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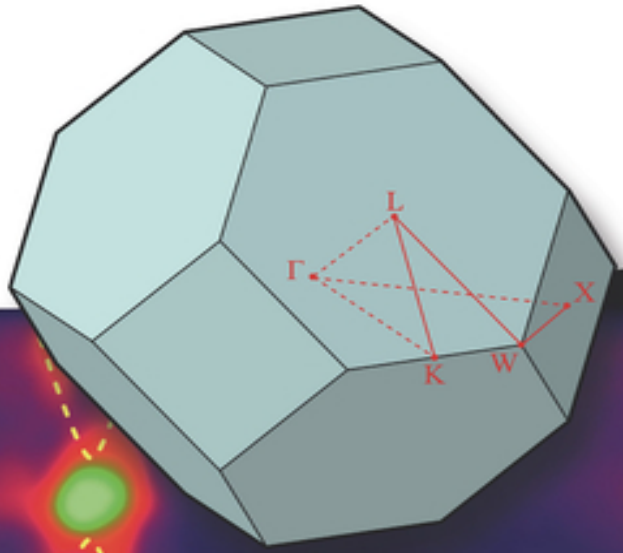
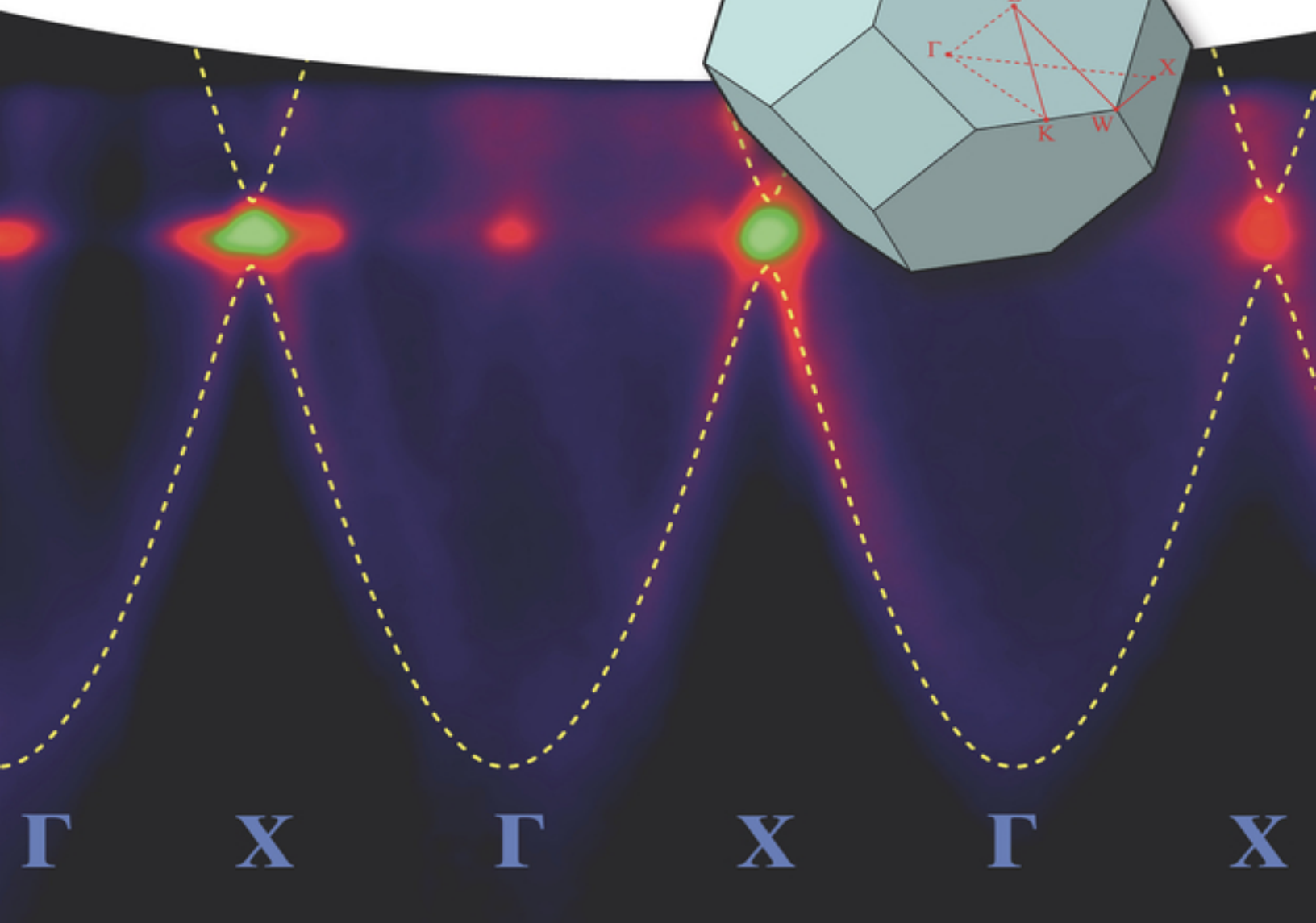
Philip Hofmann

Solid State Physics

An Introduction

Third Edition





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Third Edition

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Preface to the First Edition

This book emerged from a course on solid state physics for third-year students of physics and nanoscience, but it should also be useful for students of related fields such as chemistry and engineering. The aim is to provide a bachelor-level survey over the whole field without going into too much detail. With this in mind, a lot of emphasis is put on a didactic presentation and little on stringent mathematical derivations or completeness. For a more in-depth treatment, the reader is referred to the many excellent advanced solid state physics books. A few are listed in the Appendix.

To follow this text, a basic university-level physics course is required as well as some working knowledge of chemistry, quantum mechanics, and statistical physics. A course in classical electrodynamics is of advantage but not strictly necessary.

Some remarks on *how to use this book*: Every chapter is accompanied by a set of “discussion” questions and problems. The intention of the questions is to give the student a tool for testing his/her understanding of the subject. Some of the questions can only be answered with knowledge of later chapters. These are marked by an asterisk. Some of the problems are more of a challenge in that they are more difficult mathematically or conceptually or both. These problems are also marked by an asterisk. Not all the information necessary for solving the problems is given here. For standard data, for example, the density of gold or the atomic weight of copper, the reader is referred to the excellent resources available on the World Wide Web.

Finally, I would like to thank the people who have helped me with many discussions and suggestions. In particular, I would like to mention my colleagues Arne Nylandsted Larsen, Ivan Steensgaard, Maria Fuglsang Jensen, Justin Wells, and many others involved in teaching the course in Aarhus.

Preface to the Second Edition

The second edition of this book is slightly enlarged in some subject areas and improved throughout. The enlargement comprises subjects that turned out to be too essential to be missing, even in a basic introduction such as this one. One example is the tight-binding model for electronic states in solids, which is now added in its simplest form. Other enlargements reflect recent developments in the field that should at least be mentioned in the text and explained on a very basic level, such as graphene and topological insulators.

I decided to support the first edition by online material for subjects that were either crucial for the understanding of this text but not familiar to all readers, or not central enough to be included in the book but still of interest. This turned out to be a good concept, and the new edition is therefore supported by an extended number of such notes; they are referred to in the text. The notes can be found on my website www.philiphofmann.net.

The didactic presentation has been improved, based on the experience of many people with the first edition. The most severe changes have been made in the chapter on magnetism but minor adjustments have been made throughout the book. In these changes, didactic presentation was given a higher priority than elegance or conformity to standard notation, for example, in the figures on Pauli paramagnetism or band ferromagnetism.

Every chapter now contains a “Further Reading” section at the end. Since these sections are supposed to be independent of each other, you will find that the same books are mentioned several times.

I thank the many students and instructors who participated in the last few years' Solid State Physics course at Aarhus University, as well as many colleagues for their criticism and suggestions. Special thanks go to NL architects for permitting me to use the flipper-bridge picture in Figure 11.3, to Justin Wells for suggesting the analogy to the topological insulators, to James Kermode for Figure 3.7, and to Arne Nylandsted Larsen and Antonija Grubišić Čabo for advice on the sections on solar cells and magnetism, respectively.

Preface to the Third Edition

The third edition of this book introduces numerous improvements throughout the text, in particular in the description of covalent bonding in Chapter 2 and in the discussion of the Bloch theorem and the nearly-free electron model in Chapter 6.

The most significant changes are related to the problem sections in each chapter. In addition to the “traditional” type of problems that require an analytical solution, I have now included a number of problems that need to be solved numerically. Their complexity varies from plotting a simple function to calculating the carrier densities in a semiconductor. By introducing this new type of problems I hope to strengthen the students' computational skills, to overcome the restriction of being able to calculate solely what can be approximated using a simple model, and to impart upon students the capability to “play” with model parameters in order to explore what might happen in different physical situations. Moreover, exercises such as 4.4 and 6.10 are intended to help students understand the way phonon dispersions or electronic states are plotted as one-dimensional cuts through a multi-dimensional Brillouin zone. For instructors, Python scripts for individual problems are provided as part of the instructor resources that are available from the publisher.

Another major change in the problem sections is the addition of a “basic concepts” section in addition to the “discussion questions” and the more complex “problems” from the second edition. Many (but not all) of the new “basic concepts” questions are of the multiple-choice type and the solutions to all of them are given in Appendix B. As in the first two editions, the “discussion questions” can

serve as an inspiration to think about the central new concepts of each chapter or for discussing them in class, whereas the “problems” serve for a more in-depth exploration of the subjects. As in the previous editions, problems marked by an asterisk * are particularly challenging. The “basic concepts” section can be used in self-studies to test one's understanding of the most important ideas. Most of the questions do not require any calculations but they still go beyond a simple repetition of the chapter's content and involve some thinking. The number of “basic concepts” questions in a given chapter depends on the number and complexity of new concepts introduced in this chapter. Chapter 1, for instance, introduces difficult and very important ideas such as the reciprocal lattice, and therefore it contains a large number of “basic concepts” questions. Chapter 3, on the other hand, is conceptually less difficult and contains only a few of them. Many more of this type of questions along with their solutions can be found on my website at www.philiphofmann.net.

The multiple-choice questions have only one correct answer, or, if several correct answers exist, there is an explicit option to choose this, e. g., “C. Both A. and B. are correct.” In some cases, there is an overlap between a “basic concepts” question testing a conceptual understanding of a subject and a “problem” with a more in-depth treatment of the same question.

My thanks go to the 2021 class of the Statistical Physics and Solid State Physics course at Aarhus University for testing much of the new content, as well as to the teaching instructors Paulina Majchrzak, Alfred Jones, Michael Iversen and Nikolaj Rønne. I also thank Davide Curcio for introducing me to a new set of advanced writing tools and Charlotte E. Sanders for many helpful comments on the manuscript.

Physical Constants and Energy Equivalents

Planck constant	h	$6.626\ 070\ 15 \times 10^{-34}$ J s
		$4.135\ 667\ 70 \times 10^{-15}$ eV s
Boltzmann constant	k_B	$1.380\ 649 \times 10^{-23}$ J K^{-1}
		$8.617\ 333 \times 10^{-5}$ eV K^{-1}
Proton charge	e	$1.602\ 176\ 63 \times 10^{-19}$ C
Bohr radius	a_0	$5.291\ 77 \times 10^{-11}$ m
Bohr magneton	μ_B	$9.274\ 010\ 1 \times 10^{-24}$ J T^{-1}
Avogadro constant	N_A	$6.022\ 140\ 8 \times 10^{23}$ mol^{-1}
Speed of light	c	$2.997\ 924\ 58 \times 10^{8}$ m s^{-1}
Rest mass of the electron	m_e	$9.109\ 383\ 7 \times 10^{-31}$ kg
Rest mass of the proton	m_p	$1.672\ 621\ 9 \times 10^{-27}$ kg
Rest mass of the neutron	m_n	$1.674\ 927\ 5 \times 10^{-27}$ kg
Atomic mass unit	u	$1.660\ 539 \times 10^{-27}$ kg
Permeability of vacuum	μ_0	$4\pi \times 10^{-7}$ V s A^{-1} m^{-1}
Permittivity of vacuum	ε_0	$8.854\ 187\ 813 \times 10^{-12}$ C^2 J^{-1} m^{-1}

1 eV = $1.602\ 176\ 634 \times 10^{-19}$ J

1 K = $8.617\ 333 \times 10^{-5}$ eV

1
Crystal Structures

Our general objective in this book is to understand the macroscopic properties of solids on a microscopic level. In view of the many particles in solids, coming up with any microscopic description appears to be a daunting task. It is clearly impossible to solve the equations of motion (classical or quantum-mechanical) of the particles. Fortunately, it turns out that solids are often crystalline, with the atoms arranged on a regular lattice, and this symmetry permits us to solve microscopic models despite the vast number of particles involved. In a way, this situation is similar to atomic physics where the key to a quantum-mechanical description is the spherical symmetry of the atom. We will often imagine a macroscopic solid as one **single crystal**, a perfect lattice of atoms without any defects whatsoever. While it may seem that such perfect crystals are not particularly relevant for real materials, this is in fact not the case. Many solids are actually composed of small crystalline grains. Such solids are called **polycrystalline**, in contrast to a macroscopic single crystal, but the number of atoms within a perfect crystalline environment in them is still very large compared to the number of atoms on the **grain boundary**. For instance, for a grain size on the order of 1000^3 atomic distances, only about 0.1% of all atoms are at the grain boundaries.

There are, however, also solids that are not crystalline. These are called **amorphous**. The amorphous state is characterized by the absence of any long-range order. There may exist, however, a degree of short-range order between the atoms.

This chapter is divided into three parts. In the first part, we define some basic mathematical concepts needed to describe crystals. We keep things simple and mostly use two-dimensional examples to illustrate the ideas. In the second part, we discuss common crystal structures. For the moment, we will not ask *why* the atoms bind together in the way they do – this topic will be discussed in Chapter 2. Finally, we delve into a more detailed discussion of X-ray diffraction, the experimental technique that can be used to determine the microscopic structure of crystals. X-ray diffraction is used not only in solid state physics but also for a wide range of problems in nanotechnology and structural biology.

1.1 General Description of Crystal Structures

Our description of crystals starts with the mathematical definition of the **lattice**. A lattice is a set of regularly spaced points with positions defined as multiples of generating vectors. In two dimensions, a lattice can be defined as all the points that can be reached by the vectors $\mathbf{R}$, created from two non-collinear vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ as

$$\mathbf{R} = m\mathbf{a}_1 + n\mathbf{a}_2, \tag{1.1}$$

where n and m are integers. In three dimensions, the corresponding definition is

$$\mathbf{R} = m\mathbf{a}_1 + n\mathbf{a}_2 + o\mathbf{a}_3. \tag{1.2}$$

Such a lattice of points is also called a **Bravais lattice**. The number of possible Bravais lattices with different symmetries is limited to 5 in two dimensions and to 14 in three dimensions. An example of a two-dimensional Bravais

lattice is given in Figure 1.1. The lengths of the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are often called the **lattice constants**.

Having defined the Bravais lattice, we move on to the definition of the **primitive unit cell**. By this we denote any volume of space that, when translated through all the vectors of the Bravais lattice, will fill space without overlap and without leaving any voids. The primitive unit cell of a lattice contains only one lattice point. It is also possible to define **nonprimitive unit cells** containing several lattice points. These fill space without leaving voids when translated through a subset of the Bravais lattice vectors. Possible choices of a unit cell for a two-dimensional rectangular Bravais lattice are illustrated in Figure 1.2. It is evident from the figure that a nonprimitive unit cell has to be translated by a multiple of one (or two) lattice vectors to fill space without voids and overlap. A special choice of the primitive unit cell is the **Wigner–Seitz cell**, which is also shown in Figure 1.2. It is the region of space that is closer to one given lattice point than to any other.

The last definition we need in order to describe an actual crystal is that of a **basis**. The basis describes the items we "put" on the lattice points, that is, the building blocks for the real crystal. The basis can consist of one or several atoms, or even of complex molecules as in the case of protein crystals. Different cases are illustrated in Figure 1.3.

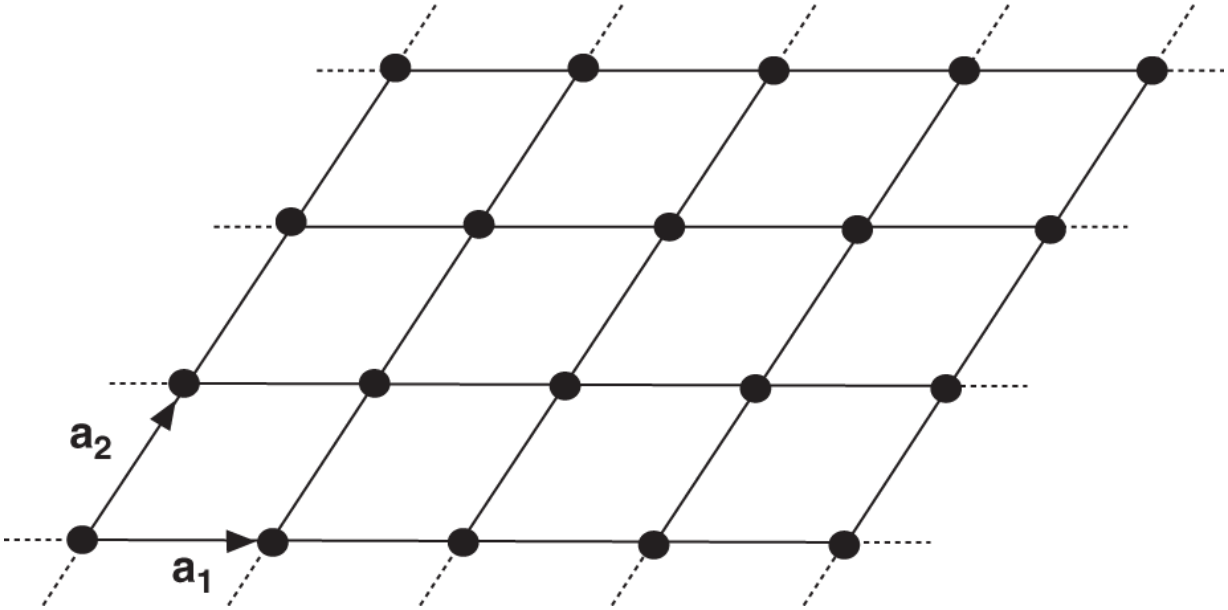

Figure 1.1 A two-dimensional Bravais lattice.

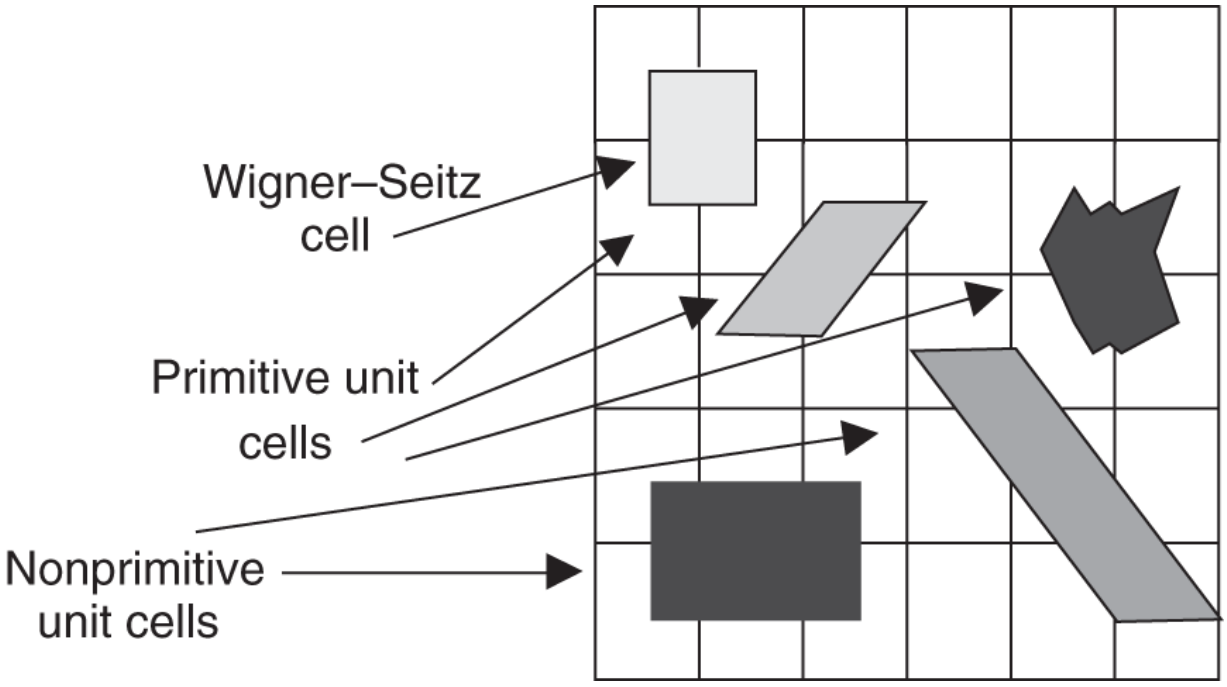

Figure 1.2 Illustration of (primitive and nonprimitive) unit cells and of the Wigner–Seitz cell for a rectangular two-dimensional lattice.

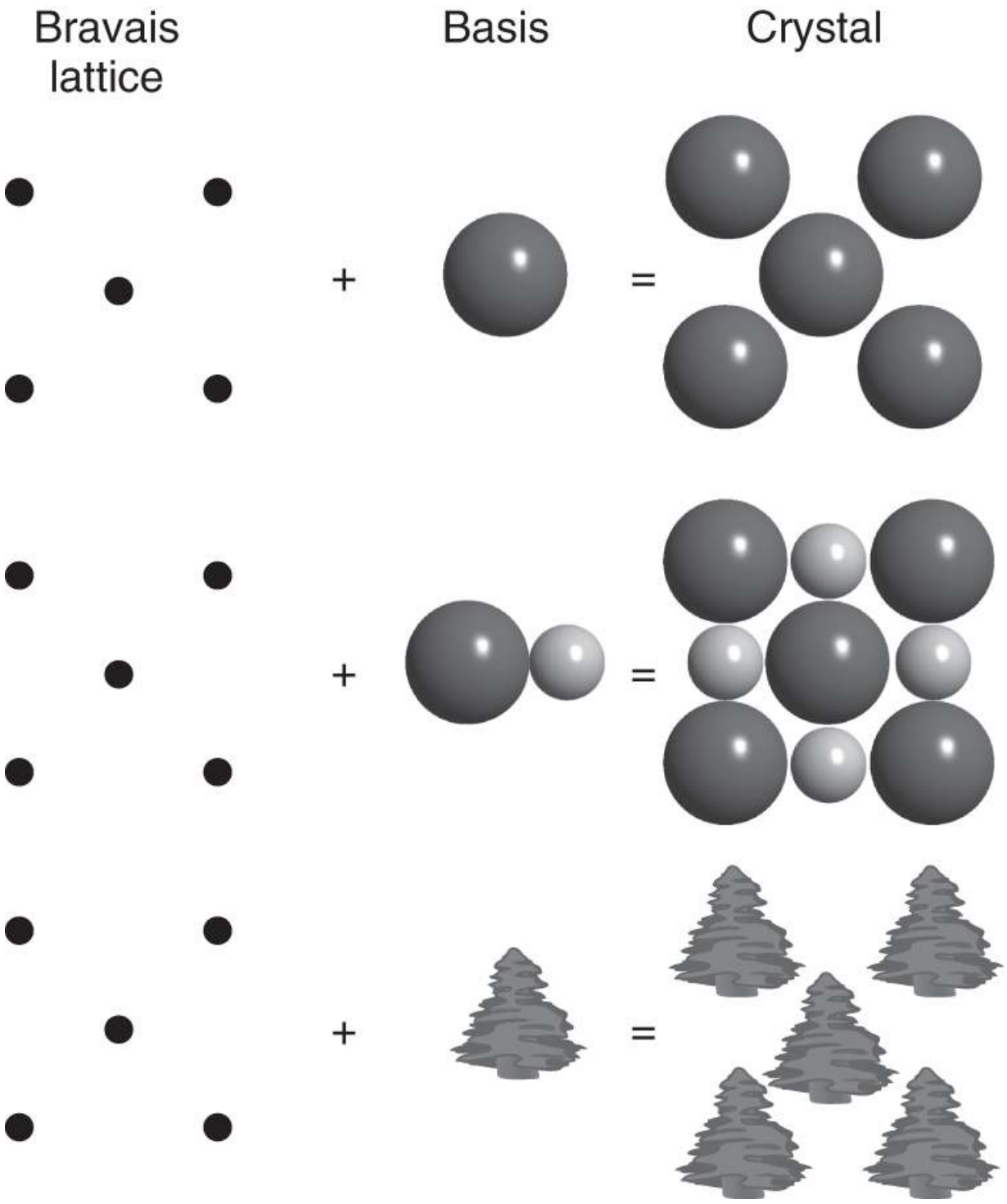

Figure 1.3 A two-dimensional Bravais lattice with different choices for the basis.

Finally, we add a remark about symmetry. So far, we discussed only **translational symmetry**. However, a real

crystal may also exhibit **point symmetry**. Compare the structures in the middle and the bottom of Figure 1.3. The former structure possesses a number of symmetry elements that are missing in the latter – for example, mirror lines, a rotational axis, and inversion symmetry. The knowledge of such symmetries can be very useful for the description of crystal properties.

1.2 Some Important Crystal Structures

After this rather formal treatment, we look at a number of common crystal structures for different types of solids, such as metals, ionic solids, or covalently bonded solids. In Chapter 2, we will take a closer look at the details of the bonding in these types of solids.

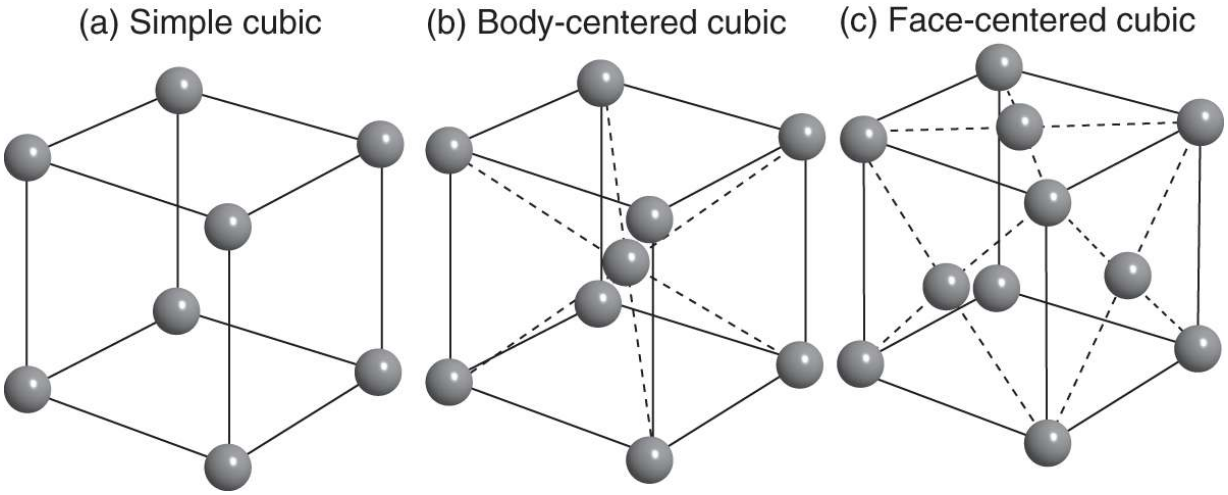

Figure 1.4 (a) Simple cubic structure; (b) body-centered cubic structure; and (c) face-centered cubic structure. Note that the spheres are depicted much smaller than in the situation of most dense packing and not all of the spheres on the faces of the cube are shown in (c).

1.2.1 Cubic Structures