Landolt-Börnstein

Numerical Data and Functional Relationships in Science and Technology

Zahlenwerte und Funktionen aus Naturwissenschaften und Technik

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Volume 17

Semiconductors

Subvolume a

Physics of Group IV Elements and III–V Compounds

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Th. Grave · G. Harbeke · K. Hübner · U. Kaufmann
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Vorwort

Die Zunahme unserer Kenntnisse der physikalischen und technologischen Eigenschaften der Halbleiter drückt sich im Umfang dieses Landolt-Börnstein (Neue Serie)-Bandes aus: fünf Teilbände (III/17a–e) mit mehr als 3000 Seiten ersetzen die 110 Seiten des 1956 erschienenen Beitrages über Halbleiterphysik (H. Weiss und H. Welker, Landolt-Börnstein, 6. Auflage, Band II/6) und die 100 Seiten des 1965 erschienenen Beitrages über Halbleitertechnologie (U. und K. Gürs, Landolt-Börnstein, 6. Auflage, Band IV/2c). Die Menge der verfügbaren Information – verstreut in Originalveröffentlichungen, zusammenfassenden Artikeln und Büchern – legt eine Zusammenstellung der wichtigsten Daten nahe. Es wird aber immer schwieriger, gleichzeitig der traditionellen Landolt-Börnstein Devise zu folgen „Was Sie nicht in diesem Band finden, wurde noch nicht gemessen“ und die Darstellung dennoch auf eine kritische Auswertung der Daten in wenigen Bänden zu beschränken, sodaß diese für die tägliche Arbeit des Experimentalphysikers brauchbar bleiben – und bei dem heute meist eingeschränkten Etat der Institute gekauft werden können.

Dieses Dilemma prägt sich im Inhalt dieses Teilbandes deutlich aus. Silicium, Germanium und einige III–V-Verbindungen sind so wichtige und eingehend untersuchte Substanzen der Halbleiterphysik und -technologie geworden, daß eine Zusammenstellung aller gemessenen Daten mehrere Bände füllen würde. Es war für die Autoren dieser Kapitel schwierig, einen Kompromiß zwischen beiden Randbedingungen zu finden und die Auswahl so zu treffen wie sie der künftige Leser erwarten wird.

Einige Worte zum Gebrauch dieses Bandes mögen nützlich sein. Für die Organisation des Datenmaterials in den Abschnitten über die einzelnen Substanzen sind verschiedene Wege möglich – wie bei jeder linearen Darstellung eines vielfach-verknüpften Problems. Das hier eingehaltene Schema ist ein Kompromiß zwischen einer nach theoretischen Gesichtspunkten geordneten Einteilung (elektronische Eigenschaften, Gittereigenschaften usw.) und einer nach experimentellen Gebieten geordneten Gliederung (Transporteigenschaften, optische Eigenschaften usw.). Dies mag zur Folge haben, daß der Leser Daten in einem anderen Abschnitt findet als er zunächst erwartet. Ein Gliederungsschema auf der Innenseite des Buchdeckels soll zum schnelleren Auffinden helfen. Bei der Auswahl der Daten war die Richtschnur, sich nicht nur auf die Halbleitereigenschaften eines Materials zu beschränken, sondern alle die Daten zu bringen, die ein Halbleiterphysiker sucht. Struktureigenschaften oder Information über Phasenübergänge u.dgl. wurden nicht ausgelassen, obwohl sie in anderen Landolt-Börnstein-Bänden ausführlicher dargestellt werden. Sie wurden in einem Rahmen gebracht, wie er von einem Benutzer dieser Bände erwartet werden mag. Für eine Resonanz der Leser zu dieser Frage, ebenso wie für Hinweise und ergänzendes Material wäre ich dankbar.

Ich möchte allen denjenigen meinen Dank ausdrücken, die geholfen haben die Herausgabe dieses Bandes zu einem glücklichen Ende zu führen – den Autoren, die alle Änderungen in ihren Manuskripten hingenommen haben, die für eine einheitliche Darstellung der Daten notwendig waren, den Mitarbeitern der Landolt-Börnstein-Redaktion, insbesondere Herrn Dr. W. Polzin, Frau B. Ade und Frau H. Weise, deren präzise und engagierte Mitarbeit mir ganz wesentlich geholfen hat und nicht zuletzt dem Springer-Verlag für ein weiteres Beispiel hervorragender Buchherstellung.

Dieser Band wurde wie alle anderen Bände des Landolt-Börnstein ohne finanzielle Hilfe von anderer Seite veröffentlicht.

Marburg, im Oktober 1981 **Der Herausgeber**

Preface

The increase in our knowledge of physical and technological properties of semiconductors is manifested by the size of this Landolt-Börnstein New Series volume III/17, Semiconductors: five subvolumes (III/17a, b, c, d, e) with more than 3000 pages replace the 110 pages of the 1956 contribution on semiconductor physics (H. Weiss, H. Welker, Landolt-Börnstein, 6th edition, vol. II/6) and the 100 pages of the 1965 contribution on semiconductor technology (U. and K. Gürs, Landolt-Börnstein, 6th edition, vol. IV/2c).

The huge amout of information available – dispersed in original papers, review articles and books – demands a compilation of the most important data. On the other hand it is more and more difficult to fulfil the traditional Landolt-Börnstein challenge "Whatever you don't find in this volume has never been measured" and at the same time to restrict the presentation to a critical evaluation of the data in a few volumes which can be used in the laboratory – and can be bought in spite of the restricted budget of most laboratories.

This dilemma is clearly reflected in the content of this subvolume III/17a. Silicon, germanium and several III–V compounds have become so important in semiconductor physics and technology and so well investigated that a compilation of all measured data would fill several volumes. It was difficult for the authors of these chapters to compromise between the conflicting boundary conditions and to present a selection the future reader is looking for.

A few words about the use of this book may be helpful. The data in the sections for the various substances can be organized in different ways – as can each linear presentation of a multi-connected problem. The organization used here is a compromise between a theoretical one (electronic properties, lattice properties etc.) and a phenomenological one (transport properties, optical properties etc.). Thus the reader may find an item in a section in which he does not expect it at first. The organization scheme printed on the inside of the front cover should help to find the way more easily. The policy for the selection of the data was not to compile only the semiconductor properties of materials but to present all data a semiconductor physicist is looking for. Thus structural data and information about phase transitions etc. – which can be found more completely in other Landolt-Börnstein volumes – have not been omitted but are presented to such an extent as may be expected by a user. A resonance by the users to these questions as well as remarks, hints and additions would be helpful to the editor.

I would like to express my gratitude to all who helped to bring the edition of this volume to a successful end – to the authors, who accepted all changes in their manuscripts necessary to reach a uniform presentation of the material, to the editorial staff of the Landolt-Börnstein office, especially Dr. W. Polzin, Frau B. Ade and Frau H. Weise, whose precise and engaged cooperation was extremely helpful to me, and last but not least to Springer-Verlag for another demonstration of their excellent standard of book production.

As all previous volumes of Landolt-Börnstein, this new one is published without any financial support from other sources.

Marburg, October 1981 **The Editor**

Table of contents

Semiconductors

Subvolume a: Physics of group IV elements and III–V compounds

(edited by O. MADELUNG)

Attention:

The distribution of the data into subvolumes a, ..., e is correctly given on the inside of the cover.

Unfortunately, some of the references to the various subvolumes (e.g. on the inner endpaper, 15th line, and in the Introduction) are not correct, due to changes during the last stage of preparation of this subvolume.

Please check the respective references against the correct inside of the cover.

A. Introduction

1 General remarks on the contents and the structure of volume 17 (subvolumes 17a···17e)

Introduction:

Each subvolume has a separate introduction which is of a more general character in this first subvolume III/17a.

Data (tables and figures):

Each subvolume 17a···17e presents *physical data* in respective chapters "Physical data of semiconductors I···V".

Subvolume 17c contains a chapter on *Semiconductor technology;* several chapters of subvolume 17e present information on *special systems* (amorphous semiconductors, semiconducting chalcogenide glasses, liquid and organic semiconductors) and on *special topics* (electronic structure of semiconducting surfaces, semiconducting surfaces and interfaces, hot electrons, electron-hole liquids).

Organization of the chapters on physical data of semiconductors:

Semiconductors are grouped into families according to the chemical nature of the constituents: IVth group elements, III-V compounds, II-VI compounds etc. A list of all chapters and their division among the subvolumes a···e is printed on the inside of the front cover.

For technical reasons, the figures of all sections have been collected to form a separate part of each subvolume, but have been numbered starting with No. 1 in each section.

Within each chapter the organization is as follows:

"0-section": Presentation of all members of the group, review of general relationships, structure, non-semiconducting phases (or members of the family not being semiconductors), high-pressure phases etc. General discussion of chemical bond within the group.

The 0-section is followed by separate sections on each member of the group and on solid solutions within the group and with members of other groups. The physical properties are listed – as far as possible – in subsections of the following order:

1 Electronic properties: Information and data about electronic and excitonic energy states as well as electron and hole parameters:

- band structure, density of states
- band gaps
- exciton data
- spin-orbit splitting energies, intraband and interband transition energies
- effective masses and *g*-factors of electrons
- effective masses of holes, other valence band parameters
- deformation potentials

2 Impurities and defects: Basic data on shallow and deep states, bound excitons and local modes (data on diffusion and distribution coefficients are presented in the technological chapters of subvolume 17b):

- shallow donors (ionization energies, excited states, ground state splittings, deformation potentials etc.)
- bound excitons (localization energies, capture cross-sections, transition lifetimes etc.)
- local modes (energies, isotope shifts etc.)
- deep traps, 3d transition metals (ionization energies, esr and endor data etc.)

3 Lattice properties: Static and dynamical properties of the lattice (for structure, space group, phase transitions, chemical bond, see the 0-section of the respective chapter; for density and melting point, see subsection 6; for static dielectric constant, see subsection 5):

lattice parameter, thermal expansion
phonon dispersion relations, density of states
phonon frequencies (wavenumbers)
sound velocities
elastic moduli (also third order)
Young's modulus, torsion modulus, bulk modulus, compressibility, Poisson's ratio, Grüneisen constant, mode Grüneisen parameter, effective ion charges etc.

4 Transport properties: Electronic transport parameters (for thermal conductivity, see subsection 6):

conductivity, carrier concentrations
electron and hole mobilities, warm electron coefficient (for hot carrier effects and e-h-drops, see special chapter in subvolume 17d)
Hall effect and magnetoresistance
piezoresistance, elastoresistance, elastostriction, piezoelectric coefficients etc.
other transport parameters as Seebeck coefficient (thermoelectric power), Nernst coefficient etc.

5 Optical properties: Optical spectra, optical constants, parameters obtained from optical experiments (if not already presented in subsections 1 and 2):

refractive index, absorption index
absorption coefficient and reflectance
dielectric constant (including static dielectric constant)
optical spectra (see also the figures on optical spectra in subsection 1)
other optical coefficients (Verdet, two-phonon absorption, piezoptic coefficients etc.)
Raman and Brillouin scattering
electron energy loss
optical spectra including core levels (vacuum uv spectra, yield spectra, ESCA, XPS, UPS, Auger spectra etc.)
Schottky barrier heights (see also special chapter in subvolume 17d for surface and contact phenomena)

6 Further properties: Thermal, magnetic, thermodynamic properties, some other general data (to avoid too much overlap with other Landolt-Börnstein volumes only the most important data have been included, see e.g. for thermodynamic data, volumes II/1 and II/4 (6th ed.), for crystallographic data, volumes III/6 and III/7 (New Series)).

thermal conductivity
magnetic susceptibility
Debye temperature, heat capacity
hardness
density
melting point
thermodynamical data (characteristical data on fusion, formation, vaporization, entropy etc.)

A shortened version of this organization scheme is reprinted on the inside of the front cover. - Publications cited in the corresponding sections can be found in **7 References.**

Organization of the chapters on semiconductor technology:

Each section of these chapters in subdivided into:

1. Technological data
2. Crystal growth
3. Characterization of crystal properties
4. Device technology

2 Semiconductor properties, their definition and methods for their determination

In this chapter a short definition will be given of the most important semiconductor properties which are listed in the tables and figures of part B. Some frequently used methods for their determination will be outlined. Pecularities which arise in connection with special crystal structures will be discussed. Properties whose definition is self-evident and which are easily accessible to experiment are omitted: melting point, density, etc. Moreover the definition of crystallographic properties (crystal structure, space groups etc.) and methods of their definition are not included in the discussion below.

2.1 Basic properties of semiconductors

2.1.1 Band structure parameters

The *band structure* $E_n(\boldsymbol{k})$ of a given solid is a multi-valued function within the (first) Brillouin zone in $\boldsymbol{k}$-space. Each index n determines a *band*. In semiconductor physics the *conduction band* and the *valence band* (each consisting of several *sub-bands*) are of most importance.

Of special interest are the *edges* of the conduction band and the valence band where the electrons and holes are situated in equilibrium, moreover the edges of sub-bands and other "critical points" in $E_n(\boldsymbol{k})$ where $\nabla_{\boldsymbol{k}} E_n(\boldsymbol{k})$ vanishes. At the energy of such critical points there is a discontinuity in the slope of the density of states $g(E)$ (eq. (A.7)).

Points and axes of high symmetry in the Brillouin zone are designated by greek or latin letters (Γ, Δ, Λ, X etc.) according to their symmetry properties under operations of the point group of the crystal. Band states at such points or lines are further characterized by indices giving the irreducible representation of the respective symmetry group to which the wave functions belong ($\Gamma_{25'}$, Δ_s etc.). If necessary subscripts c or v are added to mark whether a state belongs to the conduction or valence bands.

Band parameters of general importance are:

Energy parameters:

Energy gap (band gap)	$E_g = E_c(\boldsymbol{k}_c) - E_v(\boldsymbol{k}_v)$	energy difference between the lowest conduction band state and the uppermost valence band state
Indirect gap	if $\boldsymbol{k}_c \neq \boldsymbol{k}_v$	
Direct gap	if $\boldsymbol{k}_c = \boldsymbol{k}_v$	
Higher interband transition energies:		energy differences between critical points in the conduction and valence band at the same $\boldsymbol{k}$-vector; other band-band transition energies detectable in optical spectra.
Intraband transition energies:		energy differences within the conduction or valence band, especially energies of sub-band edges relative to the band edge. An example is the *spin-orbit splitting energy* separating sub-band edges which are degenerated in a non-relativistic spin-free band structure calculation.

Effective masses:

The structure near a band edge is given in the simplest approximation by

$$\begin{aligned} E(\boldsymbol{k}) &= E_c + \hbar^2 k^2/2m_n \quad \text{for a conduction band edge} \\ E(\boldsymbol{k}) &= E_v - \hbar^2 k^2/2m_p \quad \text{for a valence band edge.} \end{aligned} \tag{A.1}$$

E_c and E_v are the band edges of the conduction band and the valence band, respectively. m_n is the *effective mass* of the electrons, m_p that of the holes. The effective masses (general designation m^*) describe the curvature of $E_n(\boldsymbol{k})$ in the vicinity of band edges. Band edges of the shape (A.1) are called *isotropic* and *parabolic*.

The following deviations from this simple approximation are important:

Deviations from parabolicity: This is expressed by a $\boldsymbol{k}$-dependent effective mass $m_{n,p}(\boldsymbol{k})$ in (A.1) or by additional terms of the order k^4:

$$E(\boldsymbol{k}) = E_{c,v} \pm (\hbar^2 k^2/2m_{n,p})(1 - ak^2 + \dots). \tag{A.2}$$

Deviations from isotropy: The curvature of a band near an extremum may depend on the direction in $\boldsymbol{k}$-space:

$$E(\boldsymbol{k}) = E(\boldsymbol{k}_0) \pm (\hbar^2/2m)\, f(\vartheta, \varphi)\, \kappa^2 \tag{A.3}$$

with $\boldsymbol{\kappa} = (\kappa, \vartheta, \varphi) = \boldsymbol{k} - \boldsymbol{k}_0$. Important examples are

Ellipsoidal surfaces:

$$f(\vartheta, \varphi) = \frac{m_0}{\kappa^2} \left\{ \frac{\kappa_x^2}{m_1} + \frac{\kappa_y^2}{m_2} + \frac{\kappa_z^2}{m_3} \right\} \tag{A.4}$$

in a suitably chosen coordinate system κ_x, κ_y, κ_z. If $\boldsymbol{k}_0 \neq 0$ several equivalent extrema occur centred at the $\boldsymbol{k}_0$-vectors of a "star" given by the point group symmetry of the Brillouin zone (*many valley structure*).

Degenerate bands: If two bands are degenerated at their extrema two relations of the type (A.1) with the same band edge energy and different effective masses have to be used. An example of a more complicated band edge degeneracy are

Warped surfaces:

$$f(\vartheta, \varphi) = A \pm (B^2 + (\kappa_x^2 \kappa_y^2 + \kappa_y^2 \kappa_z^2 + \kappa_z^2 \kappa_x^2)\, C^2/\kappa^4)^{1/2}. \tag{A.5}$$

The average curvature of such a warped band is given by

$$\frac{1}{m_{\mathrm{av}}} = \frac{1}{m_0} (A \pm (B^2 + C^2/6)^{1/2}). \tag{A.6}$$

Density of states:

The density of states $g(E)\,\mathrm{d}E$ (number of states in an energy intervall $(E, \mathrm{d}E)$ per unit volume) is given by

$$g(E)\,\mathrm{d}E = \{(2/(2\pi)^3) \textstyle\int \mathrm{d}f'/\nabla_k E'\}\, \mathrm{d}E \tag{A.7}$$

where the integration extends over the surface $E' = E$ in $\boldsymbol{k}$-space.

Near an isotropic parabolic band edge $g(E)\,\mathrm{d}E$ is given by

$$g(E)\,\mathrm{d}E = (4\pi/h^3)(2m_{\mathrm{n,p}})^{3/2} (|E - E_{\mathrm{c,v}}|)^{1/2}\, \mathrm{d}E. \tag{A.8}$$

For an anisotropic band of the ellipsoidal type (A.4) the effective mass in (A.8) has to be replaced by the *density of states mass* m_{ds}

$$m_{\mathrm{ds}} = \nu^{2/3} (m_1 m_2 m_3)^{1/3} \tag{A.9}$$

where ν is the number of equivalent extrema. Two degenerate bands have a density of states mass $m_{\mathrm{ds}} = (m_{\mathrm{ds}1}^{3/2} + m_{\mathrm{ds}2}^{3/2})^{2/3}$.

Other combinations of effective masses (optical mass, cyclotron resonance mass etc.) will be discussed in the context of special experimental methods in section 2.2.

As *combined density of states* a function which results from (A.7) by replacing $\nabla_k E'$ by $\nabla_k E_{\mathrm{c}}(\boldsymbol{k}) - \nabla_k E_{\mathrm{v}}(\boldsymbol{k})$ is used in the evaluation of optical spectra. This function gives the number of pairs of conduction and valence band states (per unit volume) which are separated by an energy between E and $E + \mathrm{d}E$.

Polaronic effects:

In *polar semiconductors* the coupling of the electrons to the LO phonons can become so strong that the introduction of a new quasi-particle, the *polaron*, may be useful. Most experiments yield the *polaronic mass* m^{**}. An interpolation formula connecting m^{**} with the "*bare*" *electron mass* m^* is

$$m^{**} = \frac{1 - 0.0008\alpha^2}{1 - (\alpha/6) + 0.0034\alpha^2}\, m^* \tag{A.10}$$

where α is the *Fröhlich coupling parameter*

$$\alpha = (e^2/8\pi\varepsilon_0 \hbar\omega_{\mathrm{LO}})(2m\omega_{\mathrm{LO}}/\hbar)^{1/2} (\varepsilon^{-1}(\infty) - \varepsilon^{-1}(0)). \tag{A.11}$$

Deformation potentials:

Application of external stress has a profound influence on the band structure. *Hydrostatic* (isotropic) *stress* causes a shift of the energy states. *Uniaxial stress* in general lowers the symmetry of the lattice and gives rise to an additional splitting of degenerate levels. Of special interest is the *shift of band edges* δE_c, δE_v, δE_g with hydrostatic or uniaxial stress. A useful parameter connecting the shift of a band edge with the components of the strain tensor e_{ik} is the *deformation potential tensor* Ξ_{ik} defined by

$$\delta E_{(\alpha)} = \sum_{ik} \Xi_{ik}^{(\alpha)} e_{ik}. \tag{A.12}$$

For an ellipsoidal band edge of the type (A.4) this can be written as

$$\Xi_{ik} = \Xi_d \delta_{ik} + (k_{0i} k_{0k}/k_0^2)\, \Xi_u \tag{A.13}$$

$\Xi_d + \Xi_u/3$ is the deformation potential for pure dilatation, Ξ_u that for pure shear.

Equation (A.13) only represents the so-called intervalley splittings. The intravalley splitting (occuring in bands of the type (A.4)) requires the introduction of other deformation potentials. Such magnitudes will be defined together with special deformation potentials for semiconductors with diamond and zincblende structure and deformation potentials of impurity levels in subsection 2.4.1.

Exciton states:

Excitons are bound electron-hole pairs. The bound states (in an isotropic parabolic approximation) are given by

$$E(\boldsymbol{K}) = E_g + \hbar^2 K^2/2M - R/n^2, \quad R = \mu e^4/2\varepsilon^2\hbar^2, \quad n = 1, 2, 3, \ldots. \tag{A.14}$$

Here $\boldsymbol{K}$ is the sum of the $\boldsymbol{k}$-vectors of electron and hole, M is the sum of their masses and $\mu^{-1} = m_n^{-1} + m_p^{-1}$. Exciton states - being states of a theory including electron-electron interaction - cannot be included in the one electron approximation of the band structure. Results for optical spectra including the exciton contributions as well as band structure contributions will be presented in subsection 2.2.2.

Deviations from the hydrogenic spectrum given by eq. (A.14) are either due to pecularities of the band structure (anisotropic or warped energy bands) or to a more complex electron-hole interaction (influence of electron-phonon coupling in polar materials).

Optical measurements yield either information on the excitation energies from the crystal ground state (corresponding to the valence band maximum), e.g. reflectivity, absorption, or excitation from the exciton ground state, e.g. far-infrared absorption. To make this information comparable, numbers are usually given for the excitation energy of the lowest ground state component and excited state energies are referred to this level. Exciton binding energies E_b can only be obtained from experimental data by applying a model (usually a hydrogenic series for excited states). If the excitonic spectra are analyzed using an exciton theory which includes the pecularities of the band structure the characteristic parameters of this band structure can be determined with high accuracy.

Band structure in high magnetic fields:

In strong magnetic fields the structure near an isotropic parabolic conduction band edge is

$$E(k_B, l) = E_c + \hbar^2 k^2/2m_n + (l + \tfrac{1}{2})\, \hbar\omega_{cn} \pm \beta g^* B \tag{A.15}$$

with $l = 0, 1, 2 \ldots$. k_B is the component of $\boldsymbol{k}$ parallel to the magnetic field $\boldsymbol{B}$, $\omega_{cn} = \dfrac{eB}{m_n}$ is the *cyclotron resonance frequency* of the electrons, β the gyromagnetic ratio and g^* an *effective g-factor*. A similar equation holds for the top of an isotropic parabolic valence band.

2.1.2 Lattice parameters

The vibrational energy E of a lattice can be described as consisting of energy quanta of *phonons* $\hbar\omega_j(\boldsymbol{q})$

$$E=\sum_{j\boldsymbol{q}}\left(n_j(\boldsymbol{q})+\tfrac{1}{2}\right)\hbar\omega_j(\boldsymbol{q}) \tag{A.16}$$

$n_j(\boldsymbol{q})$ is the number of phonons in a vibrational mode with frequency ω_j and wave vector $\boldsymbol{q}$. The terms $\hbar\omega_j(\boldsymbol{q})/2$ contribute to the zero-point energy of the lattice.

The function $\omega_j(\boldsymbol{q})$ is called *phonon dispersion relation.* Just like the band structure it is a multi-valued function in the (first) Brillouin zone in $\boldsymbol{q}$-space. The indices j designate the *branches* of $\omega_j(\boldsymbol{q})$. If r is the number of atoms in a Wigner-Seitz cell of the lattice, j takes on $3r$ values, each triple of values representing one *longitudinal* and two *transverse branches.* Three *acoustic branches* are characterized by $\omega\rightarrow 0$ when $\boldsymbol{q}\rightarrow 0$, whereas the $3(r-1)$ *optical branches* have non-zero phonon energies at $\boldsymbol{q}=0$. Phonons belonging to these branches are consequently cited as LA-, TA-, LO- and TO-phonons.

Characteristic parameters of the dispersion relation are:

Phonon energies:	energies $\hbar\omega$ of TO-, LO-, TA- and LA-phonons at lines and points of high symmetry in the Brillouin zone. Instead of energies (in eV) often the frequencies $\nu(\mathrm{s}^{-1})$ or wavenumbers $\bar{\nu}(\mathrm{cm}^{-1})$ are tabulated.
Velocity of elastic waves $v_{\mathrm{LA,TA}}$:	slope of $\omega_{\mathrm{ac}}(\boldsymbol{q})$ near $\boldsymbol{q}=0$. In the LA-branch $\mathrm{d}\omega/\mathrm{d}\boldsymbol{q}$ gives the velocity of *sound waves,* in the TA-branches the velocity of *shear waves.* Note that in an anisotropic lattice only waves near $\boldsymbol{q}=0$ or along special symmetry lines are purely longitudinal or transverse!
Debye frequency ω_{D} and *Debye temperature* Θ_{D}:	if dispersion is neglected in the acoustic branches ($\mathrm{d}\omega/\mathrm{d}\boldsymbol{q}=\mathrm{const}$, Debye approximation) the density of state spectrum has to be cut off at the Debye energy (frequency) to conserve the correct number of states. The Debye temperature is defined as $\Theta_{\mathrm{D}}=\hbar\omega_{\mathrm{D}}/k$. By an evaluation of heat capacity measurements using the Debye theory a temperature dependent Debye temperature $\Theta_{\mathrm{D}}(T)$ is introduced.

Further lattice parameters:

Thermal expansion: The coefficient of linear thermal expansion is defined by

$$\alpha=\frac{1}{l}\frac{\partial l}{\partial T}\bigg|_p=\frac{1}{3V}\frac{\partial V}{\partial T}\bigg|_p=\frac{1}{3B}\frac{\partial p}{\partial T}\bigg|_V \tag{A.17}$$

where l and V are length and volume of a specimen. B is the (isothermal) *bulk modulus* $B=-V\frac{\partial p}{\partial V}\Big|_T$. Sometimes a subscript T is used: B_T in contrast to $B_S=(C_p/C_v)\,B_T$ (adiabatic bulk modulus).

The contribution of the vibrational modes to the thermal expansion is described by a dimensionless *Grüneisen parameter:*

$$\alpha=\gamma\frac{C_v}{3B},\qquad \gamma=\sum_{jq}\gamma_{jq}C_{jq}\Big/\sum_{jq}C_{jq} \tag{A.18}$$

where the summation extends over all states of the phonon spectrum and where the C_{jq} are the contributions of the corresponding modes to the heat capacity: $C_v=\sum_{jq}C_{jq}$. The γ_{jq} are called *mode Grüneisen parameter.*

Elastic moduli: Forces acting in an elastic solid and deformations produced by the forces are described by the *stress tensor* X_{ik} and the *strain tensor* e_{ik}. Both tensors are symmetric. This allows us to define six-component vectors X_l and e_m by $X_1=X_{11}$, $X_2=X_{22}$, $X_3=X_{33}$, $X_4=X_{12}=X_{21}$, $X_5=X_{23}=X_{32}$, $X_6=X_{13}=X_{31}$ and accordingly for the e_m. Both vectors are connected by the relations

$$X_l=\sum_m c_{lm}e_m,\qquad e_m=\sum_l s_{ml}X_l \tag{A.19}$$

where the c_{lm} are called *elastic moduli* (or stiffness constants) and the s_{ml} *compliance constants.*