FUNDAMENTALS OF CRYSTALLOGRAPHY

Fundamentals of Crystallography

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Preface

Crystallography, the science concerned with the study of crystals, is a very old subject. However, only in this century has it developed into a modern science, after the discovery of X-rays and their diffraction by crystals. In recent years crystallography has assumed an increasingly important role in the modern sciences because of its interdisciplinary nature, which has acted as a bridge between, and often as a stimulus for, various rapidly evolving disciplines. Indeed, Chemistry, Physics, Earth Sciences, Biology, Mathematics, and Materials Science have all provided stimuli to the development of new crystallographic interests and techniques. In turn, crystallography has significantly contributed to the advancement of these sciences. Thus, while on the one hand crystallography has been enriched, on the other hand writing a textbook describing all of its aspects has been made more difficult.

Recently, the demand for a compact book that gives a comprehensive account of the modern crystallographic subjects has increased. This volume should therefore be a useful and handy textbook for university courses that cover crystallography, fully or only partially. It should also be useful at the more advanced level required for doctorate studies as well as for experienced researchers.

It was with these ideas in mind that I first set out to co-ordinate the publication, in 1985, of a textbook in Italian (*Introduzione alla cristallografia moderna,* Edizioni Fratelli Laterza, Bari) of which *Fundamentals of crystallography* is not only an English translation, but a completely revised and updated version with a new chapter on crystal physics. It was clear to me that (a) the book had to be written by several authors in order to take advantage of their specific expertise; (b) the different chapters had to be carefully harmonized in order to conform them to a unified plan.

It seems to me that these two requirements are even more valid today and their achievement is entirely due to the creative co-operation of the co-authors of this book.

Two of the co-authors of the Italian textbook, M. Bolognesi and A. Coda, were unable to carry out the translation and revision of their chapters. I wish to express my thanks for their valuable contribution to the previous edition. In this book their topics are treated by G. Zanotti and H. L. Monaco. An additional chapter on crystal physics has been written by M. Catti. I thank the three new authors for entering our team and all the authors for their enthusiastic participation in this project.

Bari, Italy C.G.
August 1991

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Nec possunt oculi naturam noscere rerum: proinde animi vitium hoc oculis adfingere noli.

Lucretius, *De Rerum Natura,* IV, 386–7.

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Symmetry in crystals

1

CARMELO GIACOVAZZO

The crystalline state and isometric operations

Matter is usually classified into three states: gaseous, liquid, and solid. Gases are composed of almost isolated particles, except for occasional collisions; they tend to occupy all the available volume, which is subject to variation following changes in pressure. In liquids the attraction between nearest-neighbour particles is high enough to keep the particles almost in contact. As a consequence liquids can only be slightly compressed. The thermal motion has sufficient energy to move the molecules away from the attractive field of their neighbours; the particles are not linked together permanently, thus allowing liquids to flow.

If we reduce the thermal motion of a liquid, the links between molecules will become more stable. The molecules will then cluster together to form what is macroscopically observed as a rigid body. They can assume a random disposition, but an ordered pattern is more likely because it corresponds to a lower energy state. This ordered disposition of molecules is called the **crystalline state**. As a consequence of our increased understanding of the structure of matter, it has become more convenient to classify matter into the three states: gaseous, liquid, and crystalline.

Can we then conclude that all solid materials are crystalline? For instance, can common glass and calcite (calcium carbonate present in nature) both be considered as crystalline? Even though both materials have high hardness and are transparent to light, glass, but not calcite, breaks in a completely irregular way. This is due to the fact that glass is formed by long, randomly disposed macromolecules of silicon dioxide. When it is formed from the molten state (glass does not possess a definite melting point, but becomes progressively less fluid) the thermal energy which remains as the material is cooled does not allow the polymers to assume a regular pattern. This disordered disposition, characteristic of the liquid state, is therefore retained when the cooling is completed. Usually glasses are referred to as **overcooled liquids**, while non-fluid materials with a very high degree of disorder are known as **amorphous solids**.

A distinctive property of the crystalline state is a regular repetition in the three-dimensional space of an object (as postulated as early as the end of the eighteenth century by R. J. Haüy), made of molecules or groups of molecules, extending over a distance corresponding to thousands of molecular dimensions. However, a crystal necessarily has a number of defects at non-zero temperature and/or may contain impurities without losing its order. Furthermore:

1. Some crystals do not show three-dimensional periodicity because the

basic crystal periodicity is modulated by periodic distortions incommensurated with the basic periods (i.e. in incommensurately modulated structures, IMS). It has, however, been shown (p. 171 and Appendix 3.E) that IMSs are periodic in a suitable (3 + d)-dimensional space.

2. Some polymers only show a bi-dimensional order and most fibrous materials are ordered only along the fiber axis.

3. Some organic crystals, when conveniently heated, assume a state intermediate between solid and liquid, which is called the **mesomorphic** or **liquid crystal** state.

These examples indicate that periodicity can be observed to a lesser or greater extent in crystals, depending on their nature and on the thermodynamic conditions of their formation. It is therefore useful to introduce the concept of a **real crystal** to stress the differences from an ideal crystal with perfect periodicity. Although non-ideality may sometimes be a problem, more often it is the cause of favourable properties which are widely used in materials science and in solid state physics.

In this chapter the symmetry rules determining the formation of an ideal crystalline state are considered (the reader will find a deeper account in some papers devoted to the subject, or some exhaustive books,[1–5] or in the theoretical sections of the *International Tables for Crystallography*).[6]

In order to understand the periodic and ordered nature of crystals it is necessary to know the operations by which the repetition of the basic molecular motif is obtained. An important step is achieved by answering the following question: given two identical objects, placed in random positions and orientations, which operations should be performed to superpose one object onto the other?

The well known coexistence of **enantiomeric** molecules demands a second question: given two **enantiomorphous** (the term enantiomeric will only be used for molecules) objects, which are the operations required to superpose the two objects?

An exhaustive answer to the two questions is given by the theory of **isometric transformations**, the basic concepts of which are described in Appendix 1.A, while here only its most useful results will be considered.

Two objects are said to be **congruent** if to each point of one object corresponds a point of the other and if the distance between two points of one object is equal to the distance between the corresponding points of the other. As a consequence, the corresponding angles will also be equal in absolute value. In mathematics such a correspondence is called **isometric**.

The congruence may either be **direct** or **opposite**, according to whether the corresponding angles have the same or opposite signs. If the congruence is direct, one object can be brought to coincide with the other by a convenient **movement** during which it behaves as a rigid body. The movement may be:

(1) a **translation**, when all points of the object undergo an equal displacement in the same direction;

(2) a **rotation** around an axis; all points on the axis will not change their position;

(3) a **rototranslation** or **screw** movement, which may be considered as the combination (product) of a rotation around the axis and a translation along the axial direction (the order of the two operations may be exchanged).

If the congruence is opposite, then one object will be said to be enantiomorphous with respect to the other. The two objects may be brought to coincidence by the following operations:

(1) a symmetry operation with respect to a point, known as **inversion**;

(2) a symmetry operation with respect to a plane, known as **reflection**;

(3) the product of a rotation around an axis by an inversion with respect to a point on the axis; the operation is called **rotoinversion**;

(4) the product of a reflection by a translation parallel to the reflection plane; the plane is then called a **glide plane**.

(5) the product of a rotation by a reflection with respect to a plane perpendicular to the axis; the operation is called **rotoreflection**.

Symmetry elements

Suppose that the isometric operations described in the preceding section, not only bring to coincidence a couple of congruent objects, but act on the entire space. If all the properties of the space remain unchanged after a given operation has been carried out, the operation will be a **symmetry operation. Symmetry elements** are points, axes, or planes with respect to which symmetry operations are performed.

In the following these elements will be considered in more detail, while the description of translation operators will be treated in subsequent sections.

Axes of rotational symmetry

If all the properties of the space remain unchanged after a rotation of $2\pi/n$ around an axis, this will be called a symmetry axis of order n; its written symbol is n. We will be mainly interested (cf. p. 9) in the axes 1, 2, 3, 4, 6. Axis 1 is trivial, since, after a rotation of 360° around whatever direction the space properties will always remain the same. The graphic symbols for the 2, 3, 4, 6 axes (called two-, three-, four-, sixfold axes) are shown in Table 1.1. In the first column of Fig. 1.1 their effects on the space are illustrated. In keeping with international notation, an object is represented by a circle, with a + or − sign next to it indicating whether it is above or below the page plane. There is no graphic symbol for the 1 axis. Note that a 4 axis is at the same time a 2 axis, and a 6 axis is at the same time a 2 and a 3 axis.

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