Introduction to Dislocations

THIRD EDITION

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Preface to the First Edition

ALTHOUGH the presence of dislocations in crystals was first proposed 30 years ago, it is only in the last 15 years that a general realisation of their importance has developed. Today, an understanding of dislocations is essential for all those concerned with the properties of crystalline materials. In the last 15 years the subject of dislocations has been transformed from an advanced research topic to one which is commonly taught at University undergraduate and technical school level. The subject has been richly served by two outstanding books, one by Professor A. H. Cottrell and the other by Dr. T. W. Read, both published 10 years ago, and by a tremendous amount of research literature. Although many aspects of the application of dislocation ideas are still in a state of flux a body of knowledge, based on theoretical analysis and experimental observation, has now been established which forms a basis for most of the ideas and theories which are proposed. Some fundamental dislocation problems remain to be solved but it seems unlikely that the ground work of the subject will be changed or modified appreciably, particularly at an introductory level.

In view of the importance of dislocations and the establishment of generally accepted principles, it seems appropriate to present an account of dislocations and their properties which can form an introduction to the understanding of many aspects of the properties of crystalline materials. Such is the intention of this book which is based on part of a one-year course on crystal defects and mechanical properties which I give to students of metallurgy. Parts of the course are given also in introductory courses on the properties of materials to physics and engineering students.

The method of approach in the book reflects the importance I attach to the necessity of the student achieving an intimate understanding of the three-dimensional geometry of dislocations in crystals. Once this is mastered, a qualitative appreciation of most ideas relating to dislocations can be assimilated.

The book is an account of the geometry, properties and behaviour of dislocations in crystals. The subject is developed from first principles so that the approach is applicable to all crystalline materials. In the first part the basic features of the geometry, movement and elastic properties of dislocations are described along with an account of the methods of observing and studying dislocations. This is followed by a description of the more detailed features of dislocations in specific structures; face-centred cubic, hexagonal close-packed, body-centred cubic, ionic, layer and superlattice structures. Two chapters are devoted to the basic properties of dislocations associated with their movement, such as intersections with other dislocations, jogs and multiplication of dislocations. Another chapter describes the geometry and properties of arrays of dislocations. Finally, the interaction between dislocations and imperfections in crystals, e.g. impurities, point defects, and other dislocations, is described and related to the stress required to move dislocations through a crystal containing such imperfections.

As far as possible the book is written in a form appropriate for an undergraduate course up to a final honours year level. Some of the material is probably beyond the normal honours year standard, but I consider that this is advisable in view of the need to familiarise the student with the next step as an aid to understanding the preceding steps. Less extensive courses than the honours standard can be developed readily from the first four chapters and parts of the other chapters.

Although not normally recommended in a student textbook, I have included a fairly extensive bibliography at the end of each chapter. The books and research papers which are listed were chosen carefully, and it is intended that they should be used by those who wish to take the subject one step further. They introduce also many of the

more speculative aspects of the subject, and demonstrate the way dislocation theory is applied in practice. To help the student make a judicious choice, from the references given, the title of the work is included in addition to the reference source.

In attempting to collect together the available information on dislocations, it is inevitable that I should rely almost entirely on the published and unpublished work of others. I have been influenced particularly by the books by Cottrell and Read already referred to. Much of my outlook and knowledge of dislocations was developed and stimulated in a period of $3\frac{1}{2}$ years during which I carried out research in the basic irradiation group at Harwell. The group was led by Professor A. H. Cottrell, and included Drs. M. A. Adams, R. S. Barnes and M. J. Makin, and Professors R. E. Smallman and M. J. Thompson. My thanks are due to these friends for their stimulating company. I hope that I have given due recognition to all who have, by publishing their work, contributed to the contents of this book.

I have benefited greatly from the company of Professor W. S. Owen who kindly read through the manuscript and made many valuable suggestions. I should like also to thank Mr. I. L. Mogford and Mr. R. D. Garwood who read the manuscript in full, and many friends at Liverpool who read sections of the book and in so doing contributed to its final form.

A book of this kind would be impossible were it not for the many illustrations which are available. I am grateful to all authors and publishers who have freely given me permission to use their material. Specific acknowledgement is given in the captions. I am particularly grateful to many friends who have sent me copies from the original negatives of their photographs.

DEREK HULL

Preface to the Third Edition

The subject of dislocations is an essential basis for an understanding of many of the physical and mechanical properties of crystalline solids. It is therefore reassuring to learn that this book is still widely used in undergraduate courses. It must be comforting for students and teachers alike that there have been few major advances in the underlying principles which require significant modifications in the content of, and methods of approach to, the subject.

It is nearly twenty years since the first edition was published, and we have found no reason to change the main structure of the book or method of approach used. However, the present edition represents a major revision of the text and includes some substantial new sections, notably in topics relating to experimental techniques, the elastic properties of dislocations, forces on dislocations, dislocations in particular crystal structures, the dislocation content of boundaries, and the strength of crystalline solids. To avoid making the book significantly larger we have removed a few sections which have become a little dated as techniques and understanding have developed. We have also taken the opportunity to rewrite some sections to clarify the contents and make them conform to a more modern standpoint.

The emphasis on a physical understanding of the geometry and arrangement of dislocations has been retained, but a slightly more rigorous approach has been used in specifying the mathematical content of the subject. This will be of value to those who need to apply the principles of dislocations but it should not deter those who only require the briefest of introductions. No attempt has been made to change the book into a research text.

We warmly acknowledge the help we have received from many friends and colleagues with regard to comments and permission to use diagrams. Our Liverpool colleagues have given us much helpful advice and we are particularly grateful to Dr. G. J. Tatlock, Dr. R. C. Pond and Dr. F. W. Noble for assistance in the preparation of Chapters 2. 9 and 10 respectively. Dr. Noble provided us with lecture notes.

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CHAPTER 1

Defects in Crystals

1.1 Crystalline Materials

Metals and many important classes of non-metallics solids are crystalline, i.e. the constituent atoms are arranged in a pattern that repeats itself periodically in three dimensions. The actual arrangement of the atoms is described by the *crystal structure*. The crystal structures of most pure metals are simple, the three most common structures being the body-centred cubic, face-centred cubic and close-packed hexagonal structures which are described in section 1.2. In contrast, the structures of alloys and non-metallic compounds are often complex.

The arrangement of atoms in a crystal can be described with respect to a three-dimensional net of straight lines as in Fig. 1.1(a). The lines divide space
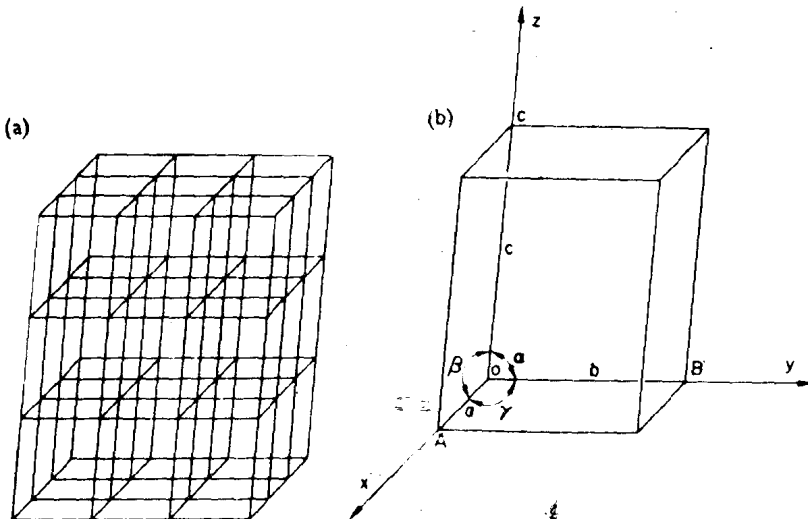

FIG. 1.1. (a) A space lattice, (b) unit cell showing positions of principal axes.

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into equal sized parallelepipeds and the intersection of the lines is called a *space lattice*. Every point of a space lattice has identical surroundings. Each parallelepiped is called a *unit cell* and the crystal is constructed by stacking identical unit cells face to face in perfect alignment in three dimensions. By placing a *motif unit* of one or more atoms at every lattice site the regular structure of a perfect crystal is obtained.

The positions of the *planes*, *directions* and *point sites* in a lattice are described by reference to the unit cell and the three principal axes, x, y and z (Fig. 1.1(b)). The cell dimensions $OA = a$, $OB = b$ and $OC = c$ are the lattice parameters, and these along with the angles $\angle BOC = \alpha$, $\angle COA = \beta$ and $\angle AOB = \gamma$ completely define the size and shape of the cell. For simplicity the discussion will be restricted to cubic and hexagonal crystal structures. In cubic crystals $a = b = c$ and $\alpha = \beta = \gamma = 90°$, and the definition of planes and directions is straight-forward. In hexagonal crystals it is convenient to use a different approach, and this is described in section 1.2.

Any *plane* $A'B'C'$ in Fig. 1.2 can be defined by the intercepts OA', OB' and OC' with the three principal axes. The usual notation (*Miller indices*) is to take the reciprocals of the ratios of the intercepts to the corresponding unit cell dimensions. Thus $A'B'C'$ is given by

$$\left(\frac{OA}{OA'}, \frac{OB}{OB'}, \frac{OC}{OC'} \right)$$

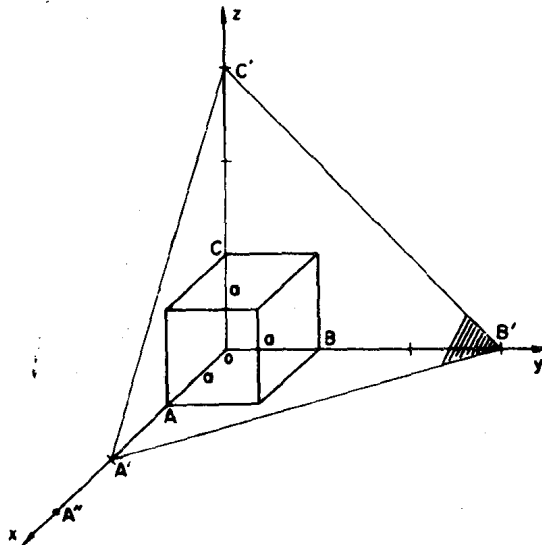and the numbers are then reduced to the three smallest integers in these ratios.

FIG. 1.2. Cubic cell illustrating method of describing positions of planes.

Thus from Fig. 1.2 $OA' = 2a$, $OB' = 3a$, and $OC' = 3a$; the Miller indices of the $A'B'C'$ plane are (322). A plane with intercepts OA, OB, and OC has Miller indices

$$\left(\frac{a}{a}, \frac{a}{a}, \frac{a}{a} \right)$$

or, more simply, (111). Similarly, a plane $DFBA$ in Fig. 1.3 is

$$\left(\frac{a}{a}, \frac{a}{a}, \frac{a}{\infty} \right)$$

or (110); a plane $DEGA$ is

$$\left(\frac{a}{a}, \frac{a}{\infty}, \frac{a}{\infty} \right)$$

or (100); and a plane $AB'C'$ in Fig. 1.2 is

$$\left(\frac{a}{a}, \frac{a}{3a}, \frac{a}{3a} \right)$$

or (311). In determining the indices of any plane it is most convenient to identify the plane of lattice points parallel to the plane which is closest to the origin O and intersects the principal axis close to the origin. Thus plane $A''B'C'$ in Fig. 1.2 is parallel to ABC and it is clear that the indices are (111). Using this approach it will be seen that the planes ABC, ABE, CEA and CEB are (111), ($1\bar{1}\bar{1}$), ($1\bar{1}1$), and ($\bar{1}11$) respectively. In a cubic crystal structure, these planes constitute a group of the same crystallographic type and are described collectively by {111}. The minus sign above an index indicates that the plane cuts the axis on the negative side of the origin.

Any *direction LM* in Fig. 1.3 is described by the line parallel to LM through the origin, in this case OE. The direction is given by the three smallest integers
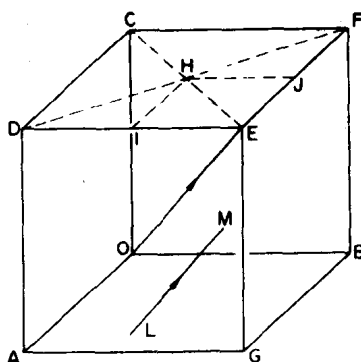

FIG. 1.3. Cubic cell illustrating the method of describing directions and point sites.

in the ratios of the lengths of OE resolved along the three principal axes, namely OA, OB and OC, as a fraction of the dimensions of the unit cell. Thus, if the unit cell is given by OA, OB and OC the direction LM is

$$\left[\frac{OA}{OA}, \frac{OB}{OB}, \frac{OC}{OC} \right]$$

or

$$\left[\frac{a}{a}, \frac{a}{a}, \frac{a}{a} \right]$$

or $[111]$. Square brackets are used for directions. The directions CG, AF, DB and EO are $[11\bar{1}]$, $[\bar{1}11]$, $[1\bar{1}\bar{1}]$ and $[\bar{1}\,\bar{1}\,\bar{1}]$ respectively and are a group of directions of the same crystallographic type described collectively by $\langle 111 \rangle$. Similarly, direction CE is

$$\left[\frac{a}{a}, \frac{a}{a}, \frac{0}{a} \right]$$

or $[110]$; direction AG is

$$\left[\frac{0}{a}, \frac{a}{a}, \frac{0}{a} \right]$$

or $[010]$; and direction GH is

$$\left[\frac{-a/2}{a}, \frac{-a/2}{a}, \frac{a}{a} \right]$$

or $[\bar{1}\,\bar{1}2]$. The rule that brackets $[\ \ ]$ and $(\ \ )$ imply specific directions and planes respectively, and that $\langle\ \ \rangle$ and $\{\ \ \}$ refer respectively to directions and planes of the same type, will be used throughout this text.

In cubic crystals the Miller indices of a plane are the same as the indices of the direction normal to that plane. Thus in Fig. 1.3 the indices of the plane $EFBG$ are (010) and the indices of the direction AG which is normal to $EFBG$ are $[010]$. Similarly, direction OE $[111]$ is normal to plane CBA (111).

Any *point* in a crystal is described by the fractional displacements of the point from the three principal axes relative to the dimensions of the unit cell. The centre of the cell in Fig. 1.3 is $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, and the points F, E, H and I are $0, 1, 1$; $1, 1, 1$; $\frac{1}{2}, \frac{1}{2}, 1$; and $1, \frac{1}{2}, 1$ respectively.

1.2 Simple Crystal Structures

In this section the atoms are considered as hard spheres which vary in size from element to element. From the hard sphere model the parameters of the unit cell can be described directly in terms of the radius of the sphere, r. In the

diagrams illustrating the crystal structures the atoms are shown as small circles in the three-dimensional drawings and as large circles representing the full hard sphere sizes in the two-dimensional diagrams. It will be shown that crystal structures can be described as a stack of atom layers in which the arrangement of atoms within each layer is identical. To see this clearly in two-dimensional figures, the atoms in one layer represented by the plane of the paper are shown as full circles, whereas those in layers above and below the first are shown as small shaded circles. The order or sequence of the atom layers in the stack, i.e. the *stacking sequence*, is referred to by fixing one layer as an *A* layer and all other layers with atoms in identical positions as *A* layers also. Layers of atoms in other positions in the stack are referred to as *B, C, D* layers, etc.

In the *simple cubic structure*, illustrated in Fig. 1.4, the atoms are situated at the corners of the unit cell. Figures 1.4(b) and (c) show the arrangements of atoms in the (100) and (110) planes respectively. The atoms touch along ⟨001⟩
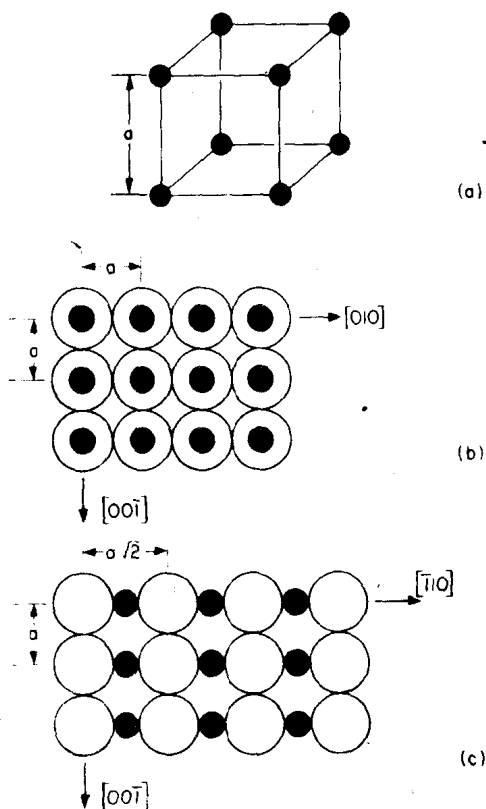
FIG. 1.4. Simple cubic structure: (a) unit cell, (b) arrangement of atoms in (100) layers, (c) arrangement of atoms in (110) layers.

directions and therefore the lattice parameter a is twice the atomic radius r $(a = 2r)$. The atoms in adjacent (100) planes are in identical atomic sites relative to the direction normal to this plane, so that the stacking sequence of (100) planes is AAA . . . The atoms in adjacent (110) planes are displaced $\frac{1}{2}a\sqrt{2}$ along $[\bar{1}10]$ relative to each other and the spacing of atoms along $[110]$ is $a\sqrt{2}$. It follows that alternate planes have atoms in the same atomic sites relative to the direction normal to (110) and the stacking sequence of (110) planes is $ABABAB$ . . . The spacing between successive (110) planes is $\frac{1}{2}a\sqrt{2}$.

In the *body-centred cubic structure* (bcc), shown in Fig. 1.5, the atoms are situated at the corners of the unit cell and at the centre site $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. The atoms touch along $\langle 111 \rangle$ directions and this is referred to as the *close-packed direction*. The lattice parameter $a = 4r/\sqrt{3}$ and the spacing of atoms along $\langle 110 \rangle$ directions is $a\sqrt{2}$. The stacking sequence of $\{100\}$ and $\{110\}$ planes is $ABABAB$ . . . (Fig. 1.5(b)). There is particular interest in the stacking of $\{112\}$ type planes. Figure 1.6 shows two body-centred cubic cells and the positions of a set of $(1\bar{1}2)$ planes. From the diagrams it is seen that the stacking sequence of these planes is $ABCDEFAB$ . . . , and the spacing between the planes is $a/\sqrt{6}$.
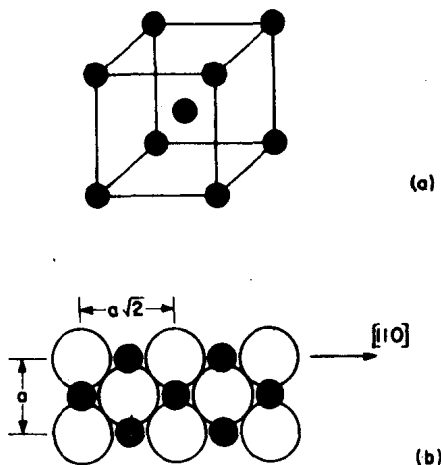

(a)

(b)

FIG. 1.5. Body-centred cubic structures: (a) unit cell, (b) arrangement of atoms in (110) layers.

In the *face-centred cubic structure* (fcc), shown in Fig. 1.7, the atoms are situated at the corners of the unit cell and at the centres of all the cube faces in sites of the type $0, \frac{1}{2}, \frac{1}{2}$. The atoms touch along the $\langle 011 \rangle$ close-packed directions. The lattice parameter $a = 2r\sqrt{2}$. The stacking sequence of $\{100\}$ and $\{110\}$ planes is $ABABAB$ . . . , and the stacking sequence of $\{111\}$ planes is $ABCABC$ . . . The latter is of considerable importance and is illustrated in Figs. 1.7(b) and (c). The atoms in the $\{111\}$ planes are in the most close-packed
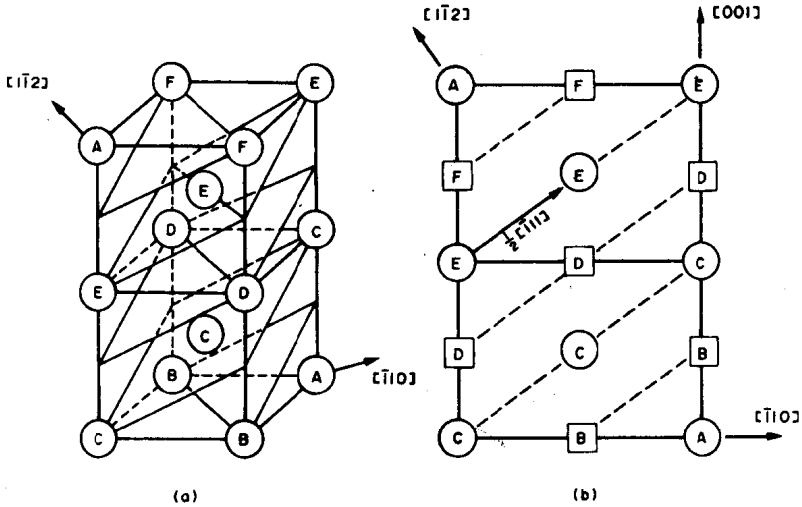
FIG. 1.6. Stacking sequence of {112} planes in a body-centred cubic crystal. (a) Two unit cells showing positions of atoms in (1$\bar{1}$2) planes. (b) Traces of the (1$\bar{1}$2) planes on a (110) projection: atom sites marked by circles lie in the plane of the diagram; those marked by squares lie $a/\sqrt{2}$ above and below.
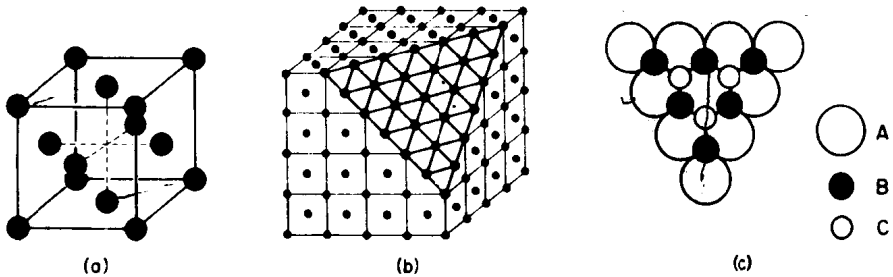

FIG. 1.7. Face-centred cubic structure: (a) unit cell, (b) arrangement of atoms in a (111) close-packed plane, (c) stacking sequence of (111) planes.

arrangement possible for spheres and contain three close-packed directions 60° apart.

The *close-packed hexagonal structure* (cph or hcp) is more complex than the cubic structures but can be described very simply with reference to the stacking sequence. The lattice is formed by the stacking of close-packed planes, as in the face-centred cubic case, but the stacking sequence is now *ABABAB....* In Fig. 1.8(a) an hexagonal lattice has been outlined in an *ABA* stack. The unit cell is outlined more heavily. Atoms are situated at the corners of the unit cell and at $\frac{2}{3}, \frac{1}{3} \frac{1}{2}$ with respect to the axes a_1, a_2, c.

For a hard sphere model the ratio of the length of the c and a axes (axial ratio) of the hexagonal structure is 1.633. In practice, the axial ratio varies