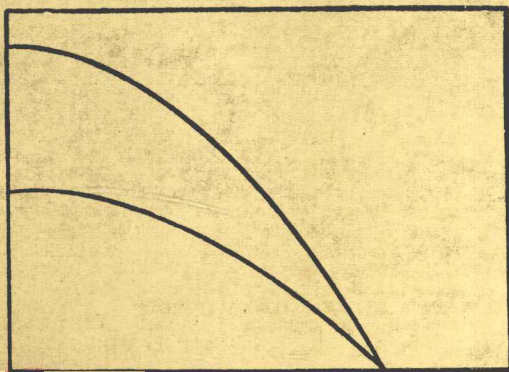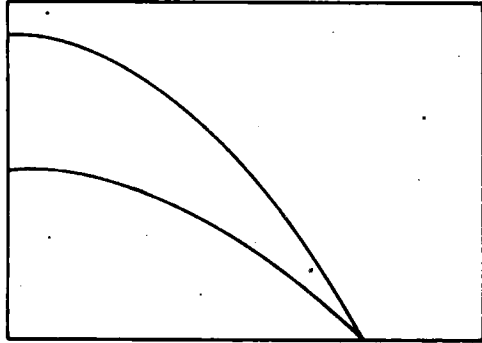# Solid
State
Physics

Harold T. Stokes

Solid State Physics

Harold T. Stokes

Brigham Young University

ALLYN AND BACON, INC.

Boston • London • Sydney • Toronto

Printed in the United States of America.

10 9 8 7 6 5 4 3 2 1   90 89 88 87 86

Preface

I wrote this book for the course, Principles of Solid State Physics, developed at Brigham Young University. The course was specifically intended for non-physics majors. The prerequisites are two semesters of introductory physics that cover mechanics and electric and magnetic fields. A course in modern physics is *not* a prerequisite. Thus, many topics of modern physics, such as quantum mechanics, are included in this course to the extent that they are needed to understand the aspects of solid state physics covered.

The purpose of this course is to acquaint the student with the fundamental physics of solids. This emphasis is on understanding the behavior of electrons in metals and semiconductors. In the first 3 chapters, crystal structure, x-ray diffraction, and lattice vibrations are discussed as a natural way to introduce concepts such as translational symmetry, wave interference, reciprocal lattice, and the first Brillouin zone. Also, two chapters (5–6) on quantum theory are included to teach the basic ideas and principles of quantum mechanics needed. All of these concepts are brought together to form an understandable modern picture of electrons in metals (chapters 7–9), in semiconductors (chapters 10–12), and in superconductors (chapter 13). Numerous examples, problems, and figures are used to illustrate the material being presented. There are 181 problems and 188 figures in this book.

The reader may note that some topics usually found in conventional solid state physics textbooks are missing from this book, such as heat capacity, magnetism, dielectrics, etc. This is a one-semester course. I wanted to treat a few central topics in great detail rather than describe superficially a great many topics.

I wish to thank Professor Dean Barnett and Professor William Evenson for critically reading portions of this book and for the many valuable suggestions they have made.

CONTENTS

Chapter 9. Electrical Conductivity of Metals

Chapter 10. Semiconductors

Chapter 11. p-n Junctions in Semiconductors

Chapter 12. Semiconductor Devices

CHAPTER 1

CRYSTAL STRUCTURE

1-1 Introduction

Many solids around us are crystalline. Obvious examples are diamonds and other precious stones which have an outward crystalline appearance. Many metals are also crystalline. However, they are usually composed of numerous small crystals fused together so that their outward appearance is *not* crystalline. In this book, we will consider only crystalline solids.

A *crystal* is a solid in which all the atoms are arranged in a periodic manner. As a simple example, consider the cubic arrangement of atoms shown in Fig. 1-1. We show only a portion of the crystal. We imagine that it extends out in all directions to infinity. Real crystals, of course, have finite dimensions, but,
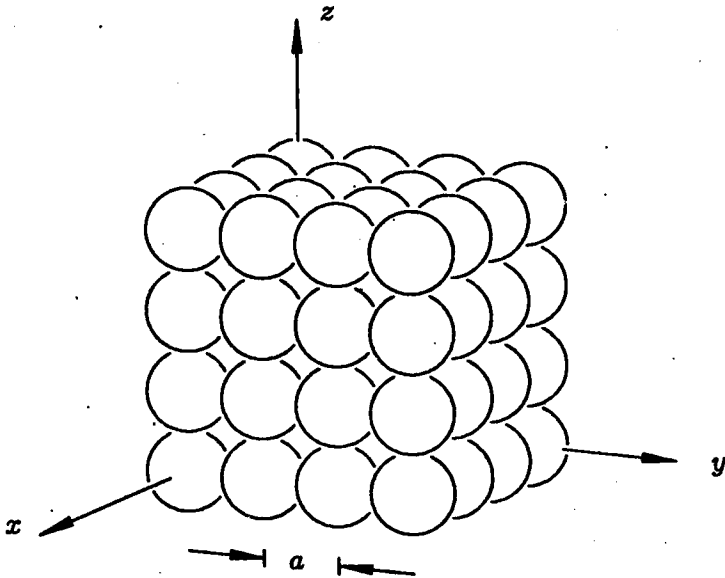
Fig. 1-1. Simple cubic arrangement of atoms.

for now, we consider the crystal to be infinitely large with no surfaces.

The atoms in the crystal shown in Fig. 1-1 are in equivalent positions. If we sit on one of the atoms, we cannot tell where we are by looking at the neighboring atoms. All atoms have exactly the same surroundings. (This, of course, is only strictly true in an *infinite* crystal.) If we move the entire crystal in some direction so that each atom is now at a position where some other atom used to be, the crystal looks the same as before. We cannot tell that it has been moved. This is called **translational symmetry**. We may now state the definition of a crystal more precisely. A **crystal** is a solid which has translational symmetry.

1-2 Lattices

In order to quantitatively describe a crystal, we introduce a group of geometric points called the crystal lattice which defines the positions of the atoms. As an example, consider the two-dimensional square lattice shown in Fig. 1-2. This lattice is a set of geometric points on a plane. If we were to place
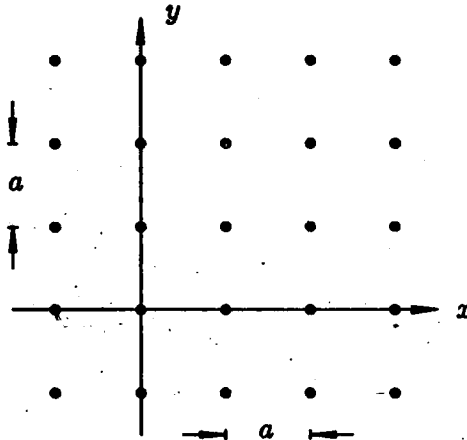
Fig. 1-2. The two-dimensional square lattice.

an atom at each point, then we would have a two-dimensional crystal. All lattice points in the figure are equivalent. This lattice has translational symmetry in two dimensions.

1-3 Basis Vectors

A lattice vector is a vector which takes us from one lattice point to any other lattice point. Obviously, all lattice vectors **R** in the two-dimensional square lattice (Fig. 1-2) have the form

$$\mathbf{R} = n_1 a\hat{\imath} + n_2 a\hat{\jmath}, \tag{1-1}$$

where n_1 and n_2 are integers (including negative values and zero), and a is the distance between adjacent lattice points in the x or y directions, as shown in Fig. 1-2. $\hat{\imath}$ and $\hat{\jmath}$ are unit vectors in the x and y directions, respectively. If we define two vectors (see Fig. 1-3),

$$\begin{aligned}\mathbf{a}_1 &= a\hat{\imath},\\ \mathbf{a}_2 &= a\hat{\jmath},\end{aligned} \tag{1-2}$$

then we can write **R** as

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2. \tag{1-3}$$
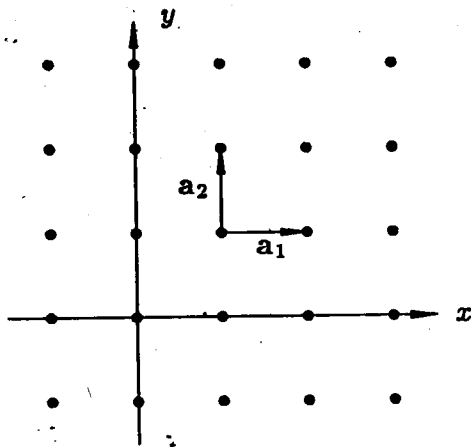
Fig. 1-3. Basis vectors for the square lattice.

Thus, *any* lattice vector **R** can be written as a linear combination of a_1 and a_2 (using integers, n_1 and n_2). Conversely, it is also true that any linear combination of a_1 and a_2 (using integers, n_1 and n_2) is a lattice vector **R**. Such vectors, a_1 and a_2, are called **basis vectors** of the lattice.

The choice of basis vectors, a_1 and a_2, is not unique. We could just as well choose (see Fig. 1-4)

$$
\begin{aligned}
\mathbf{a}_1' &= a\hat{\imath}, \\
\mathbf{a}_2' &= a\hat{\imath} + a\hat{\jmath}.
\end{aligned}
\qquad (1\text{-}4)
$$

For example, consider the lattice vector $\mathbf{R} = a\hat{\imath} + 2a\hat{\jmath}$. This can be written as $\mathbf{R} = \mathbf{a}_1 + 2\mathbf{a}_2$ or as $\mathbf{R} = -\mathbf{a}_1' + 2\mathbf{a}_2'$ as shown in Fig. 1-5.

There are an infinite number of ways to choose basis vectors for a given lattice. There is, however, usually a conventional choice of basis vectors. For example, the conventional basis vectors for the square lattice are those given in Eq. (1-2). Basis vectors can be found for any lattice of *equivalent* points.
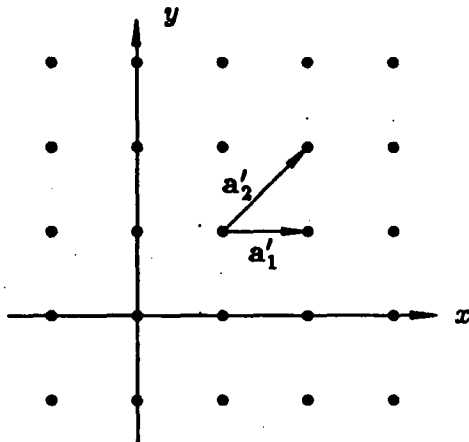
Fig. 1-4. An alternate choice of basis vectors for the square lattice.
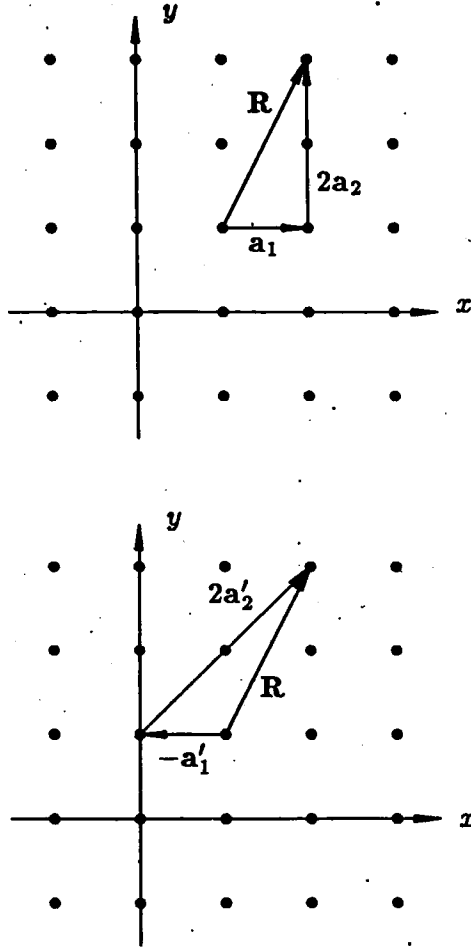
Fig. 1-5. Lattice vector $\mathbf{R}$ expressed as a linear combination of the basis vectors, $\mathbf{a}_1$ and $\mathbf{a}_2$, and also as a linear combination of the basis vectors, $\mathbf{a}_1'$ and $\mathbf{a}_2'$.

1-4 Simple Cubic Lattice

The extension to three dimensions is straightforward. The lattice which underlies the crystal structure in Fig. 1-1 has basis vectors given by

$$\mathbf{a}_1 = a\hat{\imath},$$
$$\mathbf{a}_2 = a\hat{\jmath}, \qquad\qquad (1\text{-}5)$$
$$\mathbf{a}_3 = a\hat{k},$$

and the lattice vector is given by

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3. \qquad\qquad (1\text{-}6)$$

This lattice is called simple cubic (sc).

1-5 Unit Cells

A crystal can always be divided into "building blocks" called unit cells. Each unit cell has the same shape, the same volume, and the same contents. For the sc lattice, we may choose the unit cell to be a cube of side a (see Fig. 1-6). The

Fig. 1-6. Unit cells of the sc lattice

choice of position of the lattice point within the unit cell is
arbitrary. We may arrange the cubes so that each cube con-
tains one lattice point at its center (see Fig. 1-7a). Alternately,
we may arrange the cubes so that the lattice points are at the
corners of the cube (see Fig. 1-7b). The second choice is the
conventional unit cell.

Each of these unit cells contains one lattice point. This is
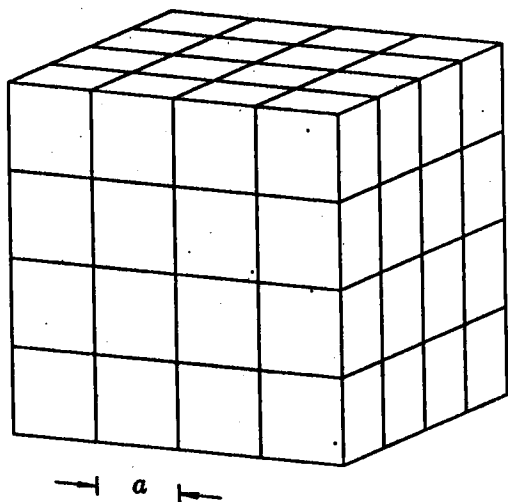obviously true for the unit cell in Fig. 1-7a which contains one
lattice point in the center. But the conventional unit cell in
Fig. 1-7b appears to contain *eight* lattice points, one at each
corner. Actually, each of those lattice points is shared by eight
neighboring unit cells that adjoin at the corner so that each
unit cell contains "$\frac{1}{8}$ lattice point" at the corner. Eight such
lattice points give us a total of one lattice point in the unit
cell.

Just as the choice of basis vectors for a lattice is not
unique, the choice of unit cells is also not unique. For example,
we could just as well choose the unit cell shown in Fig. 1-8. We
only require that the unit cells be identical to each other and
fill all space. There are an infinite number of ways to choose
the unit cell. However, the *conventional* unit cell for the sc

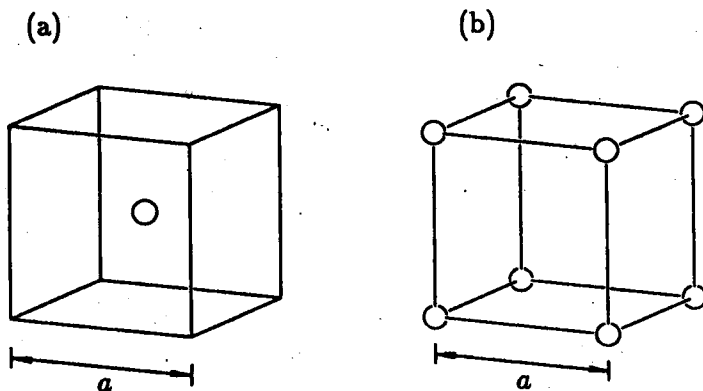(a)   (b)

Fig. 1-7. The unit cell for the sc lattice (a) with a lattice
point at the center and (b) with a lattice point at each corner
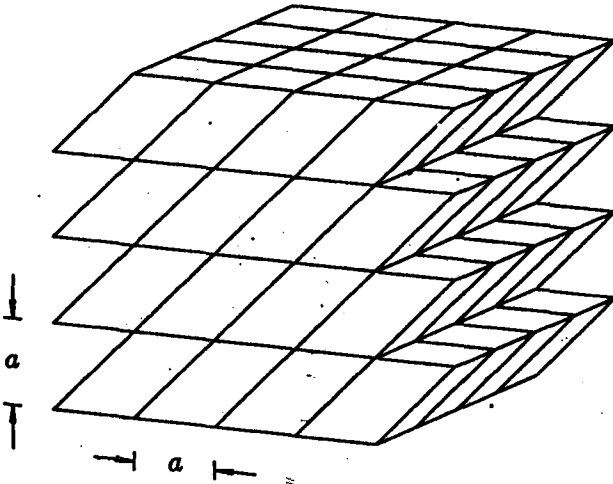(conventional unit cell).

Fig. 1-8. An alternate choice of unit cell for the sc lattice.

lattice is the cube shown in Fig. 1-7b. The distance a between adjacent atoms in the x, y, or z direction is called the **lattice parameter.**

1-6 Crystal Directions and Planes

Directions in crystals are usually represented in shorthand by three integers inside a set of square brackets. The direction $R = n_1 a\hat{i} + n_2 a\hat{j} + n_3 a\hat{k}$ in a cubic crystal, for example, is written as $[n_1, n_2, n_3]$. The integers are usually chosen to be as small as possible. Three common directions in cubic crystals with which we will deal are (see Fig. 1-9)

$$
\begin{aligned}
R &= a\hat{i} & \text{or} \quad [100], \\
R &= a\hat{i} + a\hat{j} & \text{or} \quad [110], \\
R &= a\hat{i} + a\hat{j} + a\hat{k} & \text{or} \quad [111],
\end{aligned}
\qquad (1\text{-}7)
$$

Consider a hypothetical crystal which has one atom at each lattice point of an sc lattice with $a = 5.00$ Å. (No naturally occurring element forms an sc lattice.) Starting from an atom
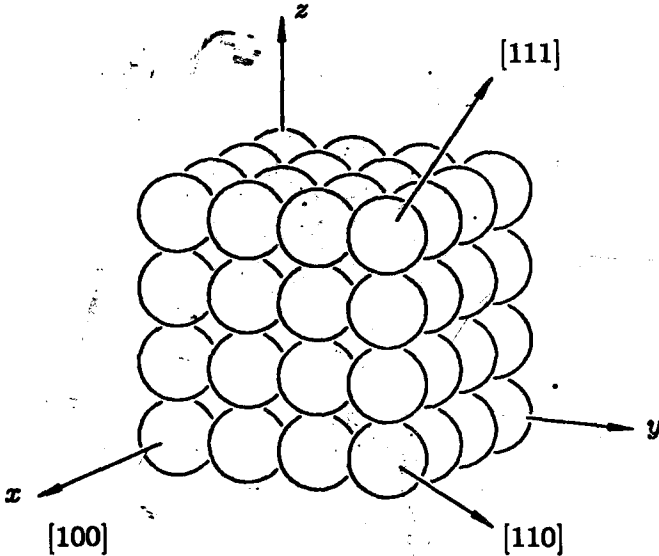
Fig. 1-9. Three common directions in cubic crystals.

at the origin, we see that along the [100] direction, there are atoms at $a\hat{i}$, $2a\hat{i}$, $3a\hat{i}$, etc. The distance between adjacent atoms along the [100] direction is $a = 5.00$ Å, which is the length of the vector $\mathbf{a}_1 = a\hat{i}$.

If we go along the [110] direction from the atom at the origin, we find atoms at $a\hat{i} + a\hat{j}$, $2a\hat{i} + 2a\hat{j}$, $3a\hat{i} + 3a\hat{j}$, etc., and the distance between adjacent atoms is the length of the vector $a\hat{i} + a\hat{j}$, which is $\sqrt{2}a = 7.07$ Å. Similarly, along the [111] direction, atoms are at $a\hat{i} + a\hat{j} + a\hat{k}$, $2a\hat{i} + 2a\hat{j} + 2a\hat{k}$, $3a\hat{i} + 3a\hat{j} + 3a\hat{k}$, etc., and the distance between adjacent atoms is the length of the vector $a\hat{i} + a\hat{j} + a\hat{k}$, which is $\sqrt{3}a = 8.66$ Å.

We would find, in general, that along any given direction in a crystal, atoms are evenly spaced. The distance between adjacent atoms is smallest along the [100] direction. These atoms are **nearest neighbors** to each other. If we imagine the atoms to be "hard" spheres such as those shown in Fig. 1-1, then we see that the nearest neighbors "touch" each other, and