

LANDOLT-BÖRNSTEIN

Numerical Data and Functional Relationships
in Science and Technology

Zahlenwerte und Funktionen
aus Naturwissenschaften und Technik

Group III: Crystal and Solid State Physics

Volume 17
Semiconductors

Editors: O. Madelung · M. Schulz · H. Weiss †

Subvolume g

Physics of Non-Tetrahedrally
Bonded Binary Compounds III



Springer-Verlag Berlin · Heidelberg · New York · Tokyo 1984

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New Series

Editors in Chief: K.-H. Hellwege · O. Madelung

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Zahlenwerte und Funktionen
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Neue Serie

Gesamtherausgabe: K.-H. Hellwege · O. Madelung

Gruppe III: Kristall- und Festkörperphysik

Band 17

Halbleiter

Herausgeber: O. Madelung · M. Schulz · H. Weiss †

Teilband g

Physik der nicht-tetraedrisch gebundenen
binären Verbindungen III

J. B. Goodenough · A. Hamnett · G. Huber · F. Hulliger

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Herausgegeben von O. Madelung



Springer-Verlag Berlin · Heidelberg · New York · Tokyo 1984

Typesetting: Universitätsdruckerei H. Stürtz AG, Würzburg; Printing: Druckhaus Langen-scheidt KG, Berlin; bookbinding: Lüderitz & Bauer GmbH, Berlin.

The use of registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Printed in Germany

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banks.

NE: Hellwege, Karl-Henning [Hrsg.]; Madelung, Otfried [Hrsg.]; Goodenough, John B. [Mitarv.].

ISBN 0-387-12744-5 New York, Heidelberg, Tokyo
ISBN 3-540-12744-5 Berlin, Heidelberg, New York, Tokyo

Springer, Parallel: Numerical data and functional relationships in science and technology. - Berlin, Heidelberg, New York
Zahlenwerte und Funktionswerte aus Naturwissenschaften und Technik/Landolt-Bornstein. - Berlin: Heidelberg; New York; Tokyo:
Springer, Herausgeber: K.-H. Hellwege; O. Madelung, Gruppe 3, Kristall- und Festkörperphysik.
NE: Landolt, Hans [Begr.]; PT, N.S., Gesamtherg.: Tellek, G., Physik der nicht-terapeutisch gebündelten Verbindungen. - III/
BD 17, Halbleiter/Hrsg.: O. Madelung, ... Hrsg. von O. Madelung - 1984.

J.B. Goodenough ... Hrsg. von O. Madelung - 1984.

Berlin, Heidelberg, New York

Springer, Parallel: Numerical data and functional relationships in science and technology. - Berlin, mit d. Erreichungsorten
Zahlenwerte und Funktionswerte aus Naturwissenschaften und Technik/Landolt-Bornstein. - Berlin: Heidelberg; New York; Tokyo:
Springer, Herausgeber: K.-H. Hellwege; O. Madelung, Gruppe 3, Kristall- und Festkörperphysik.
NE: Landolt, Hans [Begr.]; PT, N.S., Gesamtherg.: Tellek, G., Physik der nicht-terapeutisch gebündelten Verbindungen. - III/
BD 17, Halbleiter/Hrsg.: O. Madelung, ... Hrsg. von O. Madelung - 1984.

Organization of the sections in the chapters on “Physical data of semiconductors”

The data on the physical properties of semiconductors are generally arranged in subsections of the order given below. Since there is some arbitrariness in the assignment of a property to the seven subsections, physically related properties may appear in different subsections in some cases.

Structure

Static properties of the lattice as structure, space group, lattice parameters, phase transitions, chemical bond. Density, melting point, thermal expansion are sometimes listed under “Further properties”. Further static properties are given in “Lattice properties”.

Electronic properties

Information and data about electronic and excitonic energy states as well as electron and hole parameters (band structure, density of states, energy gaps, transition energies, effective masses (sometimes also presented in “Transport properties”), g-factors, other band parameters).

Impurity and defect states

Basic data on shallow and deep states (trap levels, nature of defects, point defect thermodynamics, g-factors of defects; for the influence of impurities on other properties, see also the respective subsections).

Lattice properties

Static and dynamic properties of the lattice (phonon dispersion relations, phonon frequencies, sound velocities, elastic and other moduli, Grüneisen parameter, dielectric constants (sometimes also listed under “Optical properties”); for Debye temperature, heat capacity, see also “Further properties”; for structure, density, lattice parameters, chemical bond etc., see subsection “Structure”).

Transport properties

Electronic transport parameters (conductivities, carrier concentrations, mobilities, Seebeck coefficient etc.; for thermal conductivity, see also “Further properties”).

Optical properties

Optical spectra, optical constants, parameters obtained from optical measurements if not already listed in the subsections “Electronic properties” and “Impurity and defect states” (absorption, reflection, refractive index, dielectric constants, Raman scattering etc.).

Further properties

Thermal, magnetic, thermodynamic properties, data more completely presented in other Landolt-Börnstein volumes (thermal conductivity, thermal expansion, magnetic susceptibility, magnetic transition temperatures, magnetic moments, hardness, melting point, density, heat capacity, Debye temperature etc.).



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Vorwort

Der vorliegende Band 17g schließt die in Teilband 17a begonnene und in den Teilbänden 17b, 17e und 17f fortgesetzte Behandlung der physikalischen Eigenschaften binärer Halbleiter ab. Vorgelegt werden Daten über halbleitende Borverbindungen und halbleitende Verbindungen der Übergangsmetalle und der Seltenen Erden.

Die in den früheren Bänden behandelten Familien von Verbindungen (III-V-Verbindungen, II-VI-Verbindungen etc.) enthalten eine überschaubare Anzahl von Substanzen mit wohldefinierten Halbleitereigenschaften, über die in den meisten Fällen zahlreiche Meßdaten vorliegen. Die in diesem Band behandelten Familien bestehen dagegen aus einer extrem großen Zahl von binären Verbindungen, deren Eigenschaften nur zum Teil bekannt sind und bei denen in vielen Fällen Unklarheit besteht, ob sie Halbleiter sind. Dementsprechend war es schwierig, eine sachgemäße Auswahl an Substanzen und Daten zu treffen. Die Autoren versuchten einen Mittelweg zu gehen: über die eindeutig als Halbleiter identifizierten Substanzen hinaus wurden auch solche aufgenommen, bei denen Halbleitereigenschaften zu vermuten sind oder die aus systematischen Gründen einer Gruppe als Halbleiter bekannter Stoffe zuzuordnen sind. Da bei den meisten Substanzen das Datenmaterial wesentlich geringer ist als bei den in früheren Bänden dargestellten Halbleitern, wurde vielfach auf eine detaillierte Untergliederung in strukturelle, elektronische, optische, Gittereigenschaften usw. verzichtet. Unterschieden wurde dann lediglich zwischen „strukturellen“ und „physikalischen“ Eigenschaften, in einigen Fällen wurde auch auf eine derartige Einteilung verzichtet.

Ein weiterer Unterschied zu den vorhergehenden Bänden muß erwähnt werden: bei den Verbindungen der Übergangsmetalle und Seltenen Erden sind häufig die magnetischen Eigenschaften wichtiger als die halbleitenden Eigenschaften. Solche Verbindungen (wie z.B. die Gruppe der Spinelle) sind schon in anderen Bänden dieser Serie dargestellt. Es erschien hier weder zweckmäßig, lediglich auf diese Bände zu verweisen, noch konnten alle in anderen Bänden mitgeteilten Daten hier wiederholt werden. In diesen Fällen wurden nur solche Daten aufgenommen, die einen Halbleiterphysiker in erster Linie interessieren. Für weitergehende Informationen wurde jeweils auf die anderen Bände verwiesen.

Es ist mir auch hier wieder eine Freude, den Autoren für ihre gründliche und kritische Arbeit und dem Springer-Verlag für die reibungslose Zusammenarbeit danken zu können. Den unermüdlichen Einsatz der Landolt-Börnstein-Redaktion des Verlages, insbesondere von Herrn Dr. W. Polzin, Frau R. Lettmann und Frau I. Lenhart, möchte ich besonders hervorheben.

Marburg, März 1984

Der Herausgeber

- 9.14.10 Compounds with group Vb elements
 9.14.11 Boron-hafnium compounds
 9.14.12 Boron-rhenium compounds
 9.14.13 Boron-hafnium

Preface

In this subvolume 17g, the presentation of the physical properties of binary semiconductors – started in subvolume 17a and continued in subvolumes 17b, 17e and 17f – will be completed. Data on boron compounds and on semiconducting transition-metal and rare earth compounds will be presented.

The families of III-V compounds, II-VI compounds etc. which have been treated in the previous volumes consist of a limited number of compounds with well-defined semiconducting properties. On the other side, the families treated in this volume consist of an extremely large number of compounds which are only partly investigated. For many of these compounds it is not yet clear whether they are semiconductors or not. Accordingly, the choice of substances and data to be presented in this volume was difficult. The authors tried to make a compromise: beyond substances identified definitely as semiconductors, such compounds have been included where semiconducting properties may be expected or where compounds should be added to a group of known semiconductors by systematical reasons. Since considerably less data are available for many of these compounds, the detailed subclassification (structure, electronic, optical, lattice properties etc.) used in previous volumes could frequently not be retained. The data have been then merely grouped under two headings "Structure" and "Physical properties", in some cases the data have not been classified at all.

A further difference to the previous volumes should be mentioned: for several groups of transition-metal and rare earth compounds, magnetic properties are as important as semiconducting properties. Such groups have been already treated in other Landolt-Börnstein volumes. An example is the group of transition-metal compounds with spinel structure. Here it seemed not to be appropriate to refer solely to other volumes. Nor was it possible to reprint all data presented already elsewhere. In these cases, the data have been included to such an extent as a semiconductor physicist may expect to find. For further information, references have been given to the other volumes.

I am glad to take this opportunity to thank the authors for their thorough and critical work and the Springer-Verlag for the excellent cooperation. The competent work of Dr. W. Polzin, Mrs. R. Lettmann and Mrs. I. Lenhart of the Landolt-Börnstein editorial staff is gratefully acknowledged.

Marburg, March 1984

The Editor

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	energy of critical points in optical spectra	eV	—
	energy of band edge of type I_{α}	eV	17a/2.4.1
	Young's modulus (measured in [hk0] direction)	dyn/cm ²	17a/2.4.2, eq. (A 100)
	energy of acceptor (donor) state measured from the respective band edge	eV	17a/2.3.1
	activation energy (of conductivity or other properties)	eV	—
	binding energy	eV	17a/2.1.1, eq. (A 1)
	band edge of conduction (valence) band	eV	—
	Fermi energy	eV	—
	energy gap	eV	17a/2.1.1
	energy gap extrapolated to 0 K (thermal energy E_{eff})	eV	17a/2.1.1
	direct (or direct) energy gap	eV	17a/2.1.1
	kinetic energy	eV	—
	photoluminescence (photoconductivity) peak energy	eV	—

A. Introduction

1. List of symbols

In the following list frequently used symbols are specified. The references in the last column refer to the introductory part A in subvolume 17a (cited as 17a/followed by the number for the respective section) or to that section of part B of this subvolume where the quantity is defined or introduced the first time (cited as 17g/followed by the number of the respective section). The units listed in the second-last column are the most frequently used units. In the tables of part B data are generally given in the units of the original paper. To facilitate a conversion from CGS units to SI units or vice versa conversion tables are presented in section 3 below.

Symbol	Property	Unit	Introduced in section
a, b, c	lattice parameters	Å, pm	
a_{O_2}	oxygen activity	-	17g/9.15.2
A	absorbance	-	17g/9.15.2
b	electron-hole mobility ratio (μ_n/μ_p)		
$B(B_S, B_T)$	bulk modulus (adiabatic, isothermal)	bar	17a/2.1.2, eq. (A.17)
B	Nernst coefficient	$\text{cm}^2 \text{K}^{-1} \text{s}^{-1}$	17a/2.2.1
B	magnetic induction	T, G	
B_i	internal magnetic field	T	17g/9.16
c_{lm}	elastic moduli (stiffnesses)	dyn cm^{-2}	17a/2.1.2, eq. (A.19)
C_A	Curie constant per g-atom	$\text{cm}^3 \text{K(g-atom)}^{-1}$	17g/9.15.3
C_m	molar Curie constant	$\text{cm}^3 \text{K mol}^{-1}$	17g/9.14
C_p, C_v	heat capacities	$\text{J mol}^{-1} \text{K}^{-1}$	
d	distance, bond length	cm, Å	
d	thickness of a sample	cm	
d	density	g cm^{-3}	
d_x	X-ray density	g cm^{-3}	
d_{opt}	optical density ($\log I_0/I$)	$\text{cm}^2 \text{s}^{-1}$	
$D_{n(p)}$	diffusion coefficient for electrons (holes)	eV	17g/9.16
Dq	crystal field splitting parameter	C	
e	elementary charge	e	17a/2.1.2
$e_{(T)}^*$	(transverse) effective ionic charge		
e	polarization vector	V cm ⁻¹	
E	electric field strength	eV	
E	energy	eV	
$E_{0,1,2\dots}$	energies of critical points in optical spectra	eV	17a/2.1.1
$E(\Gamma_6)\dots$	energy of band edge of type Γ_6 ...	eV	17a/2.4.1
$E_{[hkl]}$	Young's modulus (measured in [hkl] direction)	dyn cm^{-2}	17a/2.4.2, eq. (A.100)
$E_{a(d)}$	energy of acceptor (donor) state measured from the respective band edge	eV	17a/2.3.1
E_A	activation energy (of conductivity or other temperature or pressure dependent properties)	eV	
E_b	binding energy	eV	
$E_{c(v)}$	band edge of conduction (valence) band	eV	17a/2.1.1, eq. (A.1)
E_F	Fermi energy	eV	
E_g	energy gap	eV	17a/2.1.1
$E_{g, th}$	energy gap extrapolated to 0 K (thermal energy gap)	eV	17a/2.1.1
$E_{g, dir(ind)}$	direct (indirect) energy gap	eV	17a/2.2.1
E_{kin}	kinetic energy	eV	
$E_{pl(pe)}, E_{peak}$	photoluminescence (photoconductivity) peak energy	eV	

Introduction: 1. List of symbols

Symbol	Property	Unit	Introduced in section
E_t	energy of trap level	eV	
E_{thr}	ionization energy (photothermal)	eV	17g/9.16
f	frequency	Hz	
f_s	oscillator strength		17g/9.16
$g(E)$	density of states	$\text{cm}^{-3} \text{eV}^{-1}$	17a/2.1.1, eq. (A.8)
$g_c(v)$	density of conduction (valence) band states	$\text{cm}^{-3} \text{eV}^{-1}$	
g_e, g_n	g -factor of conduction electrons		
g_v, g_p	g -factor of holes (valence band)		
g_V	Gibbs energy of formation of a neutral cation vacancy	eV	17g/9.15.2
$G_{[hkl]}$	torsional (shear) modulus in [hkl] direction	dyn cm^{-2}	
ΔG_f^0	standard free energy of formation	J mol^{-1}	
ΔG_{tr}	Gibbs energy of (phase) transition	J mol^{-1}	
$H_{(B, K, V)}$	hardness (Brinell, Knoop, Vickers)	kg mm^{-2}	
H	magnetic field strength	nT , Oe	
H_A	applied magnetic field strength	A/m	
H_{ext}	external magnetic field strength	A/m	
$\Delta H_{(p-p)}$	(peak to peak) linewidth	A/m	
ΔH_f^0	standard heat of formation	J mol^{-1}	
ΔH_{tr}	(phase) transformation heat	J mol^{-1}	
i	current density	A cm^{-2}	
$I_{(lum, R)}$	intensity (of luminescence, Raman intensity)	$\text{cm}^{-2} \text{s}^{-1}$	
I_{ph}	photocurrent	A	
J	total angular momentum quantum number		
J_i	exchange energy (J/k in K)	eV	17g/9.15.2
k	extinction coefficient (absorption index)		
k	Boltzmann constant	J K^{-1}	17a/2.2.2, eq. (A.41)
k	wave vector of electrons	cm^{-1}	17a/2.1.1
K	absorption coefficient	cm^{-1}	17a/2.2.2, eq. (A.38)
K	equilibrium constant (for special meaning, see respective subsection)		17g/9.15.2
K_B	Knight shift		
L, l	length	cm	
L	symmetry point in the Brillouin zone		17a/2.4, Fig. A.4
$\Delta l/l$	linear thermal elongation		
m_0	electron mass	kg	
m^*	effective mass	m_0	17a/2.1.1
m^{**}	polaronic mass	m_0	17a/2.1.1, eq. (A.10)
$m_{n(p)}$	effective mass of electrons (holes)	m_0	17a/2.1.1, eq. (A.1)
$m_{ }, m_\perp$	longitudinal effective mass	m_0	17a/2.4.1, eq. (A.75)
m_{\perp}, m_\parallel	transverse effective mass	m_0	17a/2.4.1, eq. (A.75)
m_{ω_p}	effective plasma frequency mass	m_0	17a/2.2.2, eq. (A.50)
m_{ω_c}	effective cyclotron resonance mass	m_0	17a/2.2.2, eq. (A.57)
$M_{(0)}$	(saturation) magnetization per unit volume	A/m, Oe	
n	(real) refractive index		
$n_{a,b,c}$	refractive index in a, b, c direction		17a/2.2.2, eq. (A.37)
$\Delta n_{(A)}$	birefringence ($n_{ } - n_\perp$)		
n	electron concentration (also carrier concentration in general)	cm^{-3}	
n_i	intrinsic carrier concentration	cm^{-3}	17a/2.1.3, eq. (A.20)
$n_{a(d)}$	acceptor (donor) concentration	cm^{-3}	
n_H	carrier concentration determined by the Hall effect	cm^{-3}	17g/9.15.2
n_t	trap concentration	cm^{-3}	
n_{eff}, N_{eff}	effective number of electrons contributing to optical properties		17a/2.2.2, eq. (A.60)

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Symbol	Property	Unit	Introduced in section
N	count rate		
p	pressure	bar	
p_{tr}	(phase) transition pressure	bar	
p	hole concentration	cm^{-3}	
p_A	magnetic moment per atom (ion)	μ_B	[100]-axis in A·ebers
$p_{A,s}$	saturation magnetic moment per atom (ion)	μ_B	clarity of Brillouin temperature
p_{eff}	effective (paramagnetic) magnetic moment	μ_B	selection of Brillouin temperature
p_m	magnetic moment per formula unit	μ_B	exchangeability of spin
P	spontaneous polarization	C m^{-2}	17g/9.15.2
q	wave vector of phonons	cm^{-1}	
r, R	radius, distance	\AA	
R	resistance	Ω	
R	reflectance, reflectivity		17a/2.2.2, eq. (A.42)
R_H	normal Hall coefficient	$\text{cm}^3 \text{C}^{-1} \text{V s}$	17a/2.2.1
R_s	anomalous Hall coefficient	$\text{cm}^3 \text{C}^{-1} \text{V s}$	17g/9.14
S	spin quantum number		
S	Seebeck coefficient, thermoelectric power	V K^{-1}	17a/2.2.1, eq. (A.42)
ΔS_f^0	standard entropy of formation	$\text{J mol}^{-1} \text{K}^{-1}$	
ΔS_{tr}^0	entropy of phase transition	$\text{J mol}^{-1} \text{K}^{-1}$	
t	time	s	
t_i	transport numbers (t_+, t_- : for cations, anions)		17g/9.15.2
T	transmission		
T	temperature	$\text{K}, ^\circ\text{C}$	
T_C	Curie temperature	K	
T_{dec}	decomposition temperature	K	
T_m	melting temperature	K	
T_N	Néel temperature	K	
T_{perit}	peritectic (decomposition) temperature	K	
T_S	spin flip temperature	K	17g/9.15.2
T_{tr}	transition temperature	K	
T_V	Verwey temperature	K	17g/9.15.2
T_z	critical temperature for cluster formation (see section on FeS)	K	17g/9.15.2
u	position parameter		
U	voltage		
U	Hubbard-self energy (sometimes electro- static correlation energy)	eV	17g/9.15.2
U_H	Hall voltage	V	
v_b	bulk velocity	cm s^{-1}	17g/9.14
v_s	shear sound velocity	cm s^{-1}	17g/9.14
$v_{L(t)}, v_{L(T)}$	velocity of longitudinal (transverse) waves	cm s^{-1}	17a/2.1.2
$V_{(m)}$	(molar) volume	$\text{cm}^3 (\text{mol}^{-1})$	
W	width of valence or conduction bands	eV	
x, y, z	fractional coordinates of atoms in unit cell		
X	symmetry point in the Brillouin zone		17a/2.4.1, Fig. A.4
X_{ik}	stress tensor (6×6) (in the literature often labeled T_{ij})	bar	17a/2.1.2
X_k	stress vector (6-component)	bar	17a/2.1.2
Y	photoyield		17g/9.16
Z	coordination number		
$\alpha(\varepsilon_F)$	Fröhlich polaron coupling constant		17a/2.1.1, eq. (A.11)
α	linear thermal expansion coefficient	K^{-1}	17a/2.1.2, eq. (A.17)
$\alpha_{a,b,c}$	linear thermal expansion coefficient in a, b, c direction	K^{-1}	

Introduction: 1. List of symbols

Symbol	Property	Unit	Introduced in section
β	volume thermal expansion coefficient (3α)	K^{-1}	17a/2.1.2, eq. (A.17)
γ	Grüneisen constant	—	17a/2.1.2, eq. (A.18)
Γ	linewidth (e.g. of phonon wavenumber)	cm^{-1}	—
Γ	center of Brillouin zone	—	17a/2.4.1, Fig. A.4
Δ	[100]-axis in k -space	—	17a/2.4.1, Fig. A.4
A_{cf}	crystal field splitting energy	eV	17g/9.15.2
A_{el}	electronic stabilization energy	eV	17g/9.15.2
A_{ex}	exchange splitting parameter	eV	17g/9.15.2
$\tan \delta$	dielectric loss tangent ($=\epsilon_2/\epsilon_1$)	—	—
ϵ_0	permittivity of free space	$F\ cm^{-1}$	—
ϵ	dielectric constant	—	—
$\epsilon_{1(2)}$	real (imaginary) part of dielectric constant	—	17a/2.2.2, eq. (A.39)
$\epsilon(0)$	low frequency dielectric constant	—	17a/2.2.2, eq. (A.53)
$\epsilon(\infty)$	high frequency dielectric constant	—	17a/2.2.2, eq. (A.53)
ζ	reduced wave vector coordinate	—	—
Θ_a	asymptotic Curie temperature	K	—
Θ_p	paramagnetic Curie temperature	K	—
Θ_D	Debye temperature	K	17a/2.1.2
$\kappa(\kappa_{L, el})$	thermal conductivity (lattice, electronic contribution)	$W\ cm^{-1}\ K^{-1}$	17a/2.2.1, eq. (A.36)
κ	compressibility (=1/bulk modulus)	$cm^2\ dyn^{-1}$	—
$\kappa_{v(l)}$	volume (linear) compressibility	$cm^2\ dyn^{-1}$	—
λ	wavelength	cm	—
λ_L	wavelength of laser light	cm	—
Λ	phonon mean free path	cm	—
$\mu_{n(p)}$	electron (hole) mobility	$cm^2\ V^{-1}\ s^{-1}$	17g/9.14
μ_{dr}	drift mobility	$cm^2\ V^{-1}\ s^{-1}$	17a/2.2.1, eq. (A.25)
μ_H	Hall mobility	$cm^2\ V^{-1}\ s^{-1}$	17a/2.2.1
$\mu_{a,b,c}$	mobility in a, b, c direction	$cm^2\ V^{-1}\ s^{-1}$	17a/2.2.1, eq. (A.27)
ν	Poisson's ratio	$cm^2\ V^{-1}\ s^{-1}$	—
ν	frequency	s^{-1}	17a/2.4.2, eq. (A.100)
$\tilde{\nu}$	wavenumber	cm^{-1}	—
$\tilde{\nu}_p$	plasma wavenumber	cm^{-1}	—
ν_R	Raman wavenumber	cm^{-1}	—
π_{ik}	piezoresistance coefficients	$cm^2\ dyn^{-1}$	17a/2.1.1, eq. (A.32)
ϱ	resistivity	$\Omega\ cm$	—
$\varrho_{a,b,c}$	resistivity in a, b, c direction	$\Omega\ cm$	—
$\Delta\varrho/\varrho_0$	magnetoresistance	$\Omega\ cm$	—
$\sigma_{(i)}$	(intrinsic) conductivity	$\Omega^{-1}\ cm^{-1}$	17a/2.2.1, eq. (A.30)
$\sigma_{n(p)}$	conductivity of electrons (holes)	$\Omega^{-1}\ cm^{-1}$	17a/2.2.1
$\sigma_{a,b,c}$	conductivity in a, b, c direction	$\Omega^{-1}\ cm^{-1}$	—
σ_d	dark conductivity	$\Omega^{-1}\ cm^{-1}$	—
σ_{ph}	photoconductivity	$\Omega^{-1}\ cm^{-1}$	—
$\tau_{(n,p)}$	relaxation time, decay time, rise time, lifetime of carriers	s	—
Φ	work function	eV	—
χ_v	magnetic volume susceptibility	$cm^3\ g^{-1}$	—
χ_g, χ	magnetic mass susceptibility	$cm^3\ mol^{-1}$	—
χ_m	magnetic molar susceptibility	$rad\ s^{-1}$	—
ω	circular frequency	eV	—
$\hbar\omega$	photon energy	s^{-1}	17a/2.2.2, eq. (A.49)
ω_p	plasma resonance frequency	—	—

2. List of abbreviations

a	acceptor
ac.	alternating current
arb.	arbitrary
av	average
AF	antiferromagnetically ordered spin system
APB	antiphase boundary
APW	augmented plane wave method
bcc	body centered cubic
bct	base centered tetragonal
BZ	Brillouin zone
calc	calculated
cub	cubic
crit	critical
CB	conduction band
CCDW	commensurate charge density wave
CS	crystallographic shear (plane)
CVD	chemical vapor deposition
d	donor
dc	direct current
dir	direct
DOS	density of states
DTA	differential thermal analysis
e	electron
eff	effective
epr, EPR	electron paramagnetic resonance
esr, ESR	electron spin resonance
exp	experimental
EDC	energy distribution curve
EELS, ELS	electron energy loss spectroscopy
EMF	electromotive force
ESCA	electron spectroscopy for chemical analysis
fcc	face centered cubic
fir, FIR	far infrared
F	ferromagnetic ordered spin system
h	hole
hex	hexagonal
HT	high temperature
i	intrinsic; sometimes used for interstitial
ind	indirect
ion	ionic, ionization
ir, IR	infrared
I	insulator
ICDW	incommensurate charge density wave
I, L	longitudinal (sub- or superscript); sometimes abbreviation for "laser"
I, L, liq	liquid
LA	longitudinal acoustic
LO	longitudinal optical
LCAO	linear combination of atomic orbitals
Ln	lanthanides
LT	low temperature
m	monoclinic (mostly subscript)
magn	magnetic
max	maximum
min	minimum
M	metal
Mn _{Mn}	Mn ⁺ ion on Mn site, positively charged
MO	atomic orbital