Fifth Edition

Introduction to DISLOCATIONS

D. Hull • D. J. Bacon

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MATERIALS SCIENCE/ENGINEERING

THE classic introduction to dislocations and the role they play in the properties of crystalline solids — as clear and easy to understand as ever, now fully updated with the latest developments and references

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D. Hull and D. J. Bacon
Department of Engineering,
Materials Science and Engineering,
University of Liverpool, UK

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Introduction to Dislocations

Preface

We are delighted to introduce the fifth edition of this book, which was first published in 1965 and has been in press continuously since then. In the Preface to the first edition it was noted that *"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"*. Today the subject is a well-established discipline and is a powerful and essential aspect in understanding of the properties and behavior of crystalline solids.

Much of the basis of the subject, set out in relatively simple terms in the first edition, has been retained in later editions. In each subsequent edition new material has been included to broaden the detail and introduce some key aspects, which have emerged from research, without turning the book into a research monograph. In this latest edition we have taken advantage of recent research, using advanced computer modeling and very high resolution electron microscopy, to provide a better understanding of the arrangement of atoms close to the centre or core of dislocations. It is now clear that the atomic arrangement in the core has a fundamental effect on the behavior of dislocations and thereby on the properties of solids.

The development of this edition has benefited from a worldwide consultation, by the publishers, with leading authorities in the teaching and researching of dislocations. This consultation established that the fourth edition is still widely used in undergraduate and post-graduate university science and engineering courses and research schools. In preparing the fifth edition we have attempted to maintain a balance between a description of the basic properties of dislocations that are taught in introductory undergraduate courses and a more detailed treatment that is required for scientific research.

This distinction depends on the nature of courses and research although we have not attempted to make any delineation within the body of the text. Thus, for example, in Chapter 2, on the observation of dislocations, the simple methods, first developed in early studies, are set alongside the

sophisticated approaches now available to specialists who have access to powerful analytical and experimental techniques, such as high resolution microscopy and codes that exploit the power of current computer systems to simulate dislocations at atomic and continuum scales.

A similar distinction has been made in the selection of further reading lists at the end of each chapter. We have included references to some of the influential papers from the early days of 'dislocations' as well as more recent papers that offer access to frontier research studies and provide an insight into the research now conducted in this field.

We are greatly indebted to friends and colleagues in many different countries who have allowed us access to their work and readily offered help and advice. We are also grateful to our publishers for encouraging us to prepare this new edition and agreeing to produce it in a completely new format.

Liverpool, August 2010

Derek Hull
David Bacon

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CHAPTER 1

Defects in Crystals

1.1 CRYSTALLINE MATERIALS

Dislocations are an important class of defect in crystalline solids and so an elementary understanding of crystallinity is required before dislocations can be introduced. Metals and many important classes of non-metallic 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 relatively simple: the three most common are the body-centered cubic, face-centered cubic and close-packed hexagonal, and 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 formed by three sets of straight, parallel lines as in Fig. 1.1(a). The lines divide space into equal sized parallelepipeds and the points at the intersection of the lines define 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 here 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 straightforward. 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

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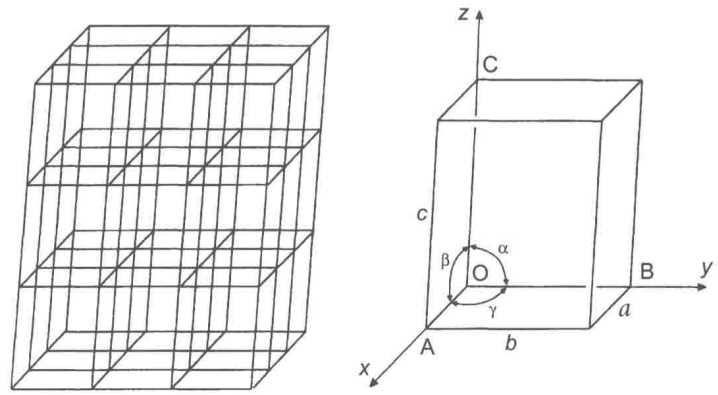

FIGURE 1.1
(a) A space lattice, (b) unit cell showing positions of principal axes.

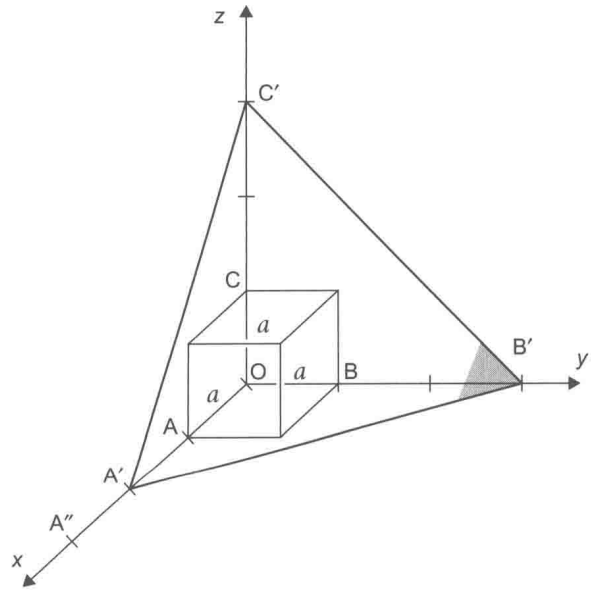

FIGURE 1.2
Cubic cell illustrating method of describing the orientation of planes.

take the reciprocals of the ratios of the intercepts to the corresponding unit cell dimensions. Thus $A'B'C'$ is represented 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.

Thus from Fig. 1.2 $OA' = 2a$, $OB' = 3a$, and $OC' = 3a$, the reciprocal intercepts are

$$\left(\frac{a}{2a}, \frac{a}{3a}, \frac{a}{3a}\right)$$

and so the Miller indices of the $A'B'C'$ plane are (322). Curved brackets are used for planes. 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 in Fig. 1.3 are (111), $(11\bar{1})$, $(1\bar{1}1)$ and $(\bar{1}11)$ respectively. The minus sign above an index indicates that the plane cuts the axis on the negative side of the origin. In a cubic crystal structure, these planes constitute a group of the same crystallographic type and are described collectively by $\{111\}$.

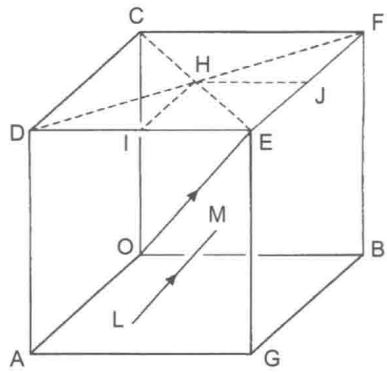

FIGURE 1.3
Cubic cell illustrating the method of describing directions and point sites. *LM* is parallel to *OE*.

Any *direction* LM in Fig. 1.3 is described by the line parallel to LM through the origin O, in this case OE. The direction is given by the three smallest integers in the ratios of the lengths of the projections of OE resolved along the three principal axes, namely OA, OB and OC, to the corresponding lattice parameters of the unit cell. Thus, if the cubic 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 $[11\bar{1}]$, $[\bar{1}11]$, $[\bar{1}1\bar{1}]$ 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

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

or [110]; direction AG is

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

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 ⟨ ⟩ 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).

The coordinates of any *point* in a crystal relative to a chosen origin site are described by the fractional displacements of the point along the three principal axes divided by the corresponding lattice parameters of the unit cell. The center of the cell in Fig. 1.3 is $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ relative to the origin *O*; 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 atomic 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 lattice planes in which the arrangement of lattice sites 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 described by labeling one layer as an *A* layer and all other layers with atoms in identical positions above the first 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* with one atom at each lattice site, illustrated in Fig. 1.4, the atoms are situated at the corners of the unit cell. (Note that no real crystals have such a simple atomic arrangement.) Figures 1.4(b) and (c) show the arrangements of atoms in the (100) and

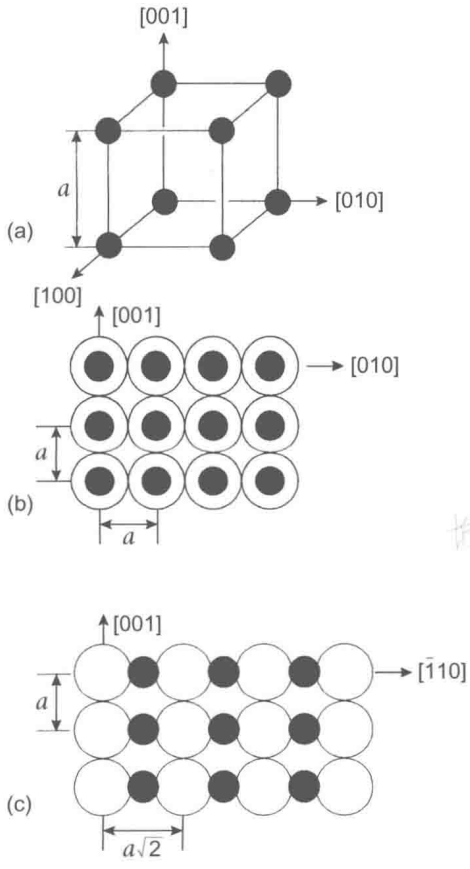

FIGURE 1.4
Simple cubic structure: (a) unit cell, (b) arrangement of atoms in (100) layers, (c) arrangement of atoms in (110) layers.

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