THEORY OF DISLOCATIONS

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PREFACE

This book is based on the lecture notes developed by the authors for courses on the theory of dislocations at Carnegie Institute of Technology, The Ohio State University, and Oslo University. The book is intended to be primarily a comprehensive text in the field of dislocations. For this reason, an exhaustive literature survey has not been attempted, although throughout the book key references are cited.

Within the past decade, studies of dislocations and their effects on material properties have expanded greatly, resulting in the apparent need for a detailed approach to the various problems in the field. We have attempted both to provide sufficient detail that much of the book could effectively be used as an undergraduate text and to extend the treatment of specific problems sufficiently to stimulate the advanced graduate student. As a result, some sections of the book are intended only for advanced students.

The book is comprised of two general groupings. Parts 1 and 2 essentially consider only fundamentals of dislocation theory. These fundamentals are solidly grounded and can be presented without problem. Parts 3 and 4 treat both fundamentals and applications of the fundamentals to the understanding of physical phenomena. Those aspects of the theory which are discussed in detail are well founded. However, the treatment of some subjects, such as work hardening, in the applications section is still moot. In such cases, we have briefly outlined current theories, pointed out their shortcomings, and suggested approaches to a general solution to the problem in question.

Throughout the book, we assume a background in mathematics through differential equations. More advanced mathematical topics are treated in the text. However, in such cases, we have attempted to outline the derivations in sufficient detail for the student to derive them either directly or with the aid of a reference book such as I. S. Sokolnikoff and R. M. Redheffer, "Mathematics of Physics and Modern Engineering," McGraw-Hill, New York, 1966. Because of the variety of topics treated, we have encountered a problem in notation. Rather than use unfamiliar symbols, we have used the same symbol for different quantities in some cases. For example, F denotes both Helmholtz free energy and force, and v denotes both velocity and volume. The context makes the definitions clear.

We are indebted to many authors and publishers for kindly supplying illustrations and permission to publish them; acknowledgements are presented in the figure captions. A number of coworkers and students contributed valuable discussions of the subject matter. We are particularly grateful for the helpful comments of W. R. Bitler, R. Bullough, P. C. J. Gallagher, T. Jøssang, M. H. Loretto, M. J. Marcinkowski, J. Weertman, and C. Wert. Finally, we are happy to acknowledge the support of the research leading to this book by the U.S. Office of Naval Research, by the U.S. Air Force Materials Laboratory, by a Battelle Visiting Professorship at Ohio State University (J. L.) and by a Mershon Travel Grant (J. P. H.).

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PART FOUR. GROUPS OF DISLOCATIONS

1

DISLOCATIONS IN ISOTROPIC CONTINUA

1

INTRODUCTORY MATERIAL

1-1. Introduction

This chapter deals largely with the historical development of the concept of a dislocation. Physical phenomena which led to the discovery of dislocations are discussed, together with early mathematical work which eventually contributed to dislocation theory. Today, of course, there is a large variety of observations which indicate directly the presence of dislocations in crystals; selected examples of these observations are presented. In the final portion of the chapter dislocations are defined formally in terms of their geometric properties. Some simple axioms follow directly from this definition.

1-2. Physical basis for dislocations

Early work

Probably the first suggestion of dislocations was provided by observations[1,2] in the nineteenth century that the plastic deformation of metals proceeded by the formation of slip bands or slip packets, wherein one portion of a specimen sheared with respect to another. Initially the interpretation of this phenomenon was obscure, but with the discovery that metals were crystalline, it was appreciated that such slip must represent the shearing of one portion of a crystal with respect to another upon a rational crystal plane.

[1] O. Mügge, *Neues Jahrb. Min.*, 13 (1883).

[2] A. Ewing and W. Rosenhain, *Phil. Trans. Roy. Soc.*, **A193**: 353 (1899).

Volterra[1] and others, notably Love,[2] in treating the elastic behavior of homogeneous, isotropic media, considered the elastic properties of a cut cylinder (Fig. 1-1*a*) deformed as shown (Figs. 1-1*b* to 1-1*g*). Some of the deformation operations clearly correspond to slip, and some of the resulting configurations correspond to dislocations. However, the relation of the work of the elasticians to crystalline slip remained unnoticed until the late 1930s, after dislocations had been postulated as crystalline defects. Configurations (*b*) and (*c*) in Fig. 1-1 correspond to edge dislocations, and (*d*) corresponds to a screw dislocation. Configurations (*e*), (*f*), and (*g*) are not discussed further here, since they do not correspond to crystalline imperfections; the essential reason for this is that the displacements produced by these configurations are proportional to the outer cylinder radius and hence do not vanish as the radius tends to infinity.

Following the discovery of x-rays and of x-ray diffraction, establishing crystallinity, Darwin[3] and Ewald[4] found that the intensity of x-ray beams reflected from crystals was about 20 times greater than that expected for a beam reflected from a perfect crystal. In a perfect crystal the intensity would be low because of the

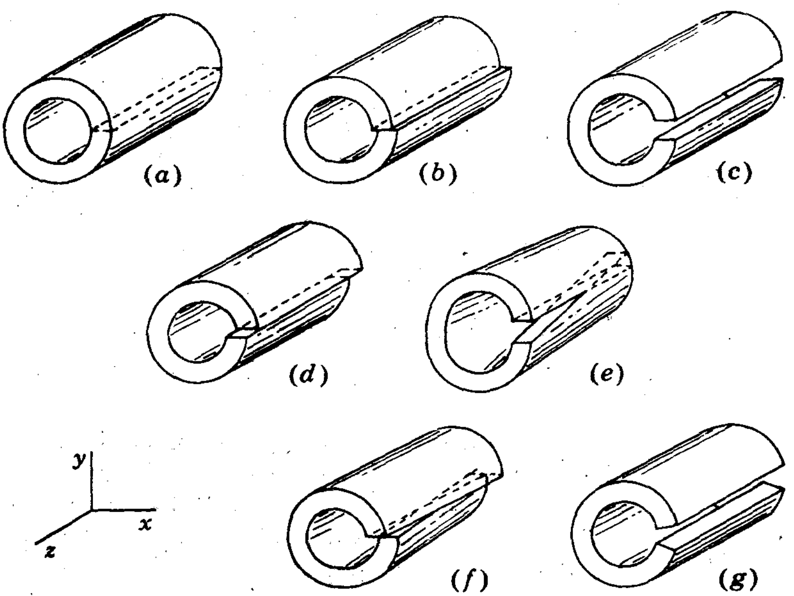

Fig. 1-1. A cylinder (*a*) as originally cut, and (*b*) to (*g*), as deformed to produce the six types of dislocations as proposed by Volterra.

[1] V. Volterra, *Ann. Ecole Norm. Super.* **24**, 400 (1907).

[2] A. E. H. Love, "The Mathematical Theory of Elasticity," Cambridge University Press, Cambridge, 1927.

[3] C. G. Darwin, *Phil. Mag.*, **27:** 315, 675 (1914).

[4] P. P. Ewald, *Ann. Phys.*, **54:** 519 (1917).

long absorption path provided by multiple internal reflections. In addition, the width of the reflected beam was about 1 to 30 minutes of arc, whereas that expected for the perfect crystal was a few seconds. To account for these results, the theory evolved that real crystals consisted of small, roughly equiaxed crystallites, 10^{-4} to 10^{-5} cm in diameter, slightly misoriented with respect to one another, with the boundaries between them consisting of amorphous material.

In this "mosaic-block" theory, the crystallite size limits the absorption path, accounting for the intensity effect, while the misorientation accounts for the beam width. The crystallite boundaries actually consist of arrays of dislocation lines. but this was not appreciated until recent times.

Crystal growth is another area of study implying the presence of dislocations. Volmer's[1] work on nucleation, following the ideas of Gibbs,[2] indicated that the layer growth of perfect crystals should not be appreciable until supersaturations of about 1.5, sufficient for nucleation of new layers, were attained. Experimentally, on the other hand, crystals were observed to grow under nearly equilibrium conditions; see, for example, the work of Volmer and Schultze[3] on iodine. This discrepancy between theory and experiment remained a puzzle until Frank[4] resolved it by postulating that growth could proceed at low supersaturations by the propagation of ledges associated with the point of emergence of a dislocation at a surface.

A number of other cases could be cited. For example, the rapid equilibration of point defects in a crystal subjected to a change in temperature suggests the presence of internal sources and sinks for point defects in crystals. It is now established that dislocations and arrays thereof can provide such sources and sinks.[5] However, these other examples in general either were developed at a later time or were less striking than those cited above, and therefore are not discussed further here.

The final case, involving the consideration of the strength of a perfect crystal, provided the major impetus for the development of dislocation theory, and serves to terminate the early work on dislocations. Because of its importance in stimulating work on dislocations, and because it involves a phenomenological approach which is applicable in many other dislocation problems, this topic is treated in detail in the following section.

[1] M. Volmer, "Kinetik der Phasenbildung," Steinkopff, Dresden and Leipsig, 1939.

[2] J. W. Gibbs, "Collected Works," vol. 1, "Thermodynamics," Yale University Press, New Haven, Conn., 1948.

[3] M. Volmer and W. Schultze, *Z. phys. Chem.*, **156**: 1 (1931).

[4] F. C. Frank, *Disc. Faraday Soc.*, **5**: 48, 67 (1949).

[5] D. N. Seidman and R. W. Balluffi [*Phys. Rev.*, **139**: A1824 (1965)] have shown that dislocations act as vacancy sources in up-quenched gold. On the other hand, R. S. Barnes [*Phil. Mag.*, **5**: 635 (1960)] showed that in α-bombarded copper, helium bubbles did *not* nucleate near single dislocations (vacancies are required for such nucleation), but that vacancies were produced at grain boundaries.

Theoretical shear strength of a perfect crystal

Once it was appreciated that metals were crystalline, interest developed in the computation of the strength of perfect crystals. The classical work in this area was that of Frenkel,[1] whose model for the shear-stress–shear-displacement relation is shown in Fig. 1-2. He supposed that a crystal plastically shearing on a rational plane passed through equivalent configurations with equal energies and with a period equal to b, the magnitude of a simple lattice-translation vector. He thus neglected the small end effects associated with the formation of surface steps by the shear. The applied shear stress required to accomplish a shear translation x is proportional to dW/dx, where W is the energy of translation per unit area of the plane. As a first approximation, Frenkel took the periodicity of the energy to be sinusoidal, so that

$$\sigma = \sigma_{\text{theor}} \sin \frac{2\pi x}{b} \tag{1-1}$$

In the limit of small shear strain x/d, where d is the interplanar spacing, Hooke's law applies in the form

$$\sigma = \mu \frac{d}{x} \tag{1-2}$$

where μ is the shear modulus. Equating (1-1) and (1-2) in the small-strain limit, where $\sin (2\pi x/b) \simeq 2\pi x/b$, one obtains for σ_{theor}, the theoretical shear stress,

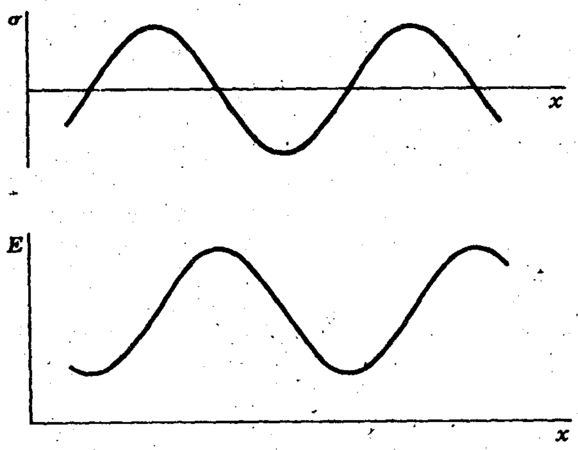

Fig. 1-2. The periodic lattice potential, and the equivalent value of the shear stress, accompanying the shear of a perfect lattice.

[1] J. Frenkel, *Z. Phys.*, 37: 572 (1926).

the value

$$\sigma_{\text{theor}} = \frac{\mu b}{2\pi d} \cong \frac{\mu}{5} \tag{1-3}$$

In marked disagreement with the prediction of Eq. (1-3), the experimental values for the maximum resolved shear stress required to initiate plastic flow in metals were in the range of 10^{-3} to $10^{-4}\,\mu$ at about the time of Frenkel's work.

To digress for a moment, later investigators noted that Eq. (1-3) was probably an overestimate of σ_{theor}, because the various semiempirical interatomic-force laws indicated that the attractive forces decreased much more rapidly with distance than did the sinusoidal force in Fig. 1-2, and because of the possibility of additional minima in the W-x plot corresponding to twin or other special orientations. Mackenzie,[1] using central forces for the case of close-packed lattices, found that σ_{theor} could be reduced to a value of $\mu/30$. This value is likely to be an underestimate, because of the neglect of the small directional forces which are also present in such lattices. Also, the contributions of thermal stresses, treated later in detail, reduce σ_{theor} below $\mu/30$ only near the melting point. Thus at room temperature σ_{theor} should be in the range $\mu/5 > \sigma_{\text{theor}} > \mu/30$, say $\sim\mu/15$. In excellent agreement with this estimate, the maximum values of the resolved shear stress for the initiation of plastic flow in (presumably perfect) whiskers of various metals[2] is $\sim\mu/15$.

Recent experimental work on bulk copper[3] and zinc,[4] on the other hand, indicates that plastic deformation begins at stresses of the order of $10^{-9}\,\mu$. Thus, except for whiskers, the discrepancy between σ_{theor} and experimental values is even larger than was first supposed.

Exercise 1-1. Carry out a calculation, analogous to that of Frenkel, using a Morse function for the interatomic potential. Such functions, given by

$$W = W_0(e^{-2a(r-r_0)} - 2e^{-a(r-r_0)}) \tag{1-4}$$

where W_0 and a are parameters and r_0 is the equilibrium separation of atoms, give good fits to P-V data, compressibility, and elastic constants in fcc crystals.[5] Taking $r_0 \sim b$, the typical value $a = 5/r_0$, and $x \sim r - r_0$, show that the use of Eq. (1-4) in place of Eq. (1-1) gives the

[1] J. K. Mackenzie, unpublished doctoral dissertation, University of Bristol, Bristol, 1949.

[2] S. S. Brenner, in R. H. Doremus *et al.* (eds.), "Growth and Perfection of Crystals," Wiley, New York, 1958, p. 3.

[3] R. F. Tinder and J. Washburn, *Acta Met.*, **12:** 129 (1964).

[4] R. F. Tinder, *J. Metals*, **16:** 94 (1964).

[5] L. A. Girifalco and V. G. Weizer, *Phys. Rev.*, **114:** 687 (1959); **120:** 837 (1960).

result $\sigma_{theor} = \mu b/20d$, and that the maximum stress occurs at $x = 0.138b$ versus $x = 0.25b$ for the case shown in Fig. 1-2. The close correspondence of this result to that of Frenkel demonstrates the reasonableness of the order of magnitude of his estimate of σ_{theor}.

After Frenkel's work, Masing and Polanyi,[1] Prandtl,[2] and Dehlinger[3] proposed various defects which were precursors of the dislocation. For example, the defects proposed by Masing and Polanyi, shown in Fig. 1-3, resemble a polygonized structure of dislocations in a crystal composed of hard atoms bound by weak directional bonds. Finally, in 1934, the edge dislocation, shown in Fig. 1-4, was proposed by Orowan,[4] Polanyi,[5] and Taylor[6] to explain the discrepancy between σ_{theor} and experiment, as discussed above. In 1939, Burgers[7] advanced the description of the screw dislocation, depicted in Fig. 1-5.

Observations of dislocations

In the past two decades an overwhelming number of observations have been made which in summary provide unequivocal evidence of the existence of dislocations in crystals. There is such an abundance of these observations that we can cite only a few examples here. The reader is referred to the reviews of such observations listed at the end of this chapter for an extensive survey.

Figure 1-6, due to Bragg and Nye, shows an edge dislocation in the two-dimensional lattice of a bubble raft. Figure 1-7 depicts a growth spiral associated with a dislocation emergent at its center in *n*-nonatriacontane; the dislocation slipped out of the crystal after growth was completed, leaving behind a slip trace. A similar spiral on a {100} face of silver is shown in Fig. 1-8; in this picture the spiral steps are one atom layer in height and are revealed by decoration and phase-contrast microscopy. Both spirals provide confirmation of Frank's postulate,[8] discussed earlier.

The strain energy of a dislocation often leads to a faster rate of chemical etching at the point of emergence of a dislocation at a free surface, resulting in the formation of etch pits at such points. Similarly, because of the strain energy, dislocations act as catalytic sites for precipitation from solid solution.

[1] G. Masing and M. Polanyi, *Ergeb. exact. Naturwiss.*, **2:** 177 (1923).

[2] L. Prandtl, *Z. ang. Math. Phys.*, **8:** 85 (1928).

[3] U. Dehlinger, *Ann. Phys.*, **2:** 749 (1929).

[4] E. Orowan, *Z. Phys.*, **89:** 605, 634 (1934).

[5] M. Polanyi, *Z. Phys.*, **89:** 660 (1934).

[6] G. I. Taylor, *Proc. Roy. Soc.*, **A145:** 362 (1934).

[7] J. M. Burgers, *Proc. Kon. Ned. Akad. Wetenschap.*, **42:** 293, 378 (1939).

[8] F. C. Frank, *Disc. Faraday Soc.*, **5:** 48, 67 (1949).