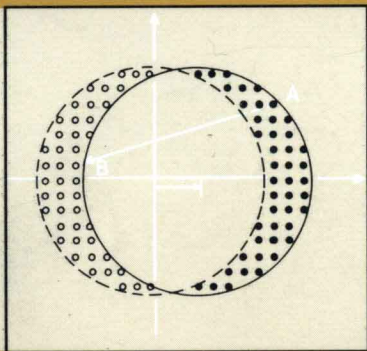


Harald Ibach Hans Lüth

Solid-State Physics

An Introduction to Principles of Materials Science

Second Edition



Springer

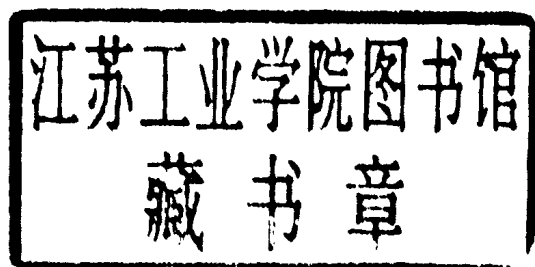
Harald Ibach · Hans Lüth

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With 232 Figures



Springer

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Periodic Table of the Elements

Periodic Table of the Elements																	α - ⁴ He P6 ₃ /mmc 3.531 — 5.693	
H₁ P6 ₃ /mmc 3.776 — 6.162	Li Im3m 3.510 — —	α -Be P6 ₃ /mmc 2.287 — 3.583											α -B R3m rhomb. 5.057 — —	C Fd3m 3.567 — —	α -N ₂ P2 ₁ 3 5.644 — —	α -O ₂ C2/m 5.403 3.429 5.086	α -F ₂ C2/m — — —	Ne Fm3m 4.455 — —
α -Na P6 ₃ /mmc 3.767 — 6.154	Mg P6 ₃ /mmc 3.209 — 5.210	Element Space group symbol Lattice constant a Lattice constant b Lattice constant c										Al Fm3m 4.050 — —	Si Fd3m 5.431 — —	P Cmca 3.314 10.478 4.376	α -S ₈ Fddd 10.465 12.866 24.486	Cl ₂ Cmca 6.24 4.48 8.26	Ar Fm3m 5.311 — —	
K Im3m 5.32 — —	α -Ca Fm3m 5.588 — —	α -Sc P6 ₃ /mmc 3.309 — 5.273	α -Ti P6 ₃ /mmc 2.951 — 4.684	V Im3m 3.024 — —	Cr Im3m 2.885 — —	α -Mn I43m 8.914 — —	α -Fe Im3m 2.866 — —	α -Co Fm3m 3.544 — —	Ni Fm3m 3.524 — —	Cu Fm3m 3.615 — —	Zn P6 ₃ /mmc 2.664 — 4.947	α -Ga Cmca 4.519 7.657 4.526	Ge Fd3m 5.658 — —	α -As R3m 4.132 — —	Se P3 _{1/2} 2 ₁ 4.366 — 4.959	Br ₂ Cmca 6.737 4.548 8.761	Kr Fm3m 5.721 — —	
Rb Im3m 5.700 — —	α -Sr Fm3m 6.085 — —	α -Y P6 ₃ /mmc 3.647 — 5.731	α -Zr P6 ₃ /mmc 3.232 — 5.148	Nb Im3m 3.299 — —	Mo Im3m 3.147 — —	Tc P6 ₃ /mmc 2.743 — 4.400	Ru P6 ₃ /mmc 2.706 — 4.281	Rh Fm3m 3.804 — —	Pd Fm3m 3.891 — —	Ag Fm3m 4.086 — —	Cd P6 ₃ /mmc 2.979 — 5.619	In I4/mmm 3.253 — 4.946	α -Sn Fd3m 6.489 — —	Sb R3m 4.308 — 11.247	Te P3 _{1/2} 2 ₁ 4.457 — 5.927	I ₂ Cmca 7.265 4.786 9.791	Xe Fm3m 6.197 — —	
Cs Im3m 6.14 — —	Ba Im3m 5.025 — —	α -La P6 ₃ /mmc 3.770 — 12.159	α -Hf P6 ₃ /mmc 3.195 — 5.051	Ta Im3m 3.303 — —	W Im3m 3.165 — —	Re P6 ₃ /mmc 2.761 — 4.458	Os P6 ₃ /mmc 2.735 — 4.319	Ir Fm3m 3.839 — —	Pt Fm3m 3.924 — —	Au Fm3m 4.078 — —	α -Hg R3m 2.993 — —	α -Tl P6 ₃ /mmc 3.456 — 5.525	Pb Fm3m 4.950 — —	Bi R3m 4.546 — 11.862	α -Po Pm3m 3.352 — —	At — — —	Rn — — —	
Fr	Ra	Ac Fm3m 5.311 — —																
			α -Ce Fm3m 4.85 — —	α -Pr P6 ₃ /mmc 3.673 — 11.835	α -Nd P6 ₃ /mmc 3.658 — 11.799	Pm	α -Sm R3m 8.996 — —	Eu Im3m 4.582 — —	Gd P6 ₃ /mmc 3.636 — 5.783	α -Tb P6 ₃ /mmc 3.601 — 5.694	Dy P6 ₃ /mmc 3.590 — 5.648	α -Ho P6 ₃ /mmc 3.577 — 5.616	α -Er P6 ₃ /mmc 3.559 — 5.587	α -Tm P6 ₃ /mmc 3.538 — 5.555	α -Yb Fm3m 5.486 — —	α -Lu P6 ₃ /mmc 3.503 — 5.551		
			α -Th Fm3m 5.084 — —	Pa I4/mmm 3.932 — 3.238	α -U Cmcm 2.848 5.858 4.946	α -Np Pmcn 4.723 4.887 6.663	α -Pu P2 ₁ /m 6.183 4.822 10.963	α -Am P6 ₃ /mmc 3.468 — 11.240	Cm P6 ₃ /mmc 3.496 — 11.331	Bk	Cf	Es	Fm	Md	No	Lw		

Face-centered cubic structure: Fm3m, O_h⁵
 Body-centered cubic structure: Im3m, O_h⁶
 Hexagonal close packing: P6₃/mmc, D_{6h}²
 Rhombohedral structure: R3m, D_{3d}³
 Diamond structure: Fd3m, O_h⁷
 Right- and left-handed selenium structure: P3₂2₁, D_{6h}⁴

Source: Landolt-Börnstein, New Series Vol. III, b
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Preface

Our German textbook "*Festkörperphysik*" has become rather popular among German-speaking students, and is currently produced in its 4th edition. Its version in English has already been adopted by many universities in the United States and other countries. This new 2nd edition corresponds to the 4th edition in German.

In addition to correcting some typographical errors and making small improvements in the presentation, in the present edition some chapters have been revised or extended. Panel V, for example, has been extended to include a description of angle-resolved photoemission and its importance for the study of electronic band structures. Section 10.10 on high-temperature superconductors has completely been rewritten. This active field of research continues to progress rapidly and many new results have emerged since the publication of the first edition. These results shed new light on much of the fundamental physics.

The new version of Sect. 10.10 has been developed in discussions with colleagues who are themselves engaged in superconductivity research. We thank, in particular, Professor C. Calandra from the University of Modena and Dr. R. Wördenweber of the Institute of Film and Ion Technology at the Research Centre Jülich.

The revision of the problems was done with the help of Dr. W. Daum, Dr. A. Förster, A. Leuther and Ch. Ohler. We would like to thank them for their efforts. We also thank Dr. Margret Giesen for numerous improvements on the manuscript as well as Dr. Angela Lahee for the competent translation of the revised or new sections.

Jülich and Aachen, April 1995

H. Ibach · H. Lüth

Preface to the First Edition

In recent decades solid state physics has seen many dramatic new developments and has become one of the largest independent branches of physics. It has simultaneously expanded into many new areas, playing a vital role in fields that were once the domain of the engineering and chemical sciences. A consequence of this explosive development is that no single university lecturer can today be expected to have a detailed knowledge of all aspects of this vast subject; likewise, it is impossible to conceive of a course that could offer students a comprehensive understanding of the entire discipline and its many applications.

In view of this situation, it is particularly valuable to have a textbook that gives a concise account of the essential elements of the physics of solids. In this book the fundamental aspects of solid state physics are presented according to the scheme: Chemical bonding, structure, lattice dynamics, and electronic properties. We believe that this sequence is the optimum choice for tutorial purposes. It enables the more difficult concepts to be introduced at a point where a basic understanding of fundamental ideas has already been achieved through the study of simple models and examples. In addition to this carefully structured exposition of classical solid state theory based on the periodic solid and the one-electron approximation, the book also includes comprehensive descriptions of the most active areas in modern research: Magnetism, superconductivity and semiconductor physics.

The chapter on magnetism discusses the exchange coupling of both localized and delocalized electrons, and will even guide the reader to the point when he or she can appreciate modern thin-film experiments. The standard picture of superconductivity is elucidated by means of a simplified presentation of BCS theory. A section is also devoted to the novel high-temperature superconductors. This field, however, remains in such a state of flux that it was necessary to confine the treatment to some selected experimental results and a few central ideas about this fascinating phenomenon. The chapter on semiconductors contains, in addition to a general introduction to these materials and their properties, detailed descriptions of semiconductor heterostructures, superlattices, epitaxy, and the quantum Hall effect.

In solid state physics, the interaction between theory and experiment has always played, and continues to play, a vital role. We have thus attempted throughout this book to steer a middle course in which both theory and experiment are adequately represented. Where a theoretical approach is helpful and not too cumbersome, we have

not hesitated in challenging the reader with the necessary abstract concepts. Furthermore, we have tried to include theoretical methods and concepts, for example, those of group theory, that are indispensable for an understanding of contemporary original publications dealing with solid state theory.

The concise presentation of the essential theoretical aspects is complemented by the inclusion of selected experimental methods and examples, summarized in the form of self-contained panels. These offer the reader the opportunity to test and consolidate the material already studied and may prove helpful in stimulating further study in areas of particular interest.

Students will also benefit significantly from working through the extensive series of problems that relate to each chapter. These examples are not restricted to calculations based on the methods described in the text; in many cases they lead into areas that lie outside the scope of the main presentation. All of the examples have been put to the test in our own lecture courses. Nonetheless, the student may often need a helping hand or some preparatory instruction from a lecturer. The problems will be useful to both students and lecturers; they are designed to stimulate further study and to illustrate the connections between different disciplines.

This book is a translation of the third edition of the original German text. The authors consider it their immensely good fortune to have been supported by Dr. Angela Lahee in the translation and editing of this work. We are also grateful to numerous colleagues who over the years have offered valuable suggestions about the presentation of the book or have supplied the experimental material described herein. For her critical reading of parts of the manuscript and the page proofs we thank in particular Dr. Angela Rizzi. Other valuable contributions were made by Dr. W. Daum, Mr. Ch. Stuhlman, Dr. M. Wuttig and Mr. G. Bogdanyi. The figures were prepared with great care and patience by Mrs. U. Marx-Birmans and Mr. H. Mattke. The German manuscript was typed by Mrs. D. Krüger, Mrs. Jürss-Nysten and Mrs. G. Offermann. We express our thanks to Dr. H. Lotsch and Mr. C.-D. Bachem of Springer-Verlag for the pleasant collaboration.

Jülich, January 1991

H. Ibach · H. Lüth

Preface to the Corrected First Edition

After this textbook on solid state physics was successfully introduced to the English-speaking scientific community, we thought it would be worthwhile to make the book available to students for a more attractive price. This paperback version therefore is a corrected reprint of the first English edition which appeared in 1991. Apart from minor corrections only, some new references to recent literature have been added.

Jülich, June 1993

H. Ibach · H. Lüth

Table of Constants

Quantity	Symbol	Value	SI Unit
Velocity of light in vacuum	c	2.997925	10^8 m s^{-1}
Permeability of vacuum	$\mu_0 = 1/\epsilon_0 c^2$	4π	10^{-7} Vs/Am
Permittivity of vacuum	$\epsilon_0 = 1/\mu_0 c^2$	8.854188	10^{-12} As/Vm
Proton restmass	m_p	1.672649	10^{-27} kg
Electron restmass	m_e	9.109534	10^{-31} kg
Elementary charge	e	1.602189	10^{-19} As
Planck's constant	h	6.626176	10^{-34} Js
Planck's constant	$\hbar = h/2\pi$	1.054589	10^{-34} Js
Flux quantum	$\Phi_0 = h/2e$	2.067851	$10^{-15} \text{ J A}^{-1}$
Sommerfeld fine-structure constant	$\alpha = \mu_0 c e^2 / 2\hbar$	7.297351	10^{-3}
Rydberg-constant	$R_\infty = \mu_0^2 m_e e^4 c^3 / 8\hbar^3$	1.097373	10^7 m^{-1}
Bohr magneton	$\mu_B = e\hbar/2m_e$	9.274078	10^{-24} Am^2
Avogadro's number	N_A	6.022045	10^{23} mol^{-1}
Atomic mass unit	$m_u = 1 \text{ u} =$ $(10^{-3} \text{ kg mol}^{-1})/N_A$	1.660566	10^{-27} kg
Boltzmann's constant	k	1.380662	$10^{-23} \text{ J K}^{-1}$

Equivalent Values

Quantity	Symbol	Value	SI Unit
Energy equivalent of the Hertz	$E[\text{Hz}] = (1 \text{ Hz})h$	6.626176	10^{-34} J
Frequency equivalent of the electron volt	$\nu[\text{eV}] = 1 \text{ eV}/h$	2.417970	10^{14} Hz
Energy equivalent of the reciprocal meter	$E[\text{m}^{-1}] = (1 \text{ m}^{-1})hc$	1.986478	10^{-25} J
Wave-number equivalent of the electron volt	$\sigma[\text{eV}] = 1 \text{ eV}/hc$	8.065479	10^5 m^{-1}
Energy equivalent of the Kelvin	$E[\text{K}] = (1 \text{ K})k$	1.380662	10^{-23} J
Temperature equivalent of the electron volt	$T[\text{eV}] = 1 \text{ eV}/k$	1.160450	10^4 K

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1 Chemical Bonding in Solids

Solid-state physics is the physics of that state of matter in which a large number of atoms are chemically bound to produce a dense solid aggregate. The emphasis in this statement is placed on the large number of atoms involved, since that number is of the order of 10^{23} cm^{-3} . At first sight it would seem to be a hopeless task to try to apply traditional scientific methods for the description of such a vast number of atoms. However, it is exactly the large number of atoms involved that in fact makes a quantitative description possible by means of new models, applicable specifically to solids. A prerequisite, though, for the success of these models, is that the participating atoms are not simply chosen at random from the periodic table of elements; the solid must be composed of a limited number of different elements whose atoms are arranged in space with a certain order. Thus, for the solid state physicist, the showpieces are the “elementary” crystals, i.e., three-dimensional periodic arrangements of atoms of one type, or chemical compounds of two elements. An understanding of solids and of their characteristic properties thus requires that we first achieve a fundamental understanding of two particular phenomena: the first is that of the forces that hold together the atoms of a solid, in other words, the chemical bonding between atoms. The second important aspect is the structural ordering of the atoms within the solid. A consideration of these two basic questions forms the content of the first two chapters. In both cases it will only be possible to give a short introduction and for a more detailed discussion of these phenomena the reader is referred to textbooks on quantum chemistry and crystallography.

1.1 The Periodic Table of the Elements

By way of introduction to the topic of chemical bonding, we will take a brief look at the construction of the periodic table of the elements.

The electronic states of an atom are classified according to the one-electron states of the radially symmetric potential. Thus we have $1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, \dots$ states where the numbers give the principal quantum number, n , and the letters s, p, d, f correspond to the values of the electron's orbital angular momentum ($l = 0, 1, 2, 3, \dots$). This classification stems from the picture in which the potential for each electron includes the effect of all other electrons by representing them as a continuous fixed charge distribution which, to a greater or lesser extent, screens the potential of the bare nucleus. In

addition to the principal quantum number n and the orbital angular momentum quantum number l , there is also a magnetic quantum number m which can take $(2l+1)$ different values (ranging from $-l$ to $+l$). According to the Pauli exclusion principle, each state can be occupied by at most two electrons of opposite spin. As a function of increasing nuclear charge this then leads to the periodic tables whose structure is outlined in Table 1.1. From the order of the energy levels of the hydrogen atom, one would expect that after the $3p$ -states are filled, the next states to be occupied would be the $3d$. But in fact, as can be seen from Table 1.1, this is not the case; following the $3p$ -levels those next occupied are the $4s$. The subsequent filling of the $3d$ -states gives rise to the first series of transition metals (the $3d$ -metals). Similarly, one also finds $4d$ - and $5d$ transition metals. The same effect for the f -states leads to the so-called rare earths. The reason for this anomaly is that the electrons in s -states have a nonvanishing probability of being located at the nucleus thereby reducing for them the screening effect of the other electrons. Hence the s -electrons possess lower energy.

If one considers a thought experiment in which several initially isolated atoms are gradually brought closer together, their interaction with one another will lead to a splitting of each of their energy levels. If a very large number of atoms are involved, as in the case of a real solid, then the energy levels will lie on a quasicontinuous scale and one therefore speaks of energy bands (Fig. 1.1). The width of the band (i.e., the broadening) depends on the overlap of the wavefunctions concerned. Thus for the deep lying levels the broadening is small, and these "core levels" retain their atomic shell-like character even in the solid. For the highest occupied levels, on the other hand, the broadening is so large that the s -, p - and where present, d -levels merge into a single band. It is the electrons in this uppermost band that are responsible for the chemical bonding between atoms, and hence one speaks of the valence band. The ultimate source of the chemical bonding is the reduction in electronic energy which results from the level broadening. This, despite the increase in repulsion between the nuclei, leads to a decrease in the total energy as a function of atomic separation until the point where the equilibrium separation is reached – i.e., the point of minimum total energy.

The type of bonding in a solid is determined essentially by the degree of overlap between the electronic wavefunctions of the atoms involved. At the one extreme, this overlap may be limited to neighbor-

Table 1.1. The build-up of the periodic table by successive filling of the electronic energy shells. Indicated on the left of each column is the outer electron level that is being progressively filled, and in brackets is its maximum allowed occupation number

1s (2) H, He	4s (2) K, Ca	5p (6) In → Xe
2s (2) Li, Be	3d (10) Transition metals Sc → Zn	6s (2) Cs, Ba
2p (6) B → Ne	4p (6) Ga → Kr	4f (14) Rare earths Ce → Lu
3s (2) Na, Mg	5s (2) Rb, Sr	5d (10) Transition metals La → Hg
3p (6) Al → Ar	4d (10) Transition metals Y → Cd	6p (6) Tl → Rn

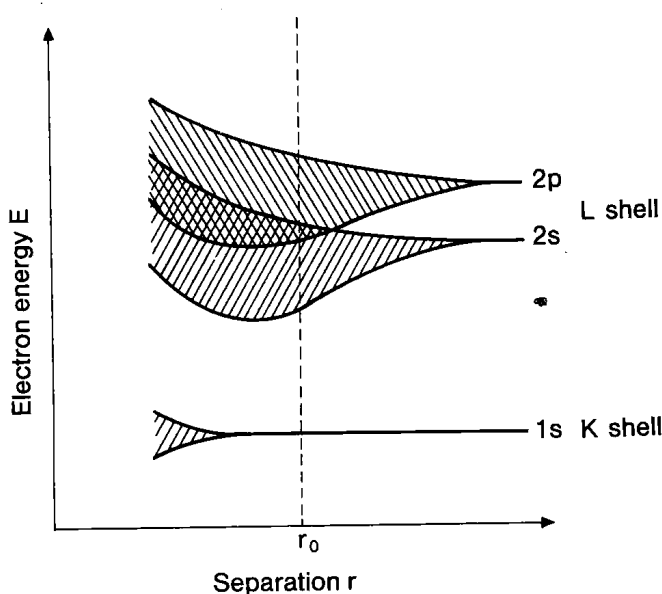


Fig. 1.1. Broadening of the energy levels as a large number of identical atoms from the first row of the periodic table approach one another (schematic). The separation r_0 corresponds to the approximate equilibrium separation of chemically bound atoms. Due to the overlap of the $2s$ and $2p$ bands, elements such as Be with two outer electrons also become metallic. Deep-lying atomic levels are only slightly broadened and thus, to a large extent, they retain their atomic character

ing atoms; in other cases the wavefunctions may be spread over many atoms. In the former case, the degree of overlap, and thus the strength of the bonding, is dependent not only on the separation of neighboring atoms, but also on the bond angles. This is referred to as *directional bonding* or *covalent bonding*.

In its purest form, covalent bonding is realized between a few elements of equal “valence”, i.e. elements with the same outer electronic configuration. However, an equal electronic configuration is neither a necessary nor a sufficient condition for covalent bonding. What is important is simply the relative extent of the wavefunctions in comparison to the interatomic separation. If the extent of the wavefunctions is large compared to the nearest-neighbor distance, then the exact position of the nearest neighbors plays an insignificant role in producing the greatest possible overlap with many atoms. In this case, the packing density is more important than the position of the next neighbors. Here one speaks of *non-directional bonding*. This regime in which the wavefunctions spread over a distance that is large in comparison to the atomic separation is characteristic of *metallic bonding*.

However, there is a further type of non-directional bonding with extremely small overlap of wavefunctions; this is the *ionic bond*. It occurs in cases where the transfer of an electron from one atom to another is sufficiently energetically favorable. A prerequisite for ionic bonding is thus a dissimilarity of the atoms involved.

In the following sections we will explore the various types of bonding in greater detail.