (AlAs)	94	
2.8	Aluminum antimonide (AlSb)	98	
2.9	Gallium nitride (GaN)	103	
2.10	Gallium phosphide (GaP)	109	
2.11	Gallium arsenide (GaAs)	117	
2.12	Gallium antimonide (GaSb).....	129	
2.13	Indium nitride (InN)	137	
2.14	Indium phosphide (InP)	139	
2.15	Indium arsenide (InAs)	148	
2.16	Indium antimonide (InSb)	154	
2.17	Ternary alloys lattice matched to binary III-V compounds	162	
2.18	Quaternary alloys lattice matched to binary III-V compounds.....	167	
3	II-VI compounds		
3.0	Crystal structure and electronic structure ...	173	
3.1	Beryllium oxide (BeO).....	180	
3.2	Beryllium sulfide (BeS)	182	
3.3	Beryllium selenide (BeSe)	182	
3.4	Beryllium telluride (BeTe).....	183	
3.5	Magnesium oxide (MgO).....	184	
3.6	Magnesium sulfide (MgS).....	186	
3.7	Magnesium selenide (MgSe).....	186	
3.8	Magnesium telluride (MgTe)	187	
3.9	Calcium oxide (CaO)	187	
3.10	Strontium oxide (SrO).....	190	
3.11	Barium oxide (BaO).....	192	
3.12	Zinc oxide (ZnO)	194	
3.13	Zinc sulfide (ZnS)	200	
3.14	Zinc selenide (ZnSe)	208	
3.15	Zinc telluride (ZnTe).....	213	
3.16	Cadmium oxide (CdO).....	218	
3.17	Cadmium sulfide (CdS).....	220	
3.18	Cadmium selenide (CdSe).....	226	
3.19	Cadmium telluride (CdTe)	232	
3.20	Mercury oxide (HgO).....	235	
3.21	Mercury sulfide (HgS)	236	
3.22	Mercury selenide (HgSe)	239	
3.23	Mercury telluride (HgTe).....	241	
4	I-VII compounds		
4.0	Crystal structure and electronic structure ...	245	
4.1	Cuprous fluoride (CuF).....	248	
4.2	Cuprous chloride (γ -CuCl).....	248	
4.3	Cuprous bromide (γ -CuBr).....	254	
4.4	Cuprous iodide (γ -CuI).....	259	
4.5	Silver fluoride (AgF).....	262	
4.6	Silver chloride (AgCl).....	263	
4.7	Silver bromide (AgBr)	268	
4.8	Silver iodide (AgI)	271	

5	III₂-VI₃ compounds		
5.0	Crystal structure of quasi-binary II ₂ -VI ₃ compounds.....	275	
5.1	Gallium sulfide (Ga ₂ S ₃)	276	
5.2	Gallium selenide (Ga ₂ Se ₃)	278	
5.3	Gallium telluride (Ga ₂ Te ₃).....	280	
5.4	Indium sulfide (In ₂ S ₃)	281	
5.5	Indium selenide (In ₂ Se ₃)	283	
5.6	Indium telluride (In ₂ Te ₃).....	286	
6	I-III-VI₂ compounds (included are I-Fe-VI ₂ compounds)		
6.0	Crystal structure and electronic structure....	289	
6.1	Copper aluminum sulfide (CuAlS ₂)	292	
6.2	Copper aluminum selenide (CuAlSe ₂)	294	
6.3	Copper aluminum telluride (CuAlTe ₂).....	297	
6.4	Copper gallium sulfide (CuGaS ₂).....	298	
6.5	Copper gallium selenide (CuGaSe ₂).....	302	
6.6	Copper gallium telluride (CuGaTe ₂)	304	
6.7	Copper indium sulfide (CuInS ₂).....	306	
6.8	Copper indium selenide (CuInSe ₂).....	309	
6.9	Copper indium telluride (CuInTe ₂).....	311	
6.10	Silver gallium sulfide (AgGaS ₂).....	313	
6.11	Silver gallium selenide (AgGaSe ₂).....	315	
6.12	Silver gallium telluride (AgGaTe ₂)	318	
6.13	Silver indium sulfide (AgInS ₂).....	319	
6.14	Silver indium selenide (AgInSe ₂).....	320	
6.15	Silver indium telluride (AgInTe ₂)	322	
6.16	Copper thallium sulfide (CuTlS ₂).....	324	
6.17	Copper thallium selenide (CuTlSe ₂).....	324	
6.18	Copper thallium telluride (CuTlTe ₂)	325	
6.19	Silver thallium selenide (AgTlSe ₂).....	325	
6.20	Silver thallium telluride (AgTlTe ₂)	325	
6.21	Copper iron sulfide (CuFeS ₂).....	326	
6.22	Copper iron selenide (CuFeSe ₂)	327	
6.23	Copper iron telluride (CuFeTe ₂).....	327	
6.24	Silver iron selenide (AgFeSe ₂)	328	
6.25	Silver iron telluride (AgFeTe ₂).....	328	
7	II-IV-V₂ compounds		
7.0	Crystal structure and electronic structure ...	329	
7.1	Magnesium silicon phosphide (MgSiP ₂)	333	
7.2	Zinc silicon phosphide (ZnSiP ₂).....	333	
7.3	Zinc silicon arsenide(ZnSiAs ₂).....	356	
7.4	Zinc germanium nitride (ZnGeN ₂).....	338	
7.5	Zinc germanium phosphide (ZnGeP ₂)	339	
7.6	Zinc germanium arsenide (ZnGeAs ₂)	342	
7.7	Zinc tin phosphide (ZnSnP ₂).....	343	
7.8	Zinc tin arsenide (ZnSnAs ₂).....	344	
7.9	Zinc tin antimonide (ZnSnSb ₂)	345	
7.10	Cadmium silicon phosphide (CdSiP ₂).....	346	
7.11	Cadmium silicon arsenide (CdSiAs ₂).....	348	
7.12	Cadmium germanium phosphide (CdGeP ₂).....	349	
7.13	Cadmium germanium arsenide..... (CdGeAs ₂)	352	
7.14	Cadmium tin phosphide (CdSnP ₂).....	355	
7.15	Cadmium tin arsenide (CdSnAs ₂)	357	
8	I₂-IV-VI₃ compounds		
8.1	Copper germanium sulfide (Cu ₂ GeS ₃).....	359	
8.2	Copper germanium selenide (Cu ₂ GeSe ₃)	360	
8.3	Copper germanium telluride (Cu ₂ GeTe ₃)	362	
8.4	Copper tin sulfide (Cu ₂ SnS ₃).....	362	
8.5	Copper tin selenide (Cu ₂ SnSe ₃)	363	
8.6	Copper tin telluride (Cu ₂ SnTe ₃).....	364	
8.7	Silver germanium selenide (Ag ₂ GeSe ₃).....	365	
8.8	Silver germanium telluride (Ag ₂ GeTe ₃)	365	
8.9	Silver tin sulfide (Ag ₂ SnS ₃).....	366	
8.10	Silver tin selenide (Ag ₂ SnSe ₃).....	366	
8.11	Silver tin telluride (Ag ₂ SnTe ₃).....	366	
9	I₃-V-VI₄ compounds		
9.0	Crystal structure	367	
9.1	Copper thiophosphate (Cu ₃ PS ₄).....	368	
9.2	Copper thioarsenide, enargite, luzonite (Cu ₃ AsS ₄)	369	
9.3	Copper arsenic selenide (Cu ₃ AsSe ₄).....	370	
9.4	Copper antimony sulfide, famatinite (Cu ₃ SbS ₄)	371	
9.5	Copper antimony selenide (Cu ₃ SbSe ₄)	371	
9.6	Copper arsenic telluride (Cu ₃ AsTe ₄)	372	
9.7	Copper antimony telluride (Cu ₃ SbTe ₄).....	372	

10 II-III₂-VI₄ compounds

10.0	Crystal structure and electronic structure.....	373
10.1	Zinc aluminum sulfide (ZnAl ₂ S ₄)	375
10.2	Zinc gallium sulfide (ZnGa ₂ S ₄).....	375
10.3	Zinc gallium selenide (ZnGa ₂ Se ₄).....	377
10.4	Zinc thioindate (ZnIn ₂ S ₄)	378
10.5	Zinc indium selenide (ZnIn ₂ Se ₄)	379
10.6	Zinc indium telluride (ZnIn ₂ Te ₄)	381
10.7	Cadmium thioaluminate (CdAl ₂ S ₄).....	381
10.8	Cadmium thiogallate (CdGa ₂ S ₄)	382
10.9	Cadmium gallium selenide (CdGa ₂ Se ₄)	384
10.10	Cadmium gallium telluride (CdGa ₂ Te ₄).....	386
10.11	Cadmium thioindate (CdIn ₂ S ₄)	387
10.12	Cadmium indium selenide (CdIn ₂ Se ₄)	389
10.13	Cadmium indium telluride (CdIn ₂ Te ₄)	391
10.14	Cadmium thallium selenide (CdTl ₂ Se ₄)	392
10.15	Mercury thiogallate (HgGa ₂ S ₄)	393
10.16	Mercury gallium selenide (HgGa ₂ Se ₄)	393
10.17	Mercury indium telluride (HgIn ₂ Te ₄).....	394
10.18	HgIn ₂ Se ₄ , Hg ₃ In ₂ Te ₆ , Hg ₅ In ₂ Te ₈	396
10.19	Further II-III ₂ -VI ₄ compounds with II = Mg, Ca	396

A Introduction

1 General remarks to the structure of this volume

This volume contains basic data of semiconductors. All data were compiled from the 17 volumes of the New Series of the Landolt-Börnstein data handbook, dealing with semiconductors. They comprise the information a scientist working on semiconductors is needing in his every-day work.

The volume consists of seven parts (A...G).

Part A contains introductory remarks.

In part B information about the properties of the important groups of tetrahedrally bonded semiconducting elements and compounds are given. The chapters 1 ... 10 cover the elements of the IVth group of the Periodic System and their isoelectronic analogues: the binary III-V, II-VI, I-VII compounds and the respective ternary compounds (vac-III₂-VI₃, I-III-VI₂, II-IV-V₂, I₂-V-VI₃, I₃-V-VI₄, II-III₂-VI₄ compounds).

The parts C, D and E cover further groups of semiconducting elements, binary and ternary compounds, respectively.

Part F summarizes informations about more than 100 substances which are described in the literature as having "semiconducting properties". Since these substances are of minor importance in semiconductor physics, the data of this chapter are only presented on the enclosed CD-ROM.

To facilitate the use of this book a Substance Index is presented in the part G, separately for the substances in chapters B ... E and for the substances in part F presented only on the CD-ROM.

The data presented in parts B ... E are ordered in chapters on specific substance groups. Most of these chapters begin with a "0"-section, presenting information about the crystal structure and the electronic structure of the semiconductors belonging to the respective substance group. Only these "0"-sections contain figures on lattice structures and on band structure.

Sections on the properties of individual substances follow. The data are ordered under the following headings:

– **Crystal structure**

lattice structure / space group / modifications / high temperature and pressure phases (as far as not mentioned in the "0"-sections).

– **Electronic properties:**

band structure / energies at symmetry points of the band structure / energy gaps (direct energy gap, indirect energy gap) / exciton energies / intra conduction band energies / intra valence band energies / critical point energies / spin-orbit splitting energies / camel's back structure of the conduction band edge / structure of the top of the valence band / effective masses (electrons, holes) / *g*-factor of electrons / valence band parameters.

– **Lattice properties:**

lattice parameters / linear thermal expansion coefficient / density / melting point / Debye temperature / heat capacity / phonon dispersion relations / phonon frequencies (wavenumbers) / sound velocities / second and third order elastic moduli / bulk modulus / Poisson ratio / internal strain parameter.

– **Transport properties:**

electrical conductivity or resistivity (intrinsic conductivity) / (intrinsic carrier concentration / carrier mobilities (electron mobility, hole mobility) / drift velocities and diffusion constants / thermal conductivity (resistivity) / Seebeck coefficient (thermoelectric power) / piezo- and elastoresistance coefficients.

– **Optical properties:**

optical constants / absorption coefficient / reflectance / extinction coefficient / refractive index / dielectric function / dielectric constants / piezo- and elastooptic coefficients.

– **Impurities and defects:**

binding energies of impurities / energy levels of impurities, defects and complexes or of deep centers.

The following restrictions should be taken in mind when using these tables:

– Only figures on crystal structure, band structures and Brillouin zones are shown in the printed part of this book. About 1000 further figures on the temperature dependence of semiconductor parameters and on optical spectra as well as all references are left to the enclosed CD-ROM. Such figures are printed in italics with the addition (CD), e.g. *Fig. 2.3.4 (CD)*. Figures in the "0"-sections of the printed volume are referred to with the page number.

– Physical data can be judged confidentially only by added information about measuring and evaluation methods, about the reference the value has been taken from etc. All this valuable information is lacking in the printed chapters because of the restriction of the number of pages. Adding such information in the present book had surpassed the frame of this volume.

– The data presented here have often to be chosen from several values, given in the Landolt-Börnstein volumes, if no unique choice had been possible for the author of the respective chapter. In such cases the "most reliable one" - according to the judgement of the author of this book - or the "newest one" has been listed.

CD-ROM

This book contains a CD-ROM with the full content of the printed pages and additionally more than 100 pages of references and about 1000 figures. Thus the reader can gain information in three stages:

- firstly by inspecting the tables of this book,
- secondly by getting additional information from the CD-ROM,
- finally by referring to the 17 Landolt-Börnstein volumes on semiconductors or their Internet version or – of course – to the original papers referred to in the Reference Lists on the CD-ROM.

2 Physical quantities tabulated in this volume

Data on the following physical quantities occur in the tables and figures of Parts B ... F:

Electronic structure

Brillouin zones:

Brillouin zones for individual semiconductors are shown in the "0"-sections at the beginning of a chapter dealing with a group of semiconducting materials. Symmetry lines and points within a Brillouin zone are designed by letters (Γ , X, L, Σ ...). Subscripts to these letters designate the irreducible representation of the respective energy state (1, 1', 2, 12, 25'...).

band structure:

The function $E(\mathbf{k})$ gives the energies of a band state at a wave vector \mathbf{k} in the Brillouin zone. Instead of the value of \mathbf{k} often the respective symmetry designation in the Brillouin zone is given ($E(\Gamma_{25'})$...). Figures on band structure show the values of $E(\mathbf{k})$ along axes and at points of high symmetry.

band structure and exciton parameters:**band energies** (unit eV):

- E_c, E_v energies of the edges of conduction and valence bands, respectively.
- E_g energy gap between conduction and valence band. Further subscripts refer to: dir: direct gap, ind: indirect gap, opt: optical gap (threshold energy for optical transitions), th: thermal gap (energy gap extrapolated to 0 K from transport measurements), \parallel, \perp electric field parallel or perpendicular to a crystal axis; L(T) superscripts for longitudinal (transverse) exciton energies.
- Δ mostly spin-orbit splittings of energy levels (subscripts 0, so, 1, 2 and dashes (')) refer to the location of the level as explained in the tables),
also other splittings of energy levels (cf: crystal-field splitting, camel's back parameters (see below) ...).
- E_0 ... the letter E with other subscripts refers to intra- and interband transitions (critical points) as explained in the tables (E_0, E_1, E_2 ...).

exciton energies (unit eV):

- E_b binding energy of an exciton.
- E_{gx} energy of the excitonic gap (defined as energy gap minus exciton binding energy).
- $E(1S)$ energy of the exciton 1S state; excited states are designated by $E(2S), E(2P)$...
- E_{L-T} longitudinal-transverse exciton splitting energy.
- E_{ex} exciton exchange interaction energy

effective masses (in units of the electron mass m_0):

- m_n, m_p effective mass of electrons (holes) defined by
 $E(k) = E(\Gamma) + \hbar^2 k^2 / 2m_n$ at the bottom of the conduction band or
 $E(k) = E(\Gamma) - \hbar^2 k^2 / 2m_p$ at the top of the valence band
 where Γ designates the center of the Brillouin zone. For very small effective electron masses the parabolic approximation $E \propto k^2$ becomes invalid (occurrence of *k-linear terms*).
- m_c ... other subscripts refer to: c: conductivity effective mass, cr: cyclotron resonance effective mass, ds: density of states mass, p,h: heavy holes, p,l: light holes, so: effective mass in the spin-orbit split band, (X ...): effective mass at symmetry point X ...

g-factor:

- g_c g -factor of electrons.

special band structure parameters (mostly for tetrahedrally bonded semiconductors, see also the "0"-sections of the respective chapters):

A, B, C anisotropy parameters of warped energy surfaces at the top of the valence band (symmetry Γ_8) of semiconductors with diamond or zincblende structure, defined by the equation

$$E(\mathbf{k}) = E(\Gamma) + (\hbar^2 k^2 / 2m_0)(A \pm (B^2 + sC^2)^{1/2}), \quad s = (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) / k^4$$

The \pm -sign refers to the two bands into which $E(\Gamma_8)$ splits for $\mathbf{k} \neq 0$. By spin-orbit splitting a second valence band of Γ_6, Γ_7 -symmetry is situated below the degenerate Γ_8 -valence band.

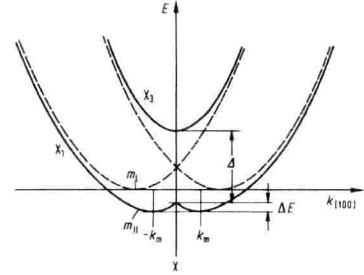
$m_{||}, m_{\perp}$ longitudinal and transverse effective masses defined by the equation

$$E(\mathbf{k}) = E(\mathbf{k}_0) + \hbar^2 \kappa_x^2 / 2m_{||} + \hbar^2 (\kappa_y^2 + \kappa_z^2) / 2m_{\perp} \quad \text{where } \kappa = \mathbf{k} - \mathbf{k}_0 \text{ and } \kappa_x \parallel k_0, \kappa_y, \kappa_z \perp k_0, \text{ if the band minima are situated at } \mathbf{k} \neq 0 \text{ along a symmetry axis } (\Delta \text{ or } \Lambda) \text{ (ellipsoidal energy surfaces).}$$

$k_{||}, k_{\perp} \dots$ parameters of the *camel's back structure* at the bottom of the conduction band in several zincblende-type semiconductors defined by the equation

$$E(\mathbf{k}) = \hbar^2 k_{||}^2 / 2m_{||} + \hbar^2 k_{\perp}^2 / 2m_{\perp} - ((\Delta/2)^2 + \Delta_0 \hbar^2 k^2 / 2m_1)^{1/2}$$

with $k_{||}$ and k_{\perp} : components of the wave vector parallel and perpendicular to the $[100]$ -direction, respectively, m_{\perp} : effective mass perpendicular to the $[100]$ -direction; Δ_0 : parameter describing the non-parabolicity; all other parameters are explained in the figure (right).



$k_{||}, k_{\perp}$ also components of the \mathbf{k} -vector near the top of the valence band in semiconductors with wurtzite lattice, defined by

$$E_1(\mathbf{k}) = E(\Gamma_6) + ak_{||}^2 + bk_{\perp}^2,$$

$$E_{2,3}(\mathbf{k}) = E(\Gamma_6) \pm \Delta/2 + ck_{||}^2 + dk_{\perp}^2 \pm ((\Delta/2 + c'k_{||}^2 + d'k_{\perp}^2)^2 + (c''k_{||}^2 + d''k_{\perp}^2)^2)^{1/2}.$$

$E_1(0)$ and $E_{2,3}(0)$ are separated by the *crystal-field splitting energy* Δ (Δ_{cf}).

Lattice properties

static lattice parameters:

a, b, c	lattice parameters (unit Å or nm)
α, β, γ	angles
α	linear thermal expansion coefficient (unit K^{-1})
d	density (unit $g\ cm^{-3}$)
T_m	melting temperature (unit K)
T_{dec}	decomposition temperature (unit K)
Θ_D	Debye temperature (unit K)
C_p, C_v	heat capacities (unit $J\ mol^{-1}K^{-1}$)

dynamic lattice parameters:

$\nu(\mathbf{k})$ phonon dispersion relation (dependence of phonon frequency on wave vector), instead of k often the reduced wave vector $\zeta = k/k_{\max}$ is used

$\nu, \bar{\nu}$ phonon frequency (unit s^{-1}), wavenumber (unit cm^{-1})

$h\nu$ photon energy (unit eV)

Subscripts to the frequencies (wavenumbers) refer to transverse and longitudinal optical and acoustic branches (TO, LO, TA, LA) and to the symmetry points in the Brillouin zone as for the band structure energies. Further subscripts refer to Raman active (R) and infrared active (ir) modes.

v_i sound velocities (unit cm s^{-1})

c_{lm}, c_{lmn} second order and third order elastic moduli (unit dyn cm^{-2})

B bulk modulus (dyn cm^{-2}) (Subscript S: adiabatic bulk modulus)

G shear modulus (unit GPa)

E Young's modulus (unit GPa)

ν Poisson's ratio (dimensionless)

ζ internal strain parameter (dimensionless)

Transport properties

R resistance (unit Ω)

R_H Hall coefficient (unit $\text{cm}^3 \text{C}^{-1}$)

$\sigma, (\sigma_i)$ (intrinsic) electrical conductivity (unit $\Omega^{-1} \text{cm}^{-1}$)

ρ electrical resistivity (unit Ωcm)

κ thermal conductivity (subscript L: lattice contribution) (unit $\text{W cm}^{-1} \text{K}^{-1}$)

E_A activation energy (mostly for temperature dependence of conductivity) (unit eV)

n, p, n_i electron and hole concentration, intrinsic carrier concentration (unit cm^{-3})

μ_n, μ_p electron and hole mobilities, respectively (unit $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$). Further subscripts refer to: dr: drift mobility, c: conductivity mobility, H: Hall mobility, \parallel, \perp : parallel (perpendicular) to a principal axis

v_n, v_p drift velocities of electrons and holes (unit cm s^{-1})

S Seebeck coefficient (thermoelectric power) (unit V/K)

π_{ik} piezoresistance coefficients (unit $\text{cm}^2 \text{dyn}^{-1}$)

m_{ik} elastoresistance coefficients (dimensionless)

$e_{ik}, d_{ik}, g_{ik}, h_{ik}$ piezoelectric coefficients

Optical properties

K absorption coefficient (unit cm^{-1})

R reflectance (dimensionless)

n	(real) refractive index (dimensionless)
k	extinction coefficient (dimensionless)
$\varepsilon, \varepsilon_{ik}$	dielectric constant (component of the dielectric tensor); subscripts and brackets refer to: 1: real part of the complex dielectric constant, 2: imaginary part of the complex dielectric constant, 0: low frequency limit, ∞ : high frequency limit, \parallel, \perp : parallel or perpendicular to a crystal axis
π_{ik}	piezooptic coefficients (unit $\text{cm}^2 \text{dyn}^{-1}$)
p_{ik}	elasto-optic coefficients (dimensionless)
r_{ik}	linear electrooptic constant (unit m/V)
R_{ik}	quadratic electrooptic coefficient (unit m^2/V^2)
$d(\text{SHG})$	second order nonlinear dielectric susceptibility (unit m/V) (SHG = second harmonic generation)
$\chi_{ijkl}^{(3)}$	third order susceptibility (unit esu)

Impurities and defects

E_b	binding energy of donors ($E_c - E_d$) or acceptors ($E_a - E_v$)
E	for deep levels the type (d, a) is given; positive values refer to the valence band edge, negative values to the conduction band edge

B Tetrahedrally bonded elements and compounds

1 Elements of the IVth group and IV-IV compounds

1.0 Crystal structure and electronic structure

1.0.1 Crystal structure

The semiconductors C (Diamond), Si, Ge, Sn (grey tin) crystallize in the diamond lattice.

In this lattice each atom is surrounded by four nearest neighbors which lie with equal distances at the corner of a tetrahedron (Fig. 1.0.1). The lattice can be seen as two interpenetrating face-centered cubic lattices (Fig. 1.0.2).

The **space group** of the diamond lattice is $O_h^7 - Fd3m$.

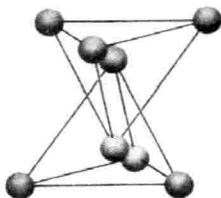


Fig. 1.0.1. Orientation of tetrahedra in the diamond structure.

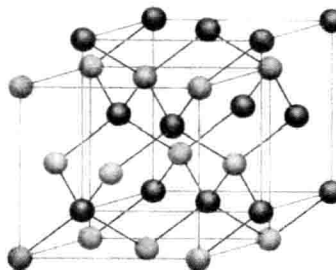


Fig. 1.0.2. The diamond lattice. The elementary cubes of the two face-centered cubic lattices are shown.

Carbon also occurs in a hexagonal modification (graphite, Fig. 1.0.3); *tin* crystallizes at room temperature normally in a tetragonal modification (white tin, β -Sn, Fig. 1.0.4), whereas the diamond-like grey tin (α -Sn) is stable only below 13.20°C.

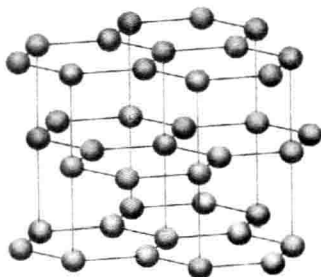


Fig. 1.0.3. The graphite lattice

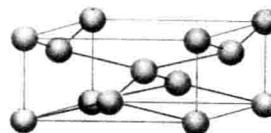


Fig. 1.0.4. Unit cell of the white tin lattice

Semiconducting phases also occur in *silicon carbide*. In this binary compound the energy differences between cubic, hexagonal and rhombohedral structures are so small, that a large number of polymorphic modifications occur. More than hundred different *polytypes* exist. In all polytypes every atom is surrounded by four atoms of the other species.

The polytypes of SiC can be described in terms of a hexagonal system, the stacking order along the *c*-axis differing from polytype to polytype; the cubic form fits into this system by taking the [111] direction as "*c*-axis". Fig. 1.0.5 shows the elementary cells of the 3C (cubic, zincblende, β -SiC), 2H (hexagonal, wurtzite, α -SiC), 4H and 6H polytypes. Other hexagonal (H) and rhombohedral (R) polytypes occur.

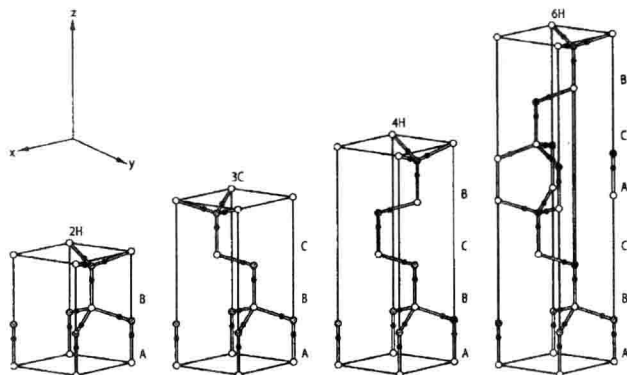


Fig. 1.0.5. Elementary cells of 3C, 2H, 4H, 6H structures. The 3C structure is also drawn in the hexagonal cell. Stacking sequences are indicated.

1.0.2 Electronic structure

General remarks on the band structure of elements with diamond structure:

The **Brillouin zone** of the diamond structure is the Brillouin zone of the face-centered lattice, Fig. 1.0.6. Symmetry lines and points within the Brillouin zone are designed by letters (Γ , X, L, Δ ...).

The qualitative **band structure** is shown in Fig. 1.0.7 along the Δ and Λ axes in the Brillouin zone. Subscripts to the letters defining the location of a given energy state in the Brillouin zone designate the irreducible representation of the respective state (1, 1', 2, 12, 25'...).

Conduction band edge: Fig 1.0.7 shows only the topological connection of the subbands of the conduction band. Two possibilities are to be considered in connection with the band structure of group IV elements:

Lowest band state at Γ : In this case the energy $E(\mathbf{k})$ can be approximated near the band edge by a scalar quadratic \mathbf{k} -dependence:

$$E(\mathbf{k}) = E(\Gamma) + \hbar^2 \mathbf{k}^2 / 2m_n$$

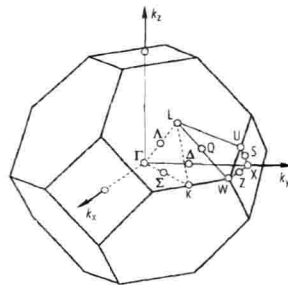


Fig. 1.0.6. Brillouin zone of the diamond lattice.

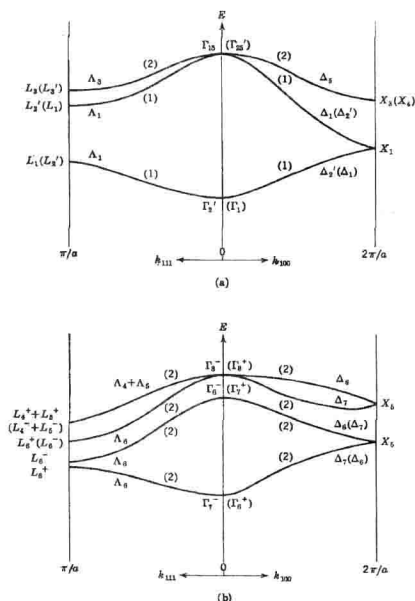


Fig. 1.0.7. Qualitative picture of the band structure of a semiconductor with diamond structure (a) without inclusion of spin, (b) with spin taken into account. This qualitative shape applies both to the valence and the conduction bands. The symmetry symbols are the same for the two cases except where valence band symbols differing from those for the conduction band are shown in brackets. Where a point or line is labeled with two symbols without brackets, it means that symmetry arguments alone cannot distinguish between the two possibilities. Degeneracies of the band are given in brackets.

Lowest band state along a symmetry axis (Δ or Λ):

In the case that the lowest band state lies at a point \mathbf{k}_0 at a symmetry axis the band edge can be approximated by $E(\mathbf{k}) = E(\mathbf{k}_0) + \hbar^2 \kappa_x^2 / 2m_{\parallel} + \hbar^2 (\kappa_y^2 + \kappa_z^2) / 2m_{\perp}$ where $\kappa = \mathbf{k} - \mathbf{k}_0$ and $\kappa_x \parallel \mathbf{k}_0$, $\kappa_y, \kappa_z \perp \mathbf{k}_0$ (ellipsoidal energy surfaces).

Valence band edge: In all group IV elements the top of the valence band is situated at the center Γ of the Brillouin zone (Γ_{25}'). According to Fig. 1.0.7 this state is triply degenerated if the spin-orbit coupling can be neglected. Taking spin into account the (now sixfold degenerated) state splits into the fourfold degenerated Γ_8^+ state and a lower lying twofold degenerated Γ_7^+ state, separated by the spin-orbit splitting energy Δ_{so} . At $\mathbf{k} \neq 0$ two subbands (degenerated at Γ) build the band edge. Their energy can be approximated by

$$E(\mathbf{k}) = E(\Gamma) + (\hbar^2 k^2 / 2m_0)(A \pm (B^2 + sC^2)^{1/2}), s = (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) k^4$$

The \pm -sign refers to the two bands into which $E(\Gamma_8^+)$ splits at $\mathbf{k} \neq 0$ (warped surfaces).

Special band structures:

According to Figs. 1.0.8 ... 1.0.13 the semiconducting group IV elements and IV-IV compounds show the following band structures:

Diamond and silicon are indirect semiconductors, the lowest minima of the conduction band being located on the Δ -axis.

Germanium is an indirect semiconductor too, but in contrast to C and Si the lowest minima of the conduction band are located at the endpoints L of the Λ -axis.

Grey tin is a zero gap semiconductor, where the top of the valence band and the bottom of the conduction band are degenerated.

Silicon carbide is an indirect semiconductor, the lowest minima of the conduction band being located at the end points X of the cubic axes (X in the cubic polytype, K in the hexagonal 2H polytype).

The valence bands of all five semiconductors are identical as shown in Fig. 1.0.7 (warped surfaces).