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Dislocations and stacking faults

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Abstract. The properties of linear defects in crystals (dislocation lines) and of planar defects (stacking faults) are important in almost every branch of solid state physics. This article is intended to give a comprehensive introduction to dislocation theory for the physicist who is not a specialist in crystal plasticity. It begins with a survey of the established theory relating to the geometrical and topological properties of dislocations, the elastic theory of dislocations in a continuum, the

atomistic or core properties of dislocations, and the dynamics of moving dislocations. General methods for finding the elastic field of an arbitrary dislocation loop are outlined, and the results of some recent calculations using anisotropic elasticity are summarized. These include the prediction, partially confirmed by experiment, that dislocations in certain ranges of orientation may have negative line tension. The current importance of atomistic calculations of core structure and related problems is emphasized, and the methods available for these calculations are discussed.

More detailed descriptions of dislocation and stacking fault configurations are given for some of the common crystal structures, and recent work on complex defects resulting from vacancy aggregation in close-packed structures is included. The experimental and theoretical evidence for the recent conclusion that screw dislocations in body-centred cubic metals have an asymmetric core is also reviewed.

The rather controversial theory of thermally activated dislocation motion is described in a separate section, and examples are given of the application of this theory to various models of the obstacles encountered by moving dislocations. The final section is concerned with the theory of dislocations in grain boundaries and interphase boundaries, and includes the concept of the surface dislocation tensor.

1. Geometrical properties of dislocations

1.1. Introduction

The theory of dislocations has two starting points. The concept of the dislocation as an elastic singularity was first introduced by considering the deformation of a body occupying a multiply connected region of space, and a systematic theory was given by Volterra (1907), following earlier work by Michell (1900), Weingarten (1901) and Timpe (1905). Volterra described the conditions under which the displacement function is continuous but multivalued (or single-valued but discontinuous), and Love (1920) gave an account of this work in his famous treatise on elasticity. The word dislocation in English is due to Love, who referred to Volterra's "distorsioni" and remarked "I have ventured to call them dislocations".

Somigliana (1914, 1915) developed further the elastic theory of dislocations, but the relation of this work to the structure of real crystals was not perceived until much later. When x-ray diffraction techniques were used to examine crystals, it very soon became evident that most real crystals have imperfect structures (Darwin 1914, 1922). In principal, crystal dislocations might then have been postulated to explain the observed magnitudes of the diffracted intensities, but in fact the model of the mosaic structure used in Darwin's paper became the generally accepted crystallographic description, and the problem of the structure of the boundaries between misorientated regions was not pursued. The first suggestions that dislocations exist in real crystals thus arose not from direct observations on structure but in order to interpret experiments on the plastic behaviour of crystals.

Crystalline defects similar to dislocations were discussed by Prandtl (1928) and Dehlinger (1929) as a possible explanation of the large discrepancy between the theoretical and experimental strength of a crystal. The real introduction of the dislocation into physics came a few years later, when edge dislocations were described by Taylor (1934), Orowan (1934) and Polanyi (1934); these papers form the second starting point for dislocation theory. Screw dislocations and dislocations of general type were first considered by Burgers (1939), and his classic papers mark the beginning of the systematic development of the theory. Other important publications at this time include the Peierls-Nabarro calculation of the stress

needed to move a dislocation (Peierls 1940, Nabarro 1947), and the first demonstration that low-angle grain boundaries may be regarded as planar arrays of dislocations (Bragg 1940, Burgers 1939).

The progress of dislocation theory since 1945 has been too rapid to permit of any short historical summary, but for many years the existence of dislocations was disputed by some physicists and metallurgists. The discoveries of experimental techniques for the observation of dislocations should thus be accorded particular significance in the development of the subject. Such techniques were reviewed by Pashley (1965).

A dislocation is (macroscopically) a linear defect, whilst a stacking fault is a planar defect. Stacking faults in layer structures and the associated x-ray diffraction effects were considered by Landau (1937) and Lifschitz (1937). The work of Edwards and Lipson (1942) and Wilson (1942) first showed that such faults are formed in pure cobalt, and hence that in principle they may exist in all metals with close-packed structures. These early studies were concerned with unbounded stacking faults, but Heidenreich and Shockley (1949) and Frank (1949) realized that faults may end within a crystal. The edge of a fault or the junction of two different faults is generally called a partial dislocation. Frank (1951 b) and Frank and Nicholas (1953) classified the various types of dislocations and stacking faults and listed those dislocations expected to occur in the common crystal structures.

Authoritative reviews of the mathematical theory of dislocations have been published by (*inter alia*) Nabarro (1952), Seeger (1955 a, 1958), Eshelby (1956 a), Indenbom (1958 a), de Wit (1960) and Mura (1969), and well known books on dislocation theory include Cottrell (1953), Read (1953), Friedel (1956, 1964) and Kröner (1958). Work on stacking faults has been reviewed by Christian and Swann (1965) and Saada (1966). Finally, two recent textbooks (Nabarro 1967, Hirth and Lothe 1968 a) provide a comprehensive description of most aspects of dislocation theory. In the present survey we shall not attempt a complete coverage of this now very large branch of solid state physics, and we have no illusions that we can substantially improve on the existing excellent accounts. Our two more modest aims are firstly to provide an up-to-date introduction to the subject written especially for the physicist who may not be interested in the details of (say) deformation theory, and secondly to attempt to highlight the more important recent developments and the probable direction of research in the next few years.

1.2. *Burgers vector and Burgers circuit*

A simple dislocation line in an elastic continuum is obtained by cutting the continuum along any surface which terminates on the line and giving the two cut surfaces a relative displacement before joining them together again. In order to avoid infinite stresses, it is necessary to bore a small hole along the termination of the cut, and material may have to be added or removed near the cut to allow the surfaces to be rejoined. Suppose the cut is made along a planar surface terminating in a straight line, and that this line and the normal to the surface are used to define an orthonormal coordinate system. Fixed vector translations of the cut surfaces parallel respectively to the three axes of this system then define the three simplest types of Volterra dislocation, and these dislocations have exact analogues in crystals. When the displacement is parallel to the line, the result is a screw dislocation. The other two translations are both perpendicular to the line and produce (equivalent)

edge dislocations. A straight dislocation of general (or mixed) type is obtained by combining these operations, so that the fixed translation of the surfaces has components both parallel and normal to the line.

A dislocation line curved in a plane or in three dimensions may be introduced in the same way, and either extends from one point on the external surface of the continuum to another or forms a closed loop in the interior. The removal of the thin cylinder along the edge of the cut illustrates that a dislocation may strictly be introduced only into a multiply connected continuum, and the virtual cuts then all terminate on surfaces of this body. The characteristics of a simple Volterra dislocation are determined by the relative displacement of the two cut surfaces, which defines the Burgers vector, and by the termination of the cut; the particular surface over which the cut is made has no significance.

Since the dislocation line has been introduced as the edge of a surface, it can terminate internally only by closing on itself or by meeting some other dislocation line. Suppose two cuts are made so that the edge of each shares a common portion with that of the other. After displacing the surfaces, it is found that three dislocation lines radiate from the point where the common edge ends, and the Burgers vector of the common edge is obtained from the vector sum of the two individual translations. Such an internal point at which three or more dislocation lines meet is called a dislocation node.

Volterra also considered three other types of 'dislocation' in which the two parts of the continuum on each side of the cut are given a relative rotation before rejoining. Following a suggestion by Frank, Nabarro (1967) uses the term 'disclination' for a line singularity of this type. The elastic strains in a medium are large at large distances from a disclination, so that such defects are not expected in solid real crystals, although they occur in some liquid crystals (e.g. Kléman and Friedel 1969). However, it is possible to envisage disclinations in internally stressed crystals of finite size, provided that planar discontinuities are also introduced. Thus, if a low-angle grain boundary terminates within a crystal, the edge of the boundary is topologically a disclination. A low-angle boundary may be regarded as an array of line dislocations (see later), and a disclination is then a discontinuity in the regular dislocation array.

Somigliana introduced a more general class of dislocation by allowing elastic distortions of the cut surfaces in addition to relative translations or rotations. The resulting defect has a variable vector translation over the cut surface and may be regarded as arising from a continuous distribution of simple Volterra dislocations.

Now consider the introduction of a simple dislocation line into a crystal instead of a continuum. If the same virtual process is used, material need not be removed along the dislocation core, but the atomic displacements in this region cannot be treated by elastic theory. Also, if the cut surfaces are to be rejoined without introducing a fault, the relative translation must be a repeat vector of the Bravais lattice.

A more formal definition of the Burgers vector invokes the concept of corresponding paths in the real crystal and in a defect-free reference crystal (Frank 1951 a). Regions of the real crystal are described as 'good' if the positions of the atoms in any small volume may be unambiguously related to those of the atoms in a reference crystal by means of displacements which are small fractions of interatomic distances. There is then a local one-to-one correspondence between the real and reference crystals, and any path composed of successive interatomic vectors in good crystal may be associated uniquely with a corresponding path in the

reference crystal. In some regions of real crystal, for example near the core of a dislocation line, the local correspondence is no longer unique. These regions are described as 'bad' crystal. The theory of linear elasticity cannot be applied to regions of bad crystal.

If a closed circuit is made in either the real or the reference crystal, the corresponding path in the other crystal will not, in general, be closed, and the closure failure is defined as the net Burgers vector of the dislocation lines which thread through the circuit in the real crystal. Consider first that the circuit encloses a single dislocation line. The sign of the Burgers vector is not defined until a positive direction has been (arbitrarily) assigned to the line, and even then either of two opposite conventions may be used. If a path S'F' in the real crystal forms a right-handed closed circuit around the positive direction of the line, a convention sometimes known as FS/RH (Bilby *et al.* 1955) identifies the Burgers vector with the displacement from the finish (F) to the start (S) of the associated path in the reference crystal. Note that the Burgers vector would be reversed in sign if (i) the circuit were left-handed, (ii) the closure failure SF were used in the definition, or (iii) the circuit were closed in the reference system. Any one of these would define an opposite convention, so $FS/RH \equiv SF/LH \equiv F'S'/LH \equiv S'F'/RH \equiv -F'S'/RH$, etc. With any convention, a reversal of the sign of the positive direction of the line also reverses the Burgers vector. Two dislocation lines which can mutually annihilate may be regarded as parallel lines with opposite Burgers vectors, or as anti-parallel lines with the same Burgers vector. A closed dislocation loop is composed of opposite elements; it is usually most convenient to define the positive direction of any element by traversing the loop in a given sense, so that the sign of the Burgers vector is constant round the loop.

A slight difference between the FS/RH and the S'F'/RH conventions should be noted, since it may be important in some circumstances. The vector FS is a repeat vector of the (ideal) Bravais lattice and is independent of the circuit chosen. However, the vector S'F' differs slightly from FS because of the displacements in the real crystal, and it thus varies spatially with the starting point S'. Thus the closure failure in the real crystal strictly defines a *local Burgers vector* (Bilby and Smith 1956). In this review the FS/RH convention will be used, except where it is necessary to refer explicitly to the local Burgers vector.

Any two circuits which may be continuously transformed into each other by adding atomic translations entirely in good crystal have the same closure failure. It follows that Burgers vectors are conserved at a node, so that if the positive directions of the n dislocation lines of Burgers vectors b_i meeting at a point are either all inwards towards or all outwards from the node, then

$$\sum_{i=1}^n b_i = 0. \quad (1.1)$$

1.3. Stacking faults and partial dislocations

In an isotropic elastic continuum, the cut surface used to introduce a Volterra dislocation or disclination cannot be distinguished after completion of the virtual operations. This is true of a defect in a real crystal only if the net displacement of a point or the net rotation of a vector respectively when carried around a circuit corresponds to a symmetry operation of the lattice. The Burgers vector of a normal lattice dislocation must thus be a repeat vector of the Bravais lattice, and the

rotation associated with a complete disclination is restricted to integral multiples of $2\pi/S$ when the axis of this rotation is an S -fold symmetry axis. Crystallographically possible disclinations thus have large strengths and do not occur in real crystals. However, if a surface across which a discontinuous orientation change takes place is associated with the disclination, the amount of rotation may be made indefinitely small. The defect should then perhaps be called a partial disclination, by analogy with the corresponding situation in which a surface of discontinuity in displacement ends within the crystal. This latter situation is important in dislocation theory.

Consider a crystal which is cut into two along a planar surface, and the two halves are given either a relative translation f or a relative rotation \mathbf{R} before being rejoined (material is added or removed as necessary in the rejoining operation). The resulting planar defect may be described as a generalized stacking fault in the first case and as a generalized grain boundary in the second case. If the translation or rotation is a symmetry operation, the surface defect vanishes; the situations of physical interest arise when this condition is not satisfied but when the specific free energy of the defect is nevertheless not unduly large. The rotation matrix used to describe the misorientation across a particular grain boundary is not unique but may be taken as any one of a set of values $\mathbf{R}_1 + \bar{\mathbf{R}}$ where \mathbf{R}_1 is any matrix of the set and $\bar{\mathbf{R}}$ is any symmetry operation of the lattice. Similarly, a stacking fault may be described by a set of translation vectors $f_1 + \mathbf{u}$ where f_1 is any vector of the set and \mathbf{u} is any vector of the Bravais lattice.

Grain boundaries of low energy are obtained if the relative rotation is simply related to a symmetry operation and to the boundary itself. In particular, a rotation of π about an axis either in the plane of the boundary or normal to this plane produces a low-energy coherent twin interface at which the lattices match exactly.

The plane of a stacking fault automatically has an equal arrangement of lattice points in each half crystal, and is thus closely related to a coherent twin boundary; Frank (1951 a) suggested the alternative term 'translation twin'. Frank also distinguished between intrinsic faults, in which the atomic arrangement of each half crystal extends to the composition plane, and extrinsic faults with at least one atomic plane which does not fit on to either lattice. One way to form an intrinsic fault is thus to remove a layer of material from an unfaulted crystal, and an extrinsic fault may similarly be created by inserting an additional layer of material. Corresponding physical processes are the assembling of point defects (vacancies or interstitials respectively) into sheets parallel to the fault plane. The displacement f is then normal to the plane of the fault, and if the spacing of the lattice planes is not changed, f is a rational fraction of the lattice repeat vector normal to the fault. Intrinsic faults and some extrinsic faults may also be produced by non-lattice translations within the plane of the fault, and hence physically by deformation processes. Once again the usual description of faulting begins with the assumption that f is a simple fraction of a lattice vector in the fault plane.

Faulting in simple close-packed structures, such as those which occur in many metals and solid rare gases, is generally described in terms of a hard sphere model. The possible structures correspond to the stacking of parallel hexagonal nets of atoms in three relative positions (A, B, C) where B and C are displaced from A by translations $\pm f$ within the plane of the net, and $\pm 3f$ is a vector of the Bravais lattice. The two commonest structures (see figure 1) are formed by repetition of the sequences ...ABC... (face-centred cubic (fcc) structure) and ...AB... (hexagonal close-packed (hcp) structure), and f is then a vector of type $\frac{1}{6}a\langle 2\bar{1}\bar{1}\rangle$ in the {111}

planes of the fcc structure, or of type $\frac{1}{3}a\langle 10\bar{1}0 \rangle$ in the $\{0001\}$ planes of the hcp structure. The translations $+f(A \rightarrow B, B \rightarrow C, C \rightarrow A)$ and $-f(B \rightarrow A, A \rightarrow C, C \rightarrow B)$ are also often represented by operator symbols Δ and ∇ , so that repeated application of the operator Δ produces the fcc structure and of the operator $\Delta\nabla$ produces the hcp structure. Repeated application of ∇ (i.e. a stacking sequence ...ACB...) produces a fcc structure which is a twin of the ...ABC... structure (see Saada (1966) or Christian and Swann (1965) for more details).

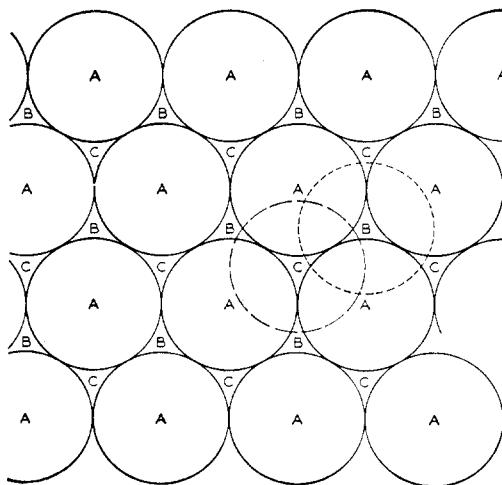


Figure 1. The hard sphere model of the fcc and hcp structures. Close-packed planes may be stacked in relative positions A, B, C, which differ by translations $\pm f$ within the planes.

The possible stacking faults of these two structures are now classified by making the assumption that successive planes remain in relative Δ or ∇ type sequences. A fault is most simply described by the number of wrong operations; for example a sequence ...ABABACBABA... represents an extrinsic 3∇ fault in the hcp structure since the sequence includes successive operations ... $\Delta\nabla(\nabla\nabla\nabla)\Delta\nabla\dots$. There are two basic faults, one intrinsic and one extrinsic, in the fcc structure and three faults, two intrinsic and one extrinsic, in the hcp structure. In both structures, faults of type Δ are completely equivalent to faults of ∇ type, and the two are interchanged by a different choice of axes. The main faults in the two structures are listed in table 1; obviously, multilayer faults could also be defined without limit, but these are best regarded as clusters of simpler faults. An alternative classification in table 1 is based on possible mechanisms for fault formation, either by mistakes in the deposition of successive atomic layers (growth faults) or by glide deformation. Growth faults in fcc structures are really twin boundaries, but it is often convenient to regard a finely twinned structure as 'faulted'. Similarly a fcc twin may be regarded as a series of 1∇ faults on successive atomic planes.

The operator notation removes the arbitrary labelling of the plane positions, but continues to assign a sense to the stacking order, so that a fcc crystal and its twin are distinguished from each other. For some purposes this is unnecessary, and it may be convenient to use configuration symbols (Jagodzinski 1949) in which each fault has a single representation. The symbol C represents three layers in cubic pattern, i.e. $\Delta\Delta\equiv\dots ABC\dots$ or $\nabla\nabla\equiv\dots ACB\dots$, and the symbol H represents three layers in

hexagonal pattern, i.e. $\Delta \nabla \equiv \dots ABA \dots$ or $\nabla \Delta \equiv \dots ACA \dots$. The perfect cubic and hexagonal structures are represented by repetitions of C and H, and as in the operator notation a fault is described by the way in which this pattern is interrupted (see table 1).

Table 1. Stacking faults in closed-packed structures

Structure	Operator symbol	Configuration symbol	Stacking sequence	Intrinsic (I) or extrinsic (E)	Other classification
fcc + twin	—	H	...ABCABACBAC...	—	Growth or twin
fcc	1∇	HH	...ABCABABCAB...	I	Deformation
fcc	2∇	HCH	...ABCABACABC...	E	Double deformation
fcc	3∇	HCCH	...ABCABACBCA...	E	Three-layer twin
fcc	4∇	HHH	...ABCABACBABC...	E	Four-layer twin
hcp	1∇	C	...ABABACACAC...	I	Growth
hcp	2∇	CC	...ABABACBCBC...	I	Deformation
hcp	3∇	CCC	...ABABACBABA...	E	—
hcp	$(1\nabla\Delta)$	CHC	...ABABACABAB...	E	—

The assumption that f is a rational fraction of a lattice vector implies that such a configuration will have a low energy relative to neighbouring configurations with slightly different f -vectors. Models of stacking faults as monolayer twins, or as thin layers of another phase, support this conclusion, but it can only be justified in detail by calculations of the relative energies of various configurations. Recent work by Vítek (1968) shows that whilst the assumption is a good approximation for the close-packed structures, it probably fails completely for the bcc structure.

Vítek defines the generalized intrinsic† fault by a vector

$$\mathbf{f} = x\mathbf{a}_1 + y\mathbf{a}_2 \quad (1.2)$$

where $\mathbf{a}_1, \mathbf{a}_2$ are the two shortest vectors which characterize the fault plane and $0 \leq x, y \leq 1$. The energy $\gamma(x, y)$ has absolute minima at $x = y = 0$, and possibly minima relative to all neighbouring configurations at other values of x and y . The fcc 1∇ faults and the hcp 2∇ faults correspond to metastable configurations of this type. A structure cannot form large stacking faults on any plane for which such relative minima do not exist, since such faults would be mechanically unstable.

The previous discussion shows that if a stacking fault ends within a crystal, its edge may be considered to be a dislocation of Burgers vector f . Since f is not a lattice vector, the dislocation is called a partial dislocation, and all partial dislocations are attached to at least one fault surface. When two faults represented by f_1 and f_2 meet along a line, this line is also a partial dislocation of Burgers vector $f_1 + f_2$. An important configuration is the intersection of two faults on non-parallel lattice planes. The straight-line defect in which they meet is then called a stair-rod dislocation.

The Burgers vector of the partial dislocation at the edge of a particular fault may be any one of the set of vectors $f_1 + u$. Since the configuration at the edge is dependent on u , the fault may be bounded in different ways, each described by a characteristic Burgers vector f . In some structures, however, a dislocation of particular Burgers vector may bound faults of different types. Thus a full description

† Strictly, generalized shear fault might be a preferable term since Vítek's use of 'intrinsic' differs somewhat from Frank's. Thus a hexagonal 1∇ fault is an intrinsic fault in Frank's terminology but involves an f -vector which is not in the plane of the fault.

of partial dislocations may require a specification of both Burgers vector and fault type.

Antiphase boundaries (APBs) in ordered, superlattice structures are stacking faults of a special type, in which the displacement vector is a lattice vector of the disordered Bravais lattice, but not of the superlattice. The transition disordered → ordered generally results in a lowering of symmetry, an increase in the size of the primitive unit cell and an increase in the lattice periodicity in some directions. A lattice vector of the disordered structure may thus correspond to some fraction of a lattice vector after ordering, and a dislocation of this Burgers vector will then become a partial and will be attached to a surface of discontinuity in the occupancy of sites. The displacement vector may lie either in or out of the plane of the APB, and these two possibilities are sometimes called APBs of types 1 and 2.

A Burgers circuit may be used in the formal definition of the Burgers vector of a partial dislocation, but this circuit must now intersect the stacking fault. Since this is strictly a region of bad crystal, a rule is required to avoid possible ambiguity in the associated paths at this point (Frank 1951 a).

1.4. Dislocation motion and dislocation sources

Consider a Volterra dislocation which is continuously displaced from an initial position to a final position. The trajectory of each line element defines an element of surface, and the movement may be represented by cutting the body along the surface linking initial and final positions, displaying the cut faces by the Burgers vector, and rejoining. No material will have to be added or removed from the body during this virtual operation provided the Burgers vector is everywhere contained in the surface to be cut. This conservative motion is described as dislocation glide, and the surface is called the virtual glide surface. If the dislocation is a straight line, or is curved only in a plane containing \mathbf{b} , the glide surface becomes a glide plane. Screw dislocations may move conservatively in any plane, so that so long as they retain their screw character they have no unique glide surface.

Dislocation glide has the property that the projected area of a dislocation loop on a plane normal to \mathbf{b} remains unchanged. When this condition is not fulfilled, material must be added or removed as the dislocation moves, and the motion is described as dislocation climb. It may only be accomplished in a crystal by diffusion of point defects (vacancies or interstitials) to or from the moving line, and the volume of material added or removed is given by the product of \mathbf{b} and the change in the projected area.

Under the action of an applied shear stress, dislocation glide on the virtual glide surface will generally increase the total length of dislocation line. In particular, loops lying in a slip plane will expand until halted by interaction with other defects, or until they reach the edges of the crystal plane. During plastic deformation, large amounts of slip occur on single planes or closely spaced groups of planes, and the dislocation density increases rapidly. This requires the existence of dislocation 'sources' within the crystal. Dislocations have energies of order 5–10 eV per atom plane, so that homogeneous nucleation of dislocation loops by external stresses plus thermal fluctuations is most improbable unless the stresses approach the theoretical shear strength of the lattice. Thus, dislocation sources are configurations of existing dislocations which enable the length of dislocation line to be increased gradually and continuously.

Figure 2 shows in (a) a dislocation line lying in a glide plane, but leaving this plane at points A and B. If these points are now fixed, the dislocation can bow out under the action of a shear stress and adopt the successive configurations shown in (b)–(f). Eventually a closed dislocation loop is produced, and a line element AB remains available to repeat the whole process. The extra energy of dislocation line created has to come from the work done by the applied stress field. The operation of the source is opposed by the line tension of the dislocation, and if the material is isotropic the critical stage is approximately that shown in figure 2(c), where the radius of curvature is a minimum.

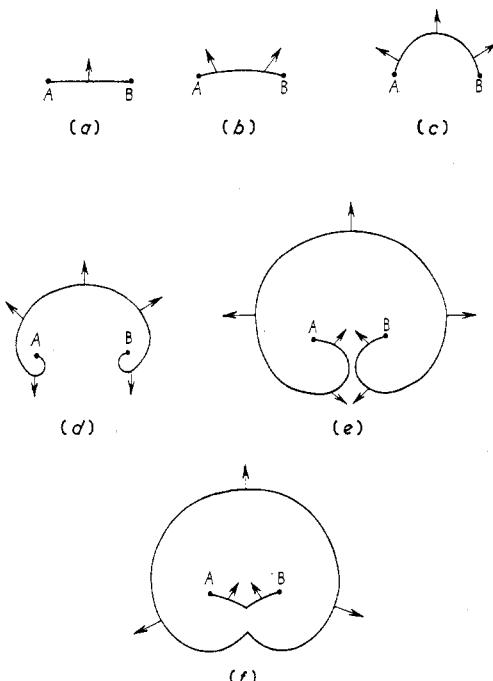


Figure 2. Successive stages in the operation of a double-ended Frank-Read source.

The configuration shown in figure 2 is known as a double-ended Frank-Read source (Frank and Read 1950). A single-ended source leaves the glide plane at only one point A, and the other end of the dislocation is on the surface of the crystal. The dislocation in the glide plane rotates about A, and since its linear velocity is initially nearly constant, a straight line soon adopts a spiral configuration. The equilibrium spiral rotates with uniform angular velocity, and the displacement across each part of the glide plane is increased by b for each complete revolution.

The points A and B of figure 2 could simply represent places where the dislocation turns out of the glide plane, but it is more probable that they are nodes of a dislocation network. If there are no nodes, the dislocation may leave the glide plane at A and B on the same or on opposite sides. In the former case, the configuration remains unchanged even after many loops have been emitted, and Orowan (1954) called this a U-mill. With the other type of source (a Z-mill), B is displaced relative to A by the Burgers vector b for each loop emitted. This implies a steady increase or decrease in the stress needed to operate the source, as the distance AB decreases or increases.

When A and B represent nodes, the geometrical action of the source requires that the new dislocations formed at the nodes do not lie in the glide plane. However, provided that equation (1.1) is satisfied, the new Burgers vectors need not be confined to the glide plane; for example, emerging dislocations at A may have equal and opposite components normal to the glide plane. The rotating dislocation is then displaced upwards or downwards through this distance for each rotation, so that the node is also displaced. Thus, dislocations are generated successively on a uniformly spaced series of lattice planes. The direction of displacement depends on the sense of rotation, and hence on the applied stress. Bilby (1955) used the term "cone source" for this configuration.

A slight modification to the Frank-Read mechanism is the double cross-slip source (Koehler 1952, Johnston and Gilman 1960). A screw dislocation which is halted in the primary glide plane cross-slips on an intersecting plane over part of its length AB to a new position A'B'. The edge elements AA', BB' can glide only in the cross-slip plane, but the screw element A'B' can cross-slip again into a plane parallel to the original glide plane. If A' and B' are immobile, for example because the edge elements are unable easily to glide, the segment A'B' may bow out in the parallel primary plane and act as a Frank-Read source. After a few turns, the process might again be repeated; there is considerable experimental evidence for this type of source.

An analogous topological configuration can lead to unlimited dislocation climb. In figure 2, AB is now a dislocation with its Burgers vector inclined to the plane of the figure. If the dislocation climbs by absorption or emission of point defects, it passes through the various configurations shown, and eventually a closed loop of prismatic dislocation is formed. As this grows outwards it either adds or removes a complete plane of material of thickness equal to the component of the Burgers vector normal to the plane of the source, whilst the element AB can repeat the whole process. This is known as a climb source or Bardeen-Herring source (Bardeen and Herring 1952) and may be regarded as a mechanism for internal crystal growth or dissolution very similar to Frank's crystal growth mechanism (Frank 1949) at a free surface.

Climb of a long dislocation of mixed character fixed at its ends may lead instead of coplanar loops to a single spiral or double spiral configuration, and by glide movements of the loops along the virtual glide surface, helices may be produced (Amelinckx *et al.*, 1957). In the limit helices may also form by the condensation of defects on pure screw dislocations. The point defects may be supposed to collapse in disks to give edge loops normal to the dislocation line, and the interaction of the screw with these disks then produces the helix. In this sense, a screw dislocation can climb, although immediately it does so it ceases to be a pure screw. Various mechanisms, e.g. the glide of the end portion of a helix, will lead to the production of a series of closed loops of dislocation aligned along a direction which is inclined to the plane of the loops. Dislocation lines of these general forms were discussed by Seitz (1952) and termed spiral prismatic dislocations; they are often observed in ionic crystals and in alloys which have been quenched to produce a supersaturation of vacancies, but they are uncommon in pure metals.

The atomic mechanism of climb requires that dislocation lines are not confined to single slip planes but contain steps where they move from one plane to a neighbouring plane. These steps are called elementary jogs and are believed to be the favourable sites for emission or absorption of point defects. If the local deviation

from equilibrium is sufficiently large, the jogs may themselves be created by homogeneous nucleation of jog-pairs, and Thomson and Balluffi (1962) believe that this is important under a wide range of conditions. Jogs may also be created by dislocation glide processes. If two dislocation lines of Burgers vectors \mathbf{b}_A and \mathbf{b}_B glide through each other, the two parts of each line separated by the point of intersection are given a relative displacement equal in length and magnitude to \mathbf{b}_B , and *vice versa*.

Suppose that line B is fixed and that line A glides through it. The jog in A can continue to move conservatively if the Burgers vector \mathbf{b}_A is contained in the slip plane of the jog. An edge dislocation gliding through another dislocation will always acquire a glissile jog, but if two perpendicular screw dislocations glide through each other, each acquires an edge jog. An edge jog in a screw dislocation can glide conservatively only along the dislocation line, so that if the screw dislocation continues to glide and drags the jog with it, a row of vacancies or interstitials must be trailed behind by the climb of the edge jog (Seitz 1952). A jog which has edge character in a general dislocation line is also unable to move conservatively if it is fixed in position along the line, but Seeger (1955 b) pointed out that it may glide in a slip plane which is not normal to the dislocation line. This requires the jog to move along the line, as the line itself moves forwards.

Accumulation of elementary jogs might lead to formation of superjogs which are many times larger than the interplanar spacing of the slip planes. Another way of forming superjogs is by the cross glide of part of a screw dislocation, which might arise for example from elastic interactions with other dislocations (Bullough and Sharp 1965). A long sessile jog will be held back when the rest of the dislocation glides, and this leads to the production of an edge dislocation dipole. Eventually the dipole may be pinched off by the cross glide of one of the parts of the original dislocation, so as to leave a closed prismatic loop. For elementary jogs of only one or two Burgers vector in height, there is no distinction between the model of a dipole (with overlapping cores) and a row of point defects; when the separation of the two parts of the dipole is reasonably large it may be alternatively regarded as a collapsed area of point defects.

Two final types of dislocation motion should be mentioned. Glide of a dislocation loop along its virtual glide surface with no change in its length does not relieve an external shear stress, but displaces the material inside the virtual glide surface relative to that outside it, as in prismatic punching. Displacement of a prismatic loop along the surface normal to \mathbf{b} without changing its size is equivalent to a bodily motion of the collapsed disk of vacancies or interstitials, and is accomplished by the diffusion of point defects from one part of the loop to the other. This is known as conservative climb, and was first observed in zinc by Kroupa and Price (1961).

2. The continuum theory of dislocations

2.1. Introduction

The continuum analogue of a crystal with defects is an elastic body with internal sources of stress which are capable of motion. As described in §1.2, some core regions must be excluded because the continuum approach fails, but this can often be allowed for by an appropriate choice of parameters in the elastic solution. Although the continuum should strictly have the elastic properties of the real crystal, it is often convenient to suppose it to be elastically isotropic; anisotropic

effects are discussed in § 2.9. Let σ_{ij} and e_{ij} be the components of the stress and strain tensors respectively, so that with the Einstein summation convention the equations of elastic equilibrium become

$$\sigma_{ij,j} + f_i = 0 \quad (2.1)$$

where f_i are the components of any body force and subscripts take values 1, 2, 3. The comma denotes differentiation with respect to orthonormal coordinates, so that $\sigma_{ij,k} = \partial\sigma_{ij}/\partial x_k$ and $u_{i,jk} = \partial^2 u_i/\partial x_j \partial x_k$. The relation between σ_{ij} and e_{ij} involves the tensor elastic stiffnesses c_{ijkl} in the form

$$\sigma_{ij} = c_{ijkl} e_{kl} \quad (2.2a)$$

but for isotropic media this reduces to

$$\sigma_{ij} = 2\mu e_{ij} + \lambda \delta_{ij} e_{kk} \quad (2.2b)$$

where δ_{ij} is the Kronecker delta, μ is the shear modulus and λ is the other Lamé constant.

When there are no internal stresses in an elastic body, the equations of compatibility

$$\epsilon_{ijk} \epsilon_{lmn} e_{km,jn} = 0 \quad (2.3)$$

have also to be satisfied. Here ϵ_{ijk} is the permutation tensor with values ± 1 when i, j, k are respectively even and odd permutations of 1–2–3 and zero unless $i \neq j \neq k$. In a single connected region, equations (2.3) are necessary and sufficient conditions for the existence of a single-valued displacement vector u_i related to e_{ij} by

$$e_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}). \quad (2.4)$$

An elastic body cut into elementary pieces which are then individually deformed in accordance with (2.3) may be reconstructed by fitting the deformed elements together again without application of any forces. If the deformed elements are not compatible in this way, forces must be applied to the elements before they can be cemented together again, and when these are removed internal stresses result. Thus the equations

$$S_{il}(\mathbf{r}) = \epsilon_{ijk} \epsilon_{lmn} e_{km,jn} \quad (2.5)$$

define a source of internal stress which is a nonzero function of the position vector \mathbf{r} . The ‘incompatibility tensor’ $S_{il}(\mathbf{r})$ usually has nonzero values only in limited regions (points, lines, planes) which are the singularities representing crystal defects. The displacement vector u_i is then not well defined; it may possess infinite values at some points in the medium and need not be both single-valued and continuous even outside the limited regions of nonzero S_{il} . The use of equation (2.5) to develop the elastic theory of dislocations (Kröner 1958) is reviewed in § 2.8. In many important cases, however, the sources of internal stress may be introduced by other methods (Volterra 1907, Somigliana 1914, 1915).

As described in § 1.2, a Somigliana dislocation involves a variable vector displacement \mathbf{d} given to two cut surfaces S terminating on the dislocation line C ; if \mathbf{d} is a smooth function, stress and strain are uniquely specified by \mathbf{d} and are everywhere finite except at C . The self energy of this defect is the elastic energy

$$U_s = \frac{1}{2} \int \sigma_{ij} e_{ij} dV \quad (2.6)$$

where the integration is restricted to that part of the body where the continuum

approximation is valid. There is another part of the energy in the region where σ_{ij} and e_{ij} become very large in a continuum, and this must either be treated atomistically or incorporated artificially in (2.6) by adjusting the limits of the integration.

Two lattice defects represented by Somigliana dislocations 1 and 2 have an interaction energy given by

$$U_{\text{int}}^{1,2} = \int \sigma_{ij}^{(1)} e_{ij}^{(2)} dV = \int \sigma_{ij}^{(2)} e_{ij}^{(1)} dV \quad (2.7)$$

provided each of them is in the region where the elastic solution of the other applies.

2.2. Volterra dislocations

2.2.1. Screw and edge dislocations. The Volterra dislocations (see §1.2) are special cases of Somigliana dislocations in which either \mathbf{d} is constant or $\mathbf{d} = \mathbf{r} \times \boldsymbol{\omega}$ where \mathbf{r} is the position vector and $\boldsymbol{\omega}$ is a constant vector. Only simple dislocations (\mathbf{d} constant) are considered in this section. In a continuum, the line integral of \mathbf{u} on a closed curve corresponds to the Burgers circuit of a lattice dislocation so that

$$\mathbf{b} = \oint d\mathbf{u}. \quad (2.8)$$

Consider a screw dislocation along the x_3 axis of an infinite cylinder of radius R . The dislocation is created by cutting along the $x_1 x_3$ surface and displacing the cut surfaces through \mathbf{b} in the x_3 direction. It is obvious from symmetry that the only component of displacement is

$$u_3 = (b/2\pi) \tan^{-1}(x_2/x_1) \quad (2.9)$$

which is discontinuous at the cut surface. The corresponding stresses are

$$\begin{aligned} \sigma_{13} &= \frac{-B_s x_2}{x_1^2 + x_2^2} & \sigma_{23} &= \frac{B_s x_1}{x_1^2 + x_2^2} \\ \sigma_{12} = \sigma_{11} = \sigma_{22} = \sigma_{33} &= 0 \end{aligned} \quad (2.10)$$

where $B_s = \mu b/2\pi$. In polar coordinates, $r(\phi)z$,

$$\sigma_{\phi z} = B_s/r \quad (2.11)$$

and all other stress components are zero.

The elastic energy per unit length between coaxial cylinders of radii r_0 and R is

$$E_s = \int_{r_0}^R \left(\frac{\sigma_{\phi z}^2}{2\mu} \right) 2\pi r . dr = \frac{1}{2} B_s b \ln \left(\frac{R}{r_0} \right). \quad (2.12)$$

The energy diverges as $R \rightarrow \infty$, and thus depends on the size of the crystal, but it is generally assumed that when a crystal contains many dislocations of opposite signs, their stress fields cancel at about half of the average separation, so that R may be set equal to this distance. The energy also diverges as $r_0 \rightarrow 0$ and the continuum theory fails in the core region $r \sim b$. It is usual to add a core energy on to (2.12), but since r_0 is not well defined it may alternatively be chosen so that (2.12) represents the whole energy.

Now introduce an edge dislocation along the axis of the same cylindrical crystal by displacing the cut surfaces in the x_1 direction. All displacements are in

the $x_1 x_2$ plane (plane strain) and equations (2.1) give

$$\begin{aligned}\sigma_{11,1} + \sigma_{12,2} &= 0 & \sigma_{12,1} + \sigma_{22,2} &= 0 \\ \sigma_{33} &= \nu(\sigma_{11} + \sigma_{22})\end{aligned}\quad (2.13)$$

where $\nu = \frac{1}{2}\lambda/(\lambda + \mu)$ is Poisson's ratio. The solution of (2.13) with the auxiliary conditions $\oint du_1 = b$ and $\oint du_2 = 0$ may be obtained by introducing an Airy stress function (e.g. Hirth and Lothe 1968 a) or by a complex variable method (Muskhelishvili 1963). This solution is

$$\begin{aligned}\frac{-\sigma_{11}}{3x_1^2 + x_2^2} &= \frac{\sigma_{22}}{x_1^2 - x_2^2} = \frac{-\sigma_{33}}{2\nu(x_1^2 + x_2^2)} \\ &= \frac{\sigma_{12}x_2}{x_1(x_1^2 - x_2^2)} = \frac{B_e x_2}{(x_1^2 + x_2^2)^2} \\ \sigma_{13} = \sigma_{23} &= 0 \quad B_e = \frac{\mu b}{2\pi(1-\nu)}.\end{aligned}\quad (2.14)$$

In polar coordinates

$$\begin{aligned}\sigma_{rr} = \sigma_{\phi\phi} &= -B_e \sin \phi/r = \sigma_{zz}/2\nu \\ \sigma_{r\phi} &= B_e \cos \phi/r.\end{aligned}\quad (2.15)$$

The elastic energy per unit length of an infinite edge dislocation is found by integration to be

$$E_e = \frac{1}{2}B_e b \ln(R/r_0). \quad (2.16)$$

The stress field (2.15) does not leave the external surface of a finite cylinder free from tractions, and additional single-valued displacements are required to achieve this. The necessary conditions ($\sigma_{rr} = \sigma_{r\phi} = 0$ at $r = R$) are obtained by adding to (2.15) stresses $\sigma_{rr} = (B_e/R^2)r \sin \phi$, $\sigma_{\phi\phi} = (3B_e/R^2)r \sin \phi$ and $\sigma_{r\phi} = -(B_e/R^2)r \cos \phi$. These stresses are negligible near the dislocation line provided $R \gg r_0$. The corresponding volume integral for the self-energy becomes

$$E_e = \frac{1}{2}B_e b \left\{ \ln\left(\frac{R}{r_0}\right) - \frac{3-4\nu}{4(1-\nu)} \right\}. \quad (2.16a)$$

The tractions across the inner (core) surface also do not disappear, and since r_0 is arbitrary they may be much larger than the true forces. If desired, these tractions may be annulled by adding further stresses

$$\sigma_{rr} = -\sigma_{\phi\phi} = B_e r_0^2 \sin \phi/r^3, \quad \sigma_{r\phi} = -B_e r_0^2 \cos \phi/r^3.$$

When both internal and external surfaces are free from tractions, the self energy is

$$E_e = \frac{1}{2}B_e b \{\ln(R/r_0) - 1\}. \quad (2.16b)$$

For a single screw dislocation in a finite cylinder, there is no traction across inner or outer cylindrical surfaces according to (2.11) but there is a finite couple across the end faces. If single-valued displacements are added to cancel this couple, the associated stress field is $\sigma_{\phi z} = -2B_s r/(R^2 + r_0^2)$ and the energy becomes

$$E_s = \frac{1}{2}B_s b \{\ln(R/r_0) - 1\}. \quad (2.12a)$$

The self-energy may alternatively be calculated as the work done on a cut surface ending on the dislocation as the displacement of the surfaces is increased from 0 to b . Bullough and Foreman (1964) emphasize that this method requires that the work done by the tractions on the core surface be included, since otherwise

inconsistent results will be obtained, from different orientations of the cut. The constant terms in equations (2.16), (2.16a) or (2.16b) are normally not important since the core radius is not defined, but in calculations on small loops this could be significant.

It follows naturally from (2.12) and (2.16) that the self-energy of any straight dislocation line is

$$E = \frac{1}{2}Bb \ln(R/r_0) \quad (2.17)$$

where B varies between limits B_s and B_e . If the Burgers vector makes an angle θ with the line, it may be regarded as a coincident screw with Burgers vector $b \cos \theta$ and an edge with Burgers vector $b \sin \theta$, so that

$$B = B_e(1 - \nu \cos^2 \theta). \quad (2.18)$$

Since the shear stress on the slip plane in the slip direction is B_s/r and B_e/r for screws (2.11) and edges (2.15) respectively, it also follows that

$$\sigma = B/r \quad (2.19)$$

is the effective shear stress produced by any straight dislocation.

As mentioned above, it is generally assumed that the stress fields of the dislocations cancel at about their mean separation R_d , so that the energy per unit volume is

$$\frac{U_s}{V} \approx \frac{E_s}{R_d^2} \approx \frac{\frac{1}{2}Bb}{R_d^2} \ln\left(\frac{R_d}{r_0}\right) \quad (2.20)$$

and the mean square internal stress is

$$\langle \sigma^2 \rangle^{1/2} \approx \mu b / R_d. \quad (2.21)$$

However, Wilkens (1967, 1968) showed that for a *random* distribution of dislocations the mean interaction energy vanishes, so that the energy of each dislocation diverges logarithmically with the outer cut-off radius which is of the order of the specimen size. This implies that a random distribution is prevented by the interaction energies; for any real distribution (2.20) and (2.21) are probably approximately valid.

2.2.2. The general dislocation loop. The displacement field $\mathbf{u}(\mathbf{r})$ of a general Volterra loop (see § 1.2) can be found using a Green function method (e.g. Seeger 1955 a, de Wit 1960) and was first derived by Burgers (1939) as an integral over the cut surface S of the function

$$R = |\mathbf{r} - \mathbf{r}'| = \{(x_i - x'_i)(x_i - x'_i)\}^{1/2}$$

where x_i are components of \mathbf{r} and x'_i of \mathbf{r}' which represents any point on the surface. Using $R_{ij} = \partial^2 R / \partial x_i \partial x_j$, etc., Burger's integral is

$$\begin{aligned} 8\pi u_i(\mathbf{r}) = & - \int_S b_j R_{,kki} dS'_j + \int_S (b_i R_{,kkj} dS'_j + b_l R_{,kkl} dS'_i) \\ & + \{2(\lambda + \mu)/(\lambda + 2\mu)\} \int_S (b_j R_{,kki} - b_k R_{,kij}) dS'_j. \end{aligned} \quad (2.22)$$

The integrals over S are transformed to integrals over the dislocation line C by means of Stokes' theorem to give

$$8\pi u_i(\mathbf{r}) = -2b_i \Omega + \oint_C \epsilon_{ijk} b_k R_{,il} dx'_j + \left(\frac{1}{1-\nu}\right) \oint_C \epsilon_{jkl} b_l R_{,ki} dx'_j \quad (2.23)$$

where x_i' is now the coordinate of any point on C and Ω is the solid angle subtended at r by the surface S and is given by

$$\Omega = -\frac{1}{2} \int_S R_{,kkj} dS_j'. \quad (2.24)$$

From these expressions, Peach and Koehler (1950) derived the stress field

$$\sigma_{ij}(\mathbf{r}) = \frac{\mu b_k}{4\pi} \oint_C \left\{ \frac{1}{2} R_{,lmn} (\epsilon_{jlk} dx_i' + \epsilon_{ilk} dx_j') + \left(\frac{1}{1-\nu} \right) \epsilon_{lmk} (R_{,mij} - \delta_{ij} R_{,mnn}) dx_l' \right\}. \quad (2.25)$$

When the stress field is known, the self-energy of the loop and the interaction energy of two dislocations may be obtained from (2.6) and (2.7). Blin (1955) obtained for the interaction energy of two dislocations

$$U_{\text{int}}^{1,2} = \frac{-\mu b_i^{(1)} b_j^{(2)}}{2\pi} \oint_{C_1} \oint_{C_2} \left\{ \epsilon_{ijk} \epsilon_{klm} R_{,nn} dx_l^{(1)} dx_m^{(2)} \right. \\ \left. - \frac{1}{2} R_{,kk} dx_i^{(1)} dx_j^{(2)} + \frac{1}{2} (\nu - 1) \epsilon_{kil} \epsilon_{mjn} R_{,km} dx_l^{(1)} dx_n^{(2)} \right\} \quad (2.26)$$

where $x_i^{(1)}$ and $x_i^{(2)}$ are now points on the curves C_1 and C_2 respectively, and

$$R = \{(x_i^{(1)} - x_i^{(2)}) (x_i^{(1)} - x_i^{(2)})\}^{1/2}.$$

The self-energy of a dislocation is one half of (2.26) for identical curves C_1 and C_2 separated by the cut-off radius r_0 . As mentioned in § 2.2.1, the work of the traction on the core surface has to be included to obtain consistent results. The self-energy would otherwise depend on the chosen relative position of the dislocation curves (Bullough and Foreman 1964). Calculation with (2.24)–(2.26) for an arbitrary loop is very difficult. The stress field of a pure prismatic circular loop (\mathbf{b} perpendicular to the plane of the loop) has been given in the form of definite integrals of Bessel functions by Kroupa (1960) and Bullough and Newman (1960). The stress field of a circular glissile loop (\mathbf{b} parallel to the plane of the loop) has been found by Kröner (1958) in the form of complete elliptic integrals. The corresponding self-energies are

$$U_{pl} = \pi B_e br \{\ln(8r/r_0) - 1\} \quad (2.27)$$

for the prismatic loop and

$$U_{sl} = \frac{1}{2}\pi(2-\nu) B_e br \{\ln(4r/r_0) - 1\} \quad (2.28)$$

for the glissile loop, where r is the loop radius in each case.

An alternative general method for the calculation of self-energies and interaction energies in which any dislocation line is constructed from angular dislocations was developed by Yoffe (1960). A rather similar approach in which the dislocation is treated as piecewise straight was suggested by Jøssang, Lothe and Skylstad (1965) and was further developed by de Wit (1967), De Wit and Ruff (1967), Asano (1968) and Jøssang (1968).

The self-energies of some complex loops have been calculated analytically by the above methods, e.g. rhombus-shaped (Bullough and Foreman 1964), n -sided regular polygon (Bacon and Crocker 1965, 1966), elliptical (Bacon 1966) and polygonal, elliptical and hexagonal (Li and Liu 1966, Liu and Li 1966 a, b). A review of calculations on dislocation loops is given by Kroupa (1966 b).

At a distance from a loop much larger than its dimensions, R in equation (2.22) may be replaced by the distance R_0 of the point \mathbf{r} from the centre of the loop, and choosing the centre of the loop as origin,

$$u_i(R_0) = -\left\{\frac{\lambda + \mu}{4\pi(\lambda + 2\mu)R_0^2}\right\} \left[\left\{\frac{\mu}{(\lambda + \mu)R_0}\right\} (b_k x_k n_i + n_k x_k b_i - b_k n_k x_i) + \left(\frac{3}{R_0^3}\right) b_k x_k n_j x_j x_i \right] \delta S \quad (2.29)$$

where \mathbf{n} is the unit normal to the loop of area δS . The stress field can then be calculated easily from (2.4) and (2.2b).

For an infinitesimal loop, δS and u_i may be replaced by dS and du_i , and the loop becomes a point singularity in an elastic continuum with a displacement field which decreases with distance as $1/R_0^2$ and stresses which decrease as $1/R_0^3$. This singularity represents a basic solution (a Green function) in the theory of dislocations in a continuum (Kroupa 1962 a). The displacement and stress field of the infinitesimal loop can be integrated over the area of a finite loop to give its displacement and stress field (Kroupa 1962 a, b, 1965).

2.3. Forces on dislocations

According to the Colonnetti principle (1915) the interaction *elastic* energy between internal and external stresses is zero, i.e. the response of a body to external forces is the same whether it is self-stressed or not. However, this does not mean that no interaction exists between dislocations and an external stress (see e.g. Eshelby 1956 a); when the virtual process of § 1.2 is used to form a dislocation loop in a body subjected to an external stress σ_{ij}^e , the total energy of the system must include the change in the potential energy of the external mechanism giving rise to the stress σ_{ij}^e . This change of the energy is equal to the work W done by the stress during the formation of the dislocation, where

$$W = - \int_S b_i \sigma_{ij}^e dS_j. \quad (2.30)$$

The integration extends over the cut surface S . More precisely, the change in the free energy of the system should be considered but possible changes in the entropy are neglected.

Now let each element δl of the dislocation be displaced through δr so that the vector area of the cut surface changes by $\delta r \times \delta l$ with components $\delta S_j = \epsilon_{jlk} \delta r_l \delta l_k$. During the displacement the stress σ_{ij}^e does additional work

$$\delta W = - \oint b_i \sigma_{ij}^e \epsilon_{jlk} dr_l dl_k \\ \oint = dF_l dr_l \quad (2.31)$$

where each element dl is acted upon by a force dF with components

$$dF_l = \epsilon_{jlk} \sigma_{ij}^e b_i dl_k. \quad (2.32)$$

This formula was derived by Peach and Koehler (1950) and may be expressed in the alternative form that the force per unit length of dislocation line, F , is related

to the unit vector \mathbf{l} giving the direction of the line by

$$F_l = \epsilon_{ijk} \sigma_{ij}^e b_i l_k \quad (2.33)$$

In using this equation, it is immaterial whether σ_{ij}^e is an externally imposed stress field or is the field of another defect. The component of force tending to produce glide, i.e. the maximum force in the plane containing \mathbf{b} and \mathbf{l} , is often more important than the total force and is given by

$$F_g = \sigma_{ij}^e b_i n_j \quad (2.34)$$

where \mathbf{n} is the unit normal to the glide plane and \mathbf{j} is a unit vector in that plane and normal to the dislocation line. In particular, the force between two parallel dislocations with the same Burgers vector is given by (2.19) as

$$\mathbf{F} = (B\mathbf{b}/r)\mathbf{j}. \quad (2.35)$$

Forces on dislocation lines arise not only from mechanical stresses, since the concept may be used wherever displacement of the line will change the energy. Thus, for example, an edge dislocation will experience a chemical force in the presence of a nonequilibrium concentration c of vacancies which may be absorbed or emitted in climb. If the equilibrium concentration of point defects is c_0 and the volume of an atom is v , the effective chemical force is (Friedel 1964)

$$F_c = (bkT/v) \ln(c/c_0). \quad (2.36)$$

Weertman (1965) pointed out that the Peach-Koehler equation appears to give wrong results in certain cases, and he proposed that σ_{ij}^e should be replaced by the deviator stress

$$\sigma_{ij}' = \sigma_{ij}^e - \frac{1}{3}\delta_{ij}\sigma_{kk}^e.$$

Difficulties arise because the division of forces into mechanical, chemical and other terms is not necessarily unique when climb processes are involved. According to Lewthwaite (1966), equation (2.30) is inapplicable if material is conserved during the creation of the dislocation and should be replaced by

$$W' = - \int_S b_i \sigma_{ij}^e dS_j - \int_A d_i \sigma_{ij}^e dA_j \quad (2.37)$$

where A is the external surface and \mathbf{d} is a displacement of that surface caused by rearrangement of material after the dislocation is created. If the dislocation now moves

$$\delta W' = - b_i \sigma_{ij}^e \epsilon_{jlk} dr_i dl_k - \int_A \delta d_i \sigma_{ij}^e dA_j. \quad (2.38)$$

For a pure hydrostatic pressure, the two terms in this equation are either zero or equal and opposite, so $\delta W' = 0$.

When a straight-edge dislocation climbs in a plane normal to the end faces of a cylindrical crystal subjected to a uniform tensile or compressive stress σ_{11} , the force per unit length is $b\sigma_{11}' = \frac{2}{3}b\sigma_{11}$ if the vacancies are emitted or absorbed uniformly at the surface, and is $b\sigma_{11}$ if they are all emitted or absorbed at the cylindrical surfaces. If they are all retained within the lattice, the force is $b\sigma_{11} - b\sigma_{11}(v - v_v)/3v$ where v_v is the volume of a vacancy, and Weertman wrote this in the form $b\sigma_{11}'$ by incorporating the term in v_v in the chemical potential.

2.4. Image forces

The stress field of a dislocation near an interface or a free surface is modified by the requirement that the shear and normal components must be continuous across the boundary, and there is thus an interaction of the dislocation with the interface. Solutions to this elastic problem can often be obtained by the method of images, which is exactly analogous to that used in electrostatics. Imaginary sources of stress, e.g. other dislocations, are introduced so that the superimposed stress fields satisfy the boundary conditions. The stress field of an image source appears as an external stress field to the real dislocation, and the resultant force on the dislocation is called an image force.

As an illustration consider a screw dislocation at $x_1 = d$, $x_3 = 0$ in a medium of shear modulus μ_1 which is separated from a second medium of modulus μ_2 by a planar boundary at $x_1 = 0$. Head (1953) showed that the stress component σ_{13} will be continuous across the boundary if in the medium μ_1 is added an additional stress field due to an image dislocation with a Burgers vector

$$A_1 \mathbf{b} = \{(\mu_2 - \mu_1)/(\mu_2 + \mu_1)\} \mathbf{b}.$$

In the medium μ_2 , the field is that of a dislocation coincident with the real dislocation, but with a Burgers vector

$$A_2 \mathbf{b} = \{2\mu_1/(\mu_1 + \mu_2)\} \mathbf{b}.$$

Hence, from (2.11), the stress in μ_1 is

$$\begin{aligned} \sigma_{13} &= -B_s \left\{ \frac{x_2}{(x_1 - d)^2 + x_2^2} + \frac{A_1 x_2}{(x_1 + d)^2 + x_2^2} \right\} \\ \sigma_{23} &= B_s \left\{ \frac{x_1 - d}{(x_1 - d)^2 + x_2^2} + \frac{A_1(x_1 + d)}{(x_1 + d)^2 + x_2^2} \right\} \end{aligned} \quad (2.39)$$

whilst in the other medium

$$\begin{aligned} \sigma_{13}' &= \frac{-B_s' A_2 x_2}{(x_1 - d)^2 + x_2^2} \\ \sigma_{23}' &= \frac{B_s' A_2 (x_1 - d)}{(x_1 - d)^2 + x_2^2} \end{aligned} \quad (2.40)$$

where $B_s = \mu_1 b/2\pi$ and $B_s' = \mu_2 b/2\pi$. The image stress field exerts a force F per unit length on the real dislocation, where

$$F_1 = B_s b A_1 / 2d \quad F_2 = 0. \quad (2.41)$$

The dislocation is thus attracted towards the interface if $\mu_2 < \mu_1$, and in particular it is attracted towards a free surface ($\mu_2 = 0$). Similar results are obtained for the interaction between a free surface and a parallel edge dislocation (Head 1953) or a dislocation inclined to the surface (Lothe 1967 a). Image forces are very important in the thin foils used for transmission electron microscopy. Hartley (1969) has shown that the image force on an edge dislocation is reduced if it is part of an infinite, uniformly spaced array parallel to the free surface. The image forces on a general dislocation loop have been considered by Groves and Bacon (1970).

Eshelby (1953 a) considered the image forces acting on an axial screw dislocation in a thin cylindrical crystal. His results, which are important in the theory of whiskers, show that the dislocation is stable with respect to small displacements from the axis towards the free surfaces.

2.5. Dislocation dipoles and dislocation pile-ups

A dislocation dipole consists of two parallel, opposite dislocations which in practice are often pure edges. The dipole energy, E^{dip} per unit length, consists of the self-energies of the two dislocations plus an interaction energy, and may readily be calculated for edges from (2.7). The energy E^{dip} and the component of force in the slip plane exerted by edge dislocation 1 on unit length of dislocation 2 are plotted in figure 3 as functions of ξ/h , where ξ is the dislocation separation along the

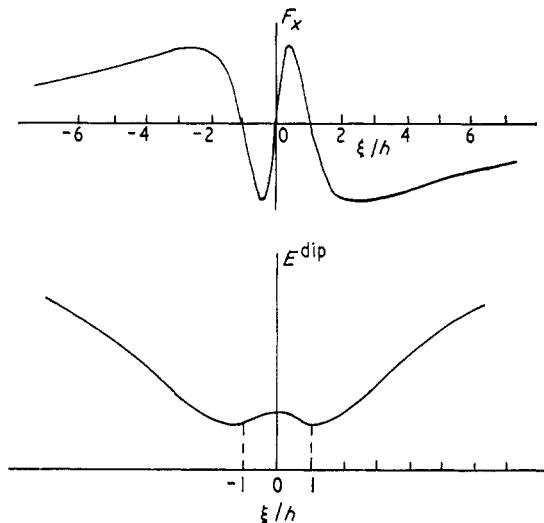


Figure 3. The energy of an edge dipole, E^{dip} , and the component F_x of the force between the two dislocations in the slip plane plotted as functions of ξ/h (after Kroupa 1966 a).

slip planes and h is the separation of the two slip planes. If the dislocations can move only in the slip planes, the elastic interaction leads to stable configurations of the dipole for $\xi = \pm h$ and an unstable equilibrium configuration at $\xi = 0$. In the stable configurations, the total elastic energy per unit length is approximately

$$E^{\text{dip}} = B_e b \ln(h/r_0) \quad (2.42)$$

and since the energy of two independent edge dislocations is approximately $B_e b \ln(R/r_0)$ it follows that the binding energy of an edge dipole (with respect to dissociation by glide) is

$$E_{\text{bind}}^{\text{dip}} = B_e b \ln(R/h). \quad (2.43)$$

When the height h of the dipole is small, i.e. less than $100b$, the binding energy is very high, i.e. about 10 eV per atom plane.

The stress field of the dipole σ_{ij}^{dip} is obtained by superposition as

$$\sigma_{ij}^{\text{dip}} = \sigma_{ij}(\mathbf{r}) - \sigma_{ij}(\mathbf{r} - \mathbf{p}) \quad (2.44)$$

where \mathbf{p} is the position vector of dislocation 2 with respect to dislocation 1 and $\sigma_{ij}(\mathbf{r})$ is given by (2.14) or (2.10). At large distances, $|\mathbf{r}| \gg |\mathbf{p}|$, a Taylor expansion gives

$$\sigma_{ij}^{\text{dip}} = \mathbf{p} \cdot \text{grad } \sigma_{ij}. \quad (2.45)$$

The long-range stress field of a dipole is thus expressed as a stress gradient of a

single dislocation, and falls off as $1/r^2$. This is because the stress fields of the component dislocations nearly cancel far from the dipole. On the other hand, the stress fields at the centre of the dipole are additive for σ_{11} , giving for an edge dipole

$$\begin{aligned}\sigma_{11} &= \pm 2B_e b/h = \sigma_{33}/\nu \\ \sigma_{12} &= \sigma_{23} = \sigma_{31} = 0.\end{aligned}\quad (2.46)$$

The alternative signs in equation (2.46) apply to opposite dipoles with tensile or compressive stresses in the centre.

An applied homogeneous shear stress σ_{12}^e exerts equal and opposite glide forces $\pm b\sigma_{12}^e$ on the component dislocations, so that there is no net force on the dipole. The effect of the stress will either be to change the equilibrium separation ('polarize' the dipole) or to decompose the dipole, depending on whether σ_{12}^e is smaller or greater than the maximum shear stress exerted by one component dislocation on the glide plane of the other. Thus, the condition for the dislocations to remain associated as a dipole is

$$\sigma_{12}^e < B_e/4h. \quad (2.47)$$

If the stress σ_{12}^e is not homogeneous, there will be a resultant force on the whole dipole which may then glide as a unit.

A dipole can form a stable tripoles configuration by combining with another straight dislocation. A tripoles has a resultant Burgers vector and a long-range stress field almost identical with that of a single dislocation, so that it experiences a force in a homogeneous stress field. Similarly a quadrupole may be formed with properties very similar to those of a dipole, and in general any number of parallel dislocations may combine to form multipoles.

Chen *et al.* (1964) and Hazzledine (1966) considered in detail the configurations and properties of various multipoles, and many other authors have published papers on the structures, mode of formation and effects on physical properties of dipoles and multipoles (e.g. Johnston and Gilman 1960, Gilman 1960, Tetelman 1962, Li 1964 a, Kroupa 1965, Washburn and Caso 1966, Steeds 1967 a, b, Hazzledine 1967, Knesl 1967, Bacon 1968, Ingram and Moore 1969). The stability and physical properties of configurations consisting of two parallel dislocations with different Burgers vectors ('quasi-dipoles') has also been studied (Seeger and Wobser 1966 a, Lejček 1968). Kroupa (1966 a) gave a detailed review of work on dipoles.

A queue of n similar dislocations on one slip plane forced against an obstacle by a shear stress σ is known as a pile-up. Some limiting properties are obvious; a virtual work argument shows that the force on the leading dislocation is $n\sigma b$, so that the pile-up is an effective stress concentrator, and at large distances the stress field is equivalent to that of a super-dislocation of Burgers vector nb . In many applications (fracture, yielding, work-hardening) the stress field close to the pile-up is required.

Problems involving planar arrays of dislocations either may be treated completely by finding the equilibrium positions of the individual dislocations, or may be approximated by smearing the dislocations into a continuous distribution of dislocations over the planar surface (Eshelby 1949 a, Leibfried 1951). The discrete dislocation problem has been solved analytically for a limited range of problems, but in many cases numerical procedures are necessary. Recently E. Smith (1968, 1969) has developed a compromise method in which one or two critical dislocations

are treated as discrete, and the remaining dislocations are smeared into a distribution. In general, the mathematical theory of planar arrays is complex, and only an outline treatment is possible here.

The equilibrium positions x_i of the dislocations in a pile-up extending from $x = -L$ to $x = 0$ (where one dislocation is fixed) under the action of a shear stress σ are given by the equations

$$\sum_{\substack{j=1 \\ j \neq i}}^n \{Bb/(x_i - x_j)\} = b\sigma \quad i = 2, 3, \dots, n \quad (2.48)$$

where n is fixed by $x_n > -L$. Eshelby *et al.* (1951) showed that this problem reduces to finding the zeros of a Laguerre polynominal

$$g(x) = (x - x_1)(x - x_2) \dots (x - x_n)$$

which is given by the differential equation

$$\frac{1}{2}g''(x) - (\sigma/B)g'(x) + (n\sigma/Bx)g(x) = 0. \quad (2.49)$$

The relation between n and σ is

$$n = (\sigma L / 2B) \quad (2.50)$$

and the spacing of the first two dislocations is

$$-x_2 = 1.84B/n\sigma. \quad (2.51)$$

The total length x_p of the first p dislocations is proportional to $p^2 B/n\sigma$ provided $p \ll n$. A related problem which has been solved by Chou (1967 a) is a pile-up in which the anchored dislocation has a Burgers vector mb ; this may be important if the leading dislocation is effectively a grain boundary ledge.

For the corresponding continuous approximation, there is a distribution of Burgers vector $f(x) dx$ and the equilibrium equation becomes

$$\int_{-L}^0 \frac{f(\lambda)}{x - \lambda} d\lambda = \frac{\sigma}{B} \quad (2.52)$$

and the appropriate solution with $f(x) = 0$, at $x = -L$, 0 is

$$f(x) = \frac{\sigma}{\pi B} \left(\frac{L+x}{x} \right)^{1/2} \quad (2.53)$$

(Leibfried 1951, Head and Louat 1955). The number of dislocations in the pile-up, $n = \int_{-L}^0 f(x) dx$, agrees with (2.50). Smith's mixed procedure gives equation (2.51) with a slightly different numerical factor (1.79) when the two leading dislocations are discrete.

Some related problems, e.g. the planar array fixed at both ends, the pile-up under a fluctuating stress and the pile-up containing dislocations of both signs, have been examined by both methods (Eshelby *et al.* 1951, Head and Louat 1955, Head and Thomson 1962). An analytical solution to the opposite-signed discrete array cannot be obtained, but numerical solutions have been given when n is small (Armstrong *et al.* 1966). Similarly numerical methods have been used to study the interaction of pile-ups on parallel planes (e.g. Head 1959) and intersecting planes (Chou *et al.* 1960, 1961).

Some features of the stress field of the simple pile-up are important. Its 'centre of gravity' is at $x = -\frac{1}{4}L$ and the field at large distances corresponds to a dislocation

of Burgers vector nb at this point (Li 1963). The net macroscopic slip produced by the dislocations thus corresponds to a movement of this super-dislocation through a distance $\frac{3}{4}L$. The shear stress ahead of the pile-up for $x < -x_2$ is practically that due to a single dislocation; for $-x_2 < x < L$ this is increased by a factor of approximately $1 + (L/x)^{1/2}$ which can be large (Stroh 1954 a).

Mitchell (1964) and Basinski and Mitchell (1966) have calculated the stress fields around various pile-ups by integrating numerically the stresses due to the infinitesimal dislocations (2.53). Similar calculations were made previously by Haasen and Leibfried (1954) and Head (1960). Mitchell resolved the stresses on to the primary slip plane and the various secondary slip planes of the fcc structure and emphasized that they are sufficiently large to induce slip on secondary systems, and that the back stress from a pile-up never exceeds the applied stress σ needed to produce the pile-up. Numerical calculations of the stress fields of discrete pile-ups and the stress needed to force a pile-up past a fixed dislocation on another slip plane were made by Hazzledine and Hirsch (1967) and Hazzledine (1968), and the last problem is treated analytically by E. Smith (1967) and Pande (1970).

Pile-ups of dissociated dislocations have been examined by Wolf (1960), Li (1969) and E. Smith (1970), and Li and Liu (1967) have considered circular pile-ups. Chou (1965 a) used the continuous distribution method to investigate a screw pile-up against an elastic half-plane (i.e. a semi-infinite second phase) and Barnett and Tetelman (1967) similarly investigated a screw pile-up against a cylindrical inclusion. Barnett (1967) solved the elastic half-plane problem for all ratios of shear moduli, and showed that the stress multiplication factor in the new medium varies as $(L/x)^a$ where $0 < a < \frac{1}{2}$ if $\mu_2 > \mu_1$ and $\frac{1}{2} < a < 1$ if $\mu_1 > \mu_2$.

2.6. Line tension

Mott and Nabarro (1948) introduced the concept of a dislocation line tension τ , in analogy with the behaviour of a taut string, and defined

$$\tau = \delta U / \delta l \quad (2.54)$$

where δU is the increase in energy for an increase in line length δl . With this definition τ depends not only on b but also on the orientation and shape of the dislocation. Thus, for a circular loop of radius r in the glide plane, equation (2.28) gives for the tension

$$\tau_1 = B_s b \left[\frac{2-\nu}{2(1-\nu)} \right] \ln \left(\frac{4r}{r_0} \right) \quad (2.55)$$

whilst for a straight dislocation

$$\tau_s = \frac{1}{2} B b \ln (R_d / r_0) \quad (2.56)$$

with B varying from B_s to B_e , and R_d equal to the average separation between dislocations. The difference between these expressions is not large when the curvature is small, and the concept of line tension is usually restricted to this condition and approximated as the energy of a straight dislocation per unit length, E , i.e. by (2.56).

Equation (2.56) is based on the assumption that the additional length, δl , has the same orientation as the original dislocation. De Wit and Koehler (1959) first suggested that any change in the orientation of the dislocation line should be

included in the definition of the line tension, so that

$$\tau = E + \frac{\partial^2 E}{\partial \theta^2} \quad (2.57)$$

where θ is the angle between \mathbf{l} and \mathbf{b} . This problem was studied in detail by Brown (1964) who introduced the concept of self-stress, that is the stress on an element of the dislocation due to the dislocation itself. This stress varies along the dislocation with the local orientation and also depends on the shape of the whole line. It is expressed as an integral (similar to (2.25)) over the dislocation line. If the curvature is small everywhere the self-stress is well approximated by the line tension introduced above. When this condition is not satisfied it is usually necessary to integrate numerically.

Further calculations of the line tension have been made recently by Jøssang, Lothe and Skystad (1965), Hirth *et al.* (1966), Jøssang (1968) and Betsch and Winchell (1968) who treated the bowed dislocation as composed of piecewise segments. Brailsford (1965) approximated the curved dislocation by a sequence of infinitesimal kinks, taking the limit as the kink-height tends to zero. de Chatel and Kovacs (1965) considered the equilibrium of a closed dislocation loop under the external and self-stresses; the effect of the self-stresses was then replaced by that of the line tension. However, it is often adequate to use the rough approximation $\tau \approx \mu b^2$ which follows from (2.56) if $R \sim 10^4 b$ and $r_0 \sim b$ (Friedel 1964).

Line tension may be used to calculate the equilibrium shape of a dislocation with fixed ends in the presence of a stress field. An element dl which subtends an angle $d\phi$ at its centre of curvature is in equilibrium under the force per unit length F from the stress field and its own line tension τ if

$$\tau d\phi = F dl \quad (2.58)$$

and hence the curvature is

$$\kappa = d\phi/dl = F/\tau. \quad (2.59)$$

Consider the action of a Frank–Read source of length l under the action of a shear stress σ (resolved parallel to \mathbf{b}). The critical configuration (see § 1.3) is when the dislocation is bent into a semicircle of radius $\frac{1}{2}l$, so that the stress needed to operate the source is

$$\sigma_c = 2\tau/lb. \quad (2.60)$$

When the shape and position of a dislocation line are required accurately, the line tension approximation is usually inadequate, and calculations must be based on the concept of self stress. At equilibrium, the force on each element of dislocation line is zero; this configuration can normally be found only by numerical calculation. An example is the equilibrium configuration of an extended node (Brown 1964), or the bowing of a dislocation segment under stress (Bacon 1967, Foreman 1967).

2.7. Interactions of dislocations with point defects

The continuum analogues of point defects (vacancies, interstitials, solute atoms) are negative or positive centres of dilatation, or strain centres of lower symmetry. If such a defect has a strain field u_i^d , Eshelby (1956 a) showed that the volume integral (2.7) representing its interaction with the stress field σ_{ij}^d of a dislocation

may be transformed into an integral

$$U_{\text{int}}^{dc} = \int_S (\sigma_{ij}^e u_i^d - \sigma_{ij}^d u_i^e) dS_j \quad (2.61)$$

over any surface S which surrounds the point defect and on which u_i^d and u_i^e exist. By taking S immediately outside the point defect, (2.61) may also be transformed into a volume integral (Eshelby 1957),

$$U_{\text{int}}^{dc} = \int_v \sigma_{ij}^d e_{ij}^T dv = \sigma_{ij}^d e_{ij}^T v \quad (2.62)$$

where v is the volume of the point defect and it is assumed that σ_{ij}^d are essentially constant over this volume. For a misfitting inclusion of elastic properties identical with those of the matrix, e_{ij}^T are the (uniform) 'stress-free strains' when the inclusion is unconstrained by the matrix; if the elastic properties are different, e_{ij}^T are the stress-free strains of the equivalent inclusion (Eshelby 1957).

An alternative procedure is to apply Gauss' theorem to transform (2.61) into

$$U_{\text{int}}^{dc} = - \int_v f_i u_i^e dV \quad (2.63)$$

where the integral is now again over the whole crystal and f_i is a distribution of body force inside the point defect which produces the same stresses and displacements on S as the defect. Point defects may be simulated by orthogonal double forces without moments (point dipoles), P_{ij} , and equation (2.63) becomes (Kröner 1958)

$$U_{\text{int}}^{dc} = - P_{ij} e_{ij}^d. \quad (2.64)$$

A point defect with a spherically symmetrical field interacts only with the hydrostatic pressure $p = -\frac{1}{3}\sigma_{ii}^d$ of the dislocation, and the interaction energy (2.62) then becomes

$$U_{\text{int}}^{dc} = - p \delta v \quad (2.65)$$

where (Eshelby 1954, 1956 a) δv is the change in the volume of the whole crystal when the point defect is introduced. The model of a solute atom as a compressible sphere in a misfitting hole is often used, and the interaction energy with an edge dislocation may then also be written (Bilby 1950) as

$$U_{\text{int}}^{dc} = \mu b \delta v^\infty \sin \phi / \pi r \quad (2.66)$$

where the atom has polar coordinates r, ϕ, z with respect to a dislocation along the z -axis. Eshelby showed that δv^∞ in this expression is the change in volume of a region enclosed by a surface immediately surrounding the solute atom, and that this differs from δv in a finite crystal because of the dilatation produced by image displacements. When the inserted sphere has compressibility K_B and shear modulus μ_B different from those of the matrix (K_A and μ_A), δv also differs from δv^{mis} , the difference in volumes of the inserted sphere (solute atom) and hole (solvent atom). The relation between δv^∞ and δv^{mis} is

$$\delta v^\infty = \left(\frac{3K_B}{3K_B + 4\mu_A} \right) \delta v^{\text{mis}}. \quad (2.67)$$

When the elastic properties are identical

$$\delta v^\infty = \left\{ \frac{1+\nu}{3(1-\nu)} \right\} \delta v^{\text{mis}} \quad (2.67a)$$

and

$$\delta v^{\text{mis}} = \delta v.$$

In principle, $U_{\text{int}}^{\text{dc}}$ can be obtained from an estimate of δv^{mis} together with (2.65) for spherically symmetrical interstitials and from (2.66) and (2.67) for solutes or vacancies. In practice, it is preferable to obtain the mean strain $e_a = d \ln a / dc$ from measurements of the change of lattice parameter a with composition c , and then in all cases (from (2.65))

$$U_{\text{int}}^{\text{dc}} = 2B_e(1+\nu)e_a v \sin \phi/r. \quad (2.68)$$

The above equations are often quoted incorrectly in the literature; a common mistake is to use equation (2.66) with δv or δv^{mis} .

The most stable position for the point defect is clearly close to the edge dislocation and at $\phi = \pm \frac{1}{2}\pi$ (depending on the relative signs of b and e_a). Putting $r \sim b$ gives the binding energy

$$U_{\text{bind}}^{\text{dc}} \approx -2B_e(1+\nu)e_a v/b. \quad (2.69)$$

Because the separation of the defects is very small, the continuum approach can no longer be valid, but numerical values obtained from (2.68) are not unreasonable.

The size effect discussed above is long range, and within the framework of linear elasticity there is no corresponding interaction with a pure screw dislocation unless the latter is dissociated into partials with edge components. Point defects of lower than cubic symmetry, however, interact with all dislocations, and tetragonal defects are of especial interest since they represent interstitial solutes in bcc metals or various other defects in fcc, ionic or diamond lattices.

If the defect is specified by principal strains $e_{11} = e_1$ and $e_{22} = e_{33} = e_2$, the interaction energy with a pure screw dislocation depends on the shear strain ($e_1 - e_2$) and for a $\langle 111 \rangle$ screw dislocation is given by (2.62) as

$$U_{\text{int}}^{\text{dc}} = \sqrt{8B_s(e_1 - e_2)v \cos \phi/r} \quad (2.70)$$

(Cochardt *et al.* 1955). The volume v with which the strains e_1 and e_2 are associated is effectively an ellipsoid, but is of ill-defined size. However, if the strains are derived from lattice parameter measurements of dilute aligned point defects (e.g. carbon martensites) which are then extrapolated to one defect per volume v , the choice of v is immaterial since the product $(e_1 - e_2)v$ is constant. Cochardt *et al.* choose $v = a^3$ which gives rather large strains, and Hirth and Cohen (1969 a, b) have argued that a more reasonable choice is $v = \frac{1}{2}a^3$ which effectively doubles the strains. They therefore suggest that the extrapolation procedure is invalid and that the relative displacements of nearest neighbours obtained by an atomistic calculation should be used in equation (2.70). Schoeck (1969) and Bacon (1969) have shown that this is incorrect and have also demonstrated by a procedure based on (2.64) that equation (2.70) is exact within the limits of continuum theory.

Equation (2.70) is appropriate for a bcc screw dislocation, and the corresponding energy for an edge dislocation is

$$U_{\text{int}}^{\text{dc}} = \{ \frac{1}{3}(e_1 + 2e_2)(1 + \nu + 2 \cos^2 \phi) - e_2 \cos 2\phi + e_1 \nu \} B_e v \sin \phi/r. \quad (2.71)$$

Equivalent equations may be given for tetragonal defects in other lattices, although lattice parameter methods for estimating the strain fields are generally not available. The interactions with edge and screw components are believed to be of similar magnitudes.

Shorter-range interactions, decreasing as $1/r^2$, arise from the concept of solute atoms as elastic inhomogeneities. For example, an atom of slightly different shear modulus has an interaction energy with a screw dislocation (Saxl 1964)

$$U_{\text{int}}^\mu = e_\mu v W_\mu = (\mu/8\pi^2) e_\mu v (b/r)^2 \quad (2.72)$$

where W_μ is the strain energy density of the dislocation and $e_\mu = -d \ln \mu / dc$. For an edge dislocation, the corresponding energy also depends on $e_K = -d \ln K / dc$ and may be written

$$U_{\text{int}}^K = v(e_K W_K + e_\mu W_\mu) = \frac{U_{\text{int}}^\mu (1 - e_{\mu K} \sin^2 \phi)}{(1 - \nu)^2} \quad (2.73)$$

(Saxl 1964) where W_μ, W_K are now the shear and dilatational energy densities of the dislocation before introduction of the solute atom, and $e_{\mu K}$ depends on ν but is approximately $1 - 0.3e_K/e_\mu$ for $\nu = \frac{1}{3}$.

Finally there is a second-order volume expansion around a screw dislocation of magnitude $Cb^2/4\pi^2 r^2$, where $0.3 \leq C \leq 1$ (Stehle and Seeger 1956). This gives a short-range interaction

$$U_{\text{int}} = \left\{ \frac{C(1+\nu)}{2\pi^2(1-2\nu)} \right\} \mu v e_a \left(\frac{b}{r} \right)^2. \quad (2.74)$$

The change of volume arises from anharmonic vibrations and Lomer (1957) pointed out that it may be assumed to be proportional to the dislocation energy and the constant of proportionality can then be derived from the Grüneisen relation between thermal expansion and specific heat. The corresponding effect for an edge dislocation can be neglected because of the first-order size effect.

2.8. Continuous distributions of dislocations

The total length of dislocation line in unit volume is a scalar called the dislocation density ρ_D , but this gives no information about the distribution of Burgers vectors among the dislocations. Nye (1953) introduced the tensor dislocation density α_{ij} which gives the i -component of the net Burgers vector \mathbf{b} of all dislocations which pass through unit area normal to the j -direction, i.e.

$$\alpha_{ij} = db_i/dS_j. \quad (2.75)$$

More generally, if C is any closed curve and S is a surface cap limited by C , the net Burgers vector of the dislocations threading C is

$$\mathbf{b}_i = \int_S \alpha_{ij} dS_j. \quad (2.76)$$

In particular if Σ is any arbitrary closed surface enclosing a volume V

$$\int_{\Sigma} \alpha_{ij} dS_j = \int_V \alpha_{ij,j} dV = 0$$

so that

$$\alpha_{ij,j} = 0. \quad (2.77)$$

In problems involving only the net dislocation content, the discrete distribution may be made continuous by allowing the density of each type of dislocation to increase without limit whilst the Burgers vector decreases so that the product remains constant. The dislocated state is then completely specified by α_{ij} and may be related to the stress via the incompatibility tensor (Kröner 1955). However, the lattice rotations associated with α_{ij} are rather complex and involve the non-Riemannian geometry of a space with torsion (Kondo 1952, Bilby *et al.*, 1955). This theory has close analogies to the general theory of relativity, but only an outline description is possible here and reference should be made to more detailed reviews (e.g. Bilby 1960, Bilby *et al.* 1966, Kröner 1958, 1966).

Let a coordinate system x_i (representing a lattice) be based on fixed orthonormal vectors a_i and be embedded in the continuum before the dislocations are introduced. At each point of the dislocated continuum, the coordinate lines represent the dislocated lattice and define a triad of vectors e_i related to a_i by

$$e_i = D_{ji} a_j \quad a_i = Q_{ji} e_j \quad (2.78)$$

where D_{ji} and Q_{ji} are reciprocal matrices. Small vectors around a point in the dislocated medium may be written $dy_i e_i$ where y_i is a tangential system of local coordinates based on e_i and

$$dy_i = Q_{ij} dx_j \quad dx_i = D_{ij} dy_j. \quad (2.79)$$

Integration of (2.79) to give y_i in terms of x_i is only possible if the deformation represented by Q is compatible, that is if

$$Q_{ijk} = Q_{ikj}. \quad (2.80)$$

When (2.80) is not valid, the Pfaffian forms (2.79) are not perfect differentials and the dislocated state cannot be obtained by applying a continuous deformation for which a displacement function exists.

A path in the dislocated continuum composed of elementary steps $dx_i a_i$ forms a closed circuit C if

$$\oint_C dx_i a_i = \oint_C Q_{ji} dx_i e_j = 0. \quad (2.81)$$

The net Burgers vector threading C is the closure failure of the corresponding path in which each e_i is replaced by a_i , so that

$$b_j = -\oint_C Q_{ji} dx_i = -\int_S \epsilon_{ikl} Q_{jil} dS_k \quad (2.82)$$

where S is any surface cap on C. Comparing with (2.76)

$$\alpha_{ij} = -\epsilon_{jkl} Q_{ilk}. \quad (2.83)$$

Alternatively, the Burgers vector could be written

$$b_j = -\oint_C (dy_j - dx_j) = -\oint_C (\delta_{ji} - D_{ji}) dy_i.$$

The expression for α_{ij} becomes

$$\alpha_{ij} = -\epsilon_{jkl} \left(\frac{\partial D_{il}}{\partial y_k} \right) \quad (2.84)$$

where the differentiation is now with respect to local coordinates.

The local Burgers vector \mathbf{b}' (§ 1.2) has the same components in the e_i system as has \mathbf{b} in the a_i system. Thus

$$b'_i = - \int_S \epsilon_{jkl} D_{im} Q_{ml,k} dS_j = - \int_S \alpha_{ij}' dS_j \quad (2.85)$$

where the local dislocation density tensor is

$$\alpha_{ij}' = \epsilon_{jkl} T_{ikl} \quad (2.86)$$

and

$$T_{ikl} = \frac{1}{2} D_{im} (Q_{ml,k} - Q_{mk,l}) \quad (2.87)$$

is called the torsion tensor. From (2.83) or (2.87) it is seen that the dislocation density is zero and the torsion tensor vanishes for a compatible deformation.

Consider two neighbouring vectors

$$q_k \mathbf{a}_k = q_k Q_{ik} e_i \quad \text{and} \quad (q_k + dq_k) \mathbf{a}_k = (q_k + dq_k) (Q_{ik} + Q_{ik,l} dx_l) e_i$$

with identical e_i components, so that

$$dq_k Q_{ik} = - q_k Q_{ik,l} dx_l$$

or

$$dq_m = - D_{mi} Q_{ik,l} q_k dx_l = - L_{klm} q_k dx_l \quad (2.88)$$

This relation is a linear connection which prescribes equivalent or parallel vectors of the generalized space. The coefficients of connection are

$$L_{klm} = D_{mi} Q_{ik,l}. \quad (2.89)$$

For a Euclidean manifold $L_{klm} = 0$, and in a Riemannian space L_{klm} is symmetric. In the geometry of a dislocated continuum, L_{klm} is not symmetric; the anti-symmetric part gives the torsion associated with \mathbf{b}' since from (2.87) and (2.89)

$$T_{klm} = \frac{1}{2} (L_{klm} - L_{lkm}). \quad (2.90)$$

The above results apply to deformations which need not be small, but a restriction $|Q_{ij} - \delta_{ij}| \ll 1$ must be imposed in order to introduce stresses by means of linear elasticity. Let $U_{ij} = Q_{ij} - \delta_{ij}$ so that $\alpha_{ij} = -\epsilon_{jkl} U_{il,k}$. The tensor U_{ij} may be divided into a symmetric strain e_{ij} and an antisymmetric rotation ω_{ij} where

$$e_{ij} = \frac{1}{2} (U_{ij} + U_{ji}) \quad \omega_{ij} = \frac{1}{2} (U_{ij} - U_{ji}). \quad (2.91)$$

The rotation may also be represented by the axial vector

$$\omega_i = -\frac{1}{2} \epsilon_{ijk} \omega_{jk} \quad \omega_{ij} = -\epsilon_{ijk} \omega_k. \quad (2.92)$$

If Q_{ij} is compatible, $U_{ij} = u_{i,j}$ where u_i is a displacement function (2.4) and

$$\omega_{ij,k} = e_{ki,j} - e_{kj,i} \quad (2.93)$$

$$\kappa_{ij} = \omega_{i,j} = -\epsilon_{ilk} e_{jl,k}. \quad (2.94)$$

The curvature κ_{ij} cannot be obtained from a rotation function for incompatible deformations. However, $U_{il} = e_{il} + \omega_{il}$ and $\alpha_{il} = 2\omega_{il}$, so that

$$\begin{aligned} \alpha_{ij} &= -\epsilon_{jkl} (e_{il,k} + \epsilon_{ilm} \omega_{m,k}) \\ &= -\epsilon_{kjl} e_{il,k} + \frac{1}{2} \delta_{ji} \alpha_{kk} + \omega_{j,i}. \end{aligned}$$

Thus

$$\kappa_{ji} = \omega_{j,i} = -\epsilon_{jlk} e_{il,k} + \alpha_{ij} - \frac{1}{2} \delta_{ij} \alpha_{kk}. \quad (2.95)$$

Equation (2.95) reduces to (2.94) when $\alpha_{ij} = 0$, and the curvature may thus be

regarded as the sum of a compatible curvature κ_{ji}' and an incompatible curvature κ_{ij}'' due to dislocations, where

$$\kappa_{ji}'' = \alpha_{ij} - \frac{1}{2}\delta_{ij}\alpha_{kk}. \quad (2.96)$$

Equation (2.96) was obtained by Nye (1953) for a special case and is a measure of the incompatibility of rotations, just as (2.5) measures incompatibility of strains. The relation between α_{ij} and S_{ij} (equation (2.5)) may now be obtained. Since

$$\begin{aligned} \epsilon_{imp}\kappa_{ji,p}'' &= \epsilon_{imp}\epsilon_{jlk}\epsilon_{il,kp} \\ S_{mj} &= \frac{1}{2}(\epsilon_{imp}\alpha_{ij,p} + \epsilon_{ijp}\alpha_{im,p}). \end{aligned} \quad (2.97)$$

The complete set of elastic equations for a continuous distribution of dislocations is now (2.1) (2.2) (2.5) (2.77) and (2.97).

An elastic-plastic deformation may be obtained by cutting a continuum into small volumes, giving each a stress-free deformation Q_{ij}^{pl} , applying elastic surface stresses to return each volume to its original shape, welding the volumes together again, and finally removing the built-in layers of stress. The total shape change of each volume Q_{ij}^{tot} is a compatible deformation, and if the deformations are small may be divided as

$$Q_{ij}^{tot} = Q_{ij}^{pl} + Q_{ij}^{el}. \quad (2.98)$$

The elastic deformations are not compatible because the plastic deformations can be arbitrary. The relations described above arise because noncompatible elastic deformations are needed to reform a compact continuum and these elastic strains imply a dislocation distribution. The division into elastic and plastic strains is used by Kröner (1966), and it follows from the discussion that the lattice rotation is ω_{ij}^{el} . An alternative terminology applies to problems involving interfaces, where the deformations can be larger but discontinuous. The deformation Q_{ij}^{tot} is then called the shape deformation, Q_{ij}^{pl} is called the lattice invariant or dislocation deformation, and Q_{ij}^{el} is called the lattice deformation (Bilby *et al.* 1955, Bilby and Christian 1956). The linear relation (2.98) is not valid for finite deformations and must be replaced by

$$Q_{ij}^{tot} = Q_{ik}^{pl}Q_{kj}^{el}. \quad (2.99)$$

Kröner (1958) has given the general solutions for the elastic equations of a continuous distribution of dislocations. With no body forces (2.1) may be satisfied by setting

$$\sigma_{ij} = \epsilon_{ikl}\epsilon_{jmn}\psi_{lm,kn} \quad (2.100)$$

where ψ_{ij} is a symmetric tensor (the stress function). Equations (2.5) become

$$\nabla^4\chi_{ij} = S_{ij} \quad (2.101)$$

where

$$\begin{aligned} \chi_{ij} &= \frac{1}{2\mu}\left(\psi_{ij} - \frac{\nu}{1+2\nu}\psi_{kk}\delta_{ij}\right) \\ \text{and} \quad \psi_{ij} &= 2\mu\left(\chi_{ij} + \frac{\nu}{1-\nu}\chi_{kk}\delta_{ij}\right). \end{aligned} \quad (2.102)$$

The interaction energy of two stress fields (2.7) transforms by partial integration and use of (2.5) and (2.100) to

$$U_{int}^{1,2} = \int \psi_{ij}^{(1)} S_{ij}^{(2)} dV. \quad (2.103)$$

The general solution of equations (2.101) for an infinite medium is known from the theory of biharmonic functions and gives

$$8\pi\chi_{ij}(\mathbf{r}) = - \int S_{ij}(\mathbf{r}') |\mathbf{r} - \mathbf{r}'| dV' \quad (2.104)$$

and this integral has to be calculated for a given distribution of dislocations.

Very few applications of real continuous distributions of dislocations have been made except to problems in which there are no far-reaching stresses (Bilby 1960, Schottky *et al.* 1965). Pile-ups have been treated as continuous planar arrays (§ 2.5) but the theory of this section is then not required. A singular dislocation loop may be treated as a continuous distribution with

$$\alpha_{ij} = l_i(\mathbf{r}_c') b_j \delta(\mathbf{r}_c' - \mathbf{r}) \quad (2.105)$$

where \mathbf{r}_c' is the position vector of points on the dislocation loop C and l is the unit vector tangent to the curve. Kröner (1958) has calculated ψ_{ij} and σ_{ij} for the general loop (see also de Wit 1960) and obtained formulae identical with those given by (2.23). Using (2.103), a useful expression for the interaction energy of two loops is

$$U_{\text{int}}^{1,2} = b_i^{(1)} b_j^{(2)} M_{ij} \quad (2.106)$$

where

$$M_{ij} = -\frac{\mu}{8\pi} \oint_{C_1} \oint_{C_2} \left\{ \frac{1+\nu}{1-\nu} R_{kk} dx_j^{(1)} dx_i^{(2)} + \frac{2}{1-\nu} (R_{,ij} - R_{,ll} \delta_{ij}) dx_k^{(1)} dx_k^{(2)} \right\} \quad (2.107)$$

is called the ‘dislocation mutual inductance’. In equation (2.107) R has the meaning defined in § 2.2.2.

2.9. The effects of elastic anisotropy

The use of anisotropic elastic theory enables the variation of properties with direction to be taken into account. Most numerical values are changed from isotropic results by no more than 20–50%, which may not be significant in view of the approximations; the more pronounced deviations naturally occur in highly anisotropic materials such as the alkali metals or β -brass. However, some results may be obtained only by the use of anisotropic theory, and increasing attention has been paid to this part of the subject in recent years. In view of the complexity of most of the algebra, this section contains only a general survey of the results which have been obtained.

In cubic crystals, there are only three independent values among the c_{ijkl} of equation (2.2a) and for hexagonal and the more symmetrical tetragonal crystals there are five values (see e.g. Nye 1957, Huntington 1958). For a large class of problems, exact solutions may be obtained in hexagonal symmetry but not in cubic symmetry (Kröner 1953, Eshelby 1956 b, Lifshitz and Rosenzweig 1947, Lejček 1969).

Eshelby *et al.* (1953) used a complex variable method to find the stress and strain fields of an infinite straight dislocation in an anisotropic continuum, and a slightly different method was developed by Stroh (1958). Except in certain symmetrical orientations, the isotropic conditions $u_1 = u_2 = 0$ for a pure screw dislocation and $u_3 = 0$ for a pure edge dislocation do not apply, and a set of linear equations together with a sixth-order algebraic equation have to be solved. Eshelby *et al.* obtained

analytical solutions for a screw dislocation normal to a symmetry plane and an edge dislocation parallel to a fourfold axis of a cubic structure. In general, analytical solutions may be obtained for dislocations parallel to symmetry axes or in planes normal to even-fold symmetry axes, and have been published, for example, for dislocations in basal planes of hcp structures (Seeger and Schoeck 1953, Chou 1962, Chou and Eshelby 1962, Fisher and Alfred 1968, Teutonico 1968, 1969) or parallel to threefold axes of cubic structures (Head 1964 a, b, Chou and Mitchell 1967, Hirth and Gehlen 1969, Steeds 1969). The self-energy of a straight dislocation in an anisotropic medium (Stroh 1958, Foreman 1955) may be expressed in the form

$$E = (Kb^2/4\pi) \ln(R/r_0) \quad (2.108)$$

where the energy factor K is a function of the elastic constants and of the orientation of the Burgers vector with respect to the dislocation line and of the dislocation line itself.

For symmetrical orientations, analytical expressions for K have been obtained, and in general K may be expressed as a Fourier series

$$K = \sum_{n=0}^{\infty} (\alpha_n \cos n\theta + \beta_n \sin n\theta) \quad (2.109)$$

where θ is the angle between b and the line direction l . In some orientations of the dislocation, the line tension becomes negative because of the elastic anisotropy, and the straight dislocation is then unstable (Head 1967). This is discussed further in § 5.1.

An anisotropic calculation of the elastic field and associated energy of a general dislocation configuration has only recently become possible. Indenbom and Orlov (1967, 1968) solved the elastic problem of a finite dislocation segment by using a Green function method which generalizes approaches due to Lothe (1967 b) and Brown (1967). This solution utilizes the derivatives with respect to orientation of the distortions produced by an infinite straight dislocation. Analytical solutions which do not require solution of a set of linear or algebraic equations have been derived by Willis (1970), also by means of a Green function method. Willis gives for the infinite straight dislocation explicit expressions which are easier to apply than the formulations of Eshelby *et al.* (1953) and Stroh (1958), and also derives equations for the distortions produced by a dislocation segment and by any planar dislocation loop. These expressions do not require the analytical solutions for infinite, straight dislocations and can be used directly for the calculation of the stress and strain fields or energies of any dislocation configuration. The expressions are rather complex and will not be reproduced here. The theory has already been applied to the elliptical dislocation loop (Willis 1970) and rhombus-shaped loop (Bacon *et al.* 1970).

The dilatational part of the strain field of a dislocation is the most important component when considering interactions with symmetrical point defects, and has been studied in particular by Chang (1962), Baštecká (1965) and Chou (1965 b). An interesting result is that a screw dislocation has a dilatational field in bcc structures, but not in fcc or hcp structures. Thus even in linear elasticity, screw dislocations interact with centres of dilatation in bcc crystals.

Dislocation reactions and dissociations have been studied by many workers (e.g. Seeger and Schoeck 1953, Spence 1962, Teutonico 1963 a, 1964, 1965 a, b, 1966, 1967, Vítek 1966 a, Thrower 1967, Hartley 1968, Yoa 1968); some of the

results are discussed in §5. Anisotropic theory has also been used in work on arrays, walls, dipoles, quasi-dipoles and pile-ups (Chou *et al.* 1960, Chou and Whitmore 1961, Chang 1962, Mitchell 1964, Jøssang *et al.* 1965, Seeger and Wobser 1966 a, Chou 1967 b, Kratochvíl and Saxlová 1967, Saxlová-Švábová 1967, Kratochvíl 1968, Lejček 1968).

One problem which requires use of anisotropic elasticity is the interaction of a dislocation with a grain or twin boundary. General expressions for the stress field of a dislocation near to a boundary have been given by Pastur *et al.* (1962), Tucker and Crocker (1967), Gemperlová and Saxl (1968) and Tucker (1969), and dislocation-boundary interactions in bcc structures have been calculated by Head (1965), Chou (1966 a, b) and Gemperlová (1968). Finally, Armstrong and Head (1965), Chou (1967 a, b) and Chou and Barnett (1967) have studied pile-ups of dislocations at grain boundaries in anisotropic materials.

3. Dislocations in crystal lattices

3.1. The Frenkel-Kontorova and Peierls-Nabarro models

The continuum approach fails in the dislocation core and other models are required to describe the atomic structure. The best known of these is due to Peierls (1940) and Nabarro (1947), but in recent years core structures have also been described in terms of dislocation dissociations. Finally, numerical calculation of atomic positions using interatomic potentials is now possible, although many difficulties remain to be overcome.

A one-dimensional model of a dislocation was suggested by Dehlinger (1929) and developed by Frenkel and Kontorova (1938). A set of mass points (atoms), connected to each other by springs, interacts with a rigid substrate through a sinusoidal potential of amplitude A and period b equal to the equilibrium atom spacing. A dislocation is obtained if the numbers of atoms and of potential minima differ by one. The equilibrium positions of the atoms are specified by a set of difference equations, which can be approximated by a differential equation, and the solution for the edge dislocation gives the displacement u_n of the n th atom as

$$u_n = \left(\frac{2b}{\pi} \right) \tan^{-1} \left[\exp \left\{ \frac{2\pi A^{1/2}(n+\alpha)}{bk^{1/2}} \right\} \right] \quad (3.1)$$

where k is the spring constant and α specifies the core symmetry with $-\frac{1}{2} \leq \alpha \leq \frac{1}{2}$. The core is symmetrical and stable for $\alpha = \pm \frac{1}{2}$ and unstable for $\alpha = 0$, and exact solutions of the difference equations are then available (Hobbart and Celli 1962, Schiller and Seeger 1963). Indenbom (1958 b) generalized the model for non-sinusoidal potentials and Kratochvíl (1965 a) solved the difference equations graphically in such a case. Representations of other configurations, e.g. a series of equally spaced dislocations (Kochendörfer and Seeger 1950) or two opposite edge dislocations (Kratochvíl 1965 b), are also possible. The Frenkel-Kontorova model is a better representation of an atomic layer on a substrate than of a lattice dislocation, and Frank and van der Merwe (1949) and Kochendörfer and Seeger (1950) applied it to epitaxial growth by introducing a difference in the spacing of the atoms in the chain and the period of the potential.

In the Peierls-Nabarro model, an edge dislocation is obtained by suitably displacing two elastic half-crystals at the plane $x_2 = 0$, and assuming that in this plane there is a non-linear periodic shear stress between the two half-crystals.

The disregistry is specified by

$$\Phi_1(x_1) = \begin{cases} 2u_1(x_1) + \frac{1}{2}b & x_1 > 0 \\ 2u_1(x_1) - \frac{1}{2}b & x_1 < 0 \end{cases} \quad (3.2)$$

where $u_1(x_1)$ is a displacement function antisymmetric about the plane $x_2 = 0$ and

$$u_1(+\infty) = -u_1(-\infty) = -\frac{1}{4}b. \quad (3.3)$$

This is equivalent (Eshelby 1949 a) to a continuous distribution of edge dislocations of density

$$\rho_D(x_1) = -\frac{2}{b} \left\{ \frac{du_1(x_1)}{dx_1} \right\} \quad (3.4)$$

and the Burgers vector between x_1 and $x_1 + dx_1$ is $-2 du_1(x_1)$. From (2.14) the elastic shear stress in the plane $x_2 = 0$ is

$$\sigma_{12}(x_1, 0) = \left\{ \frac{\mu}{\pi(1-\nu)} \right\} \int_{-\infty}^{+\infty} \frac{(du_1(x_1)/dx_1)_{x_1=x'}}{x_1 - x'} dx'. \quad (3.5)$$

The interaction between the two atomic planes $x_2 = \pm h$ leads to restoring forces with period b . In simplest approximation the restoring stress is

$$\sigma_{12} = \frac{\mu b}{2\pi h} \sin \left\{ \frac{4\pi u_1(x_1)}{b} \right\} \quad (3.6)$$

where the force law is assumed sinusoidal and the constant is fixed by requiring Hooke's law to be valid in the limit of small shear. Equations (3.5) and (3.6) give the integral equation for the equilibrium displacement, the solution of which with the boundary condition (3.3) is

$$u_1 = -\frac{b}{2\pi} \tan^{-1} \left(\frac{x_1 + \alpha b}{\zeta_e} \right) \quad (3.7)$$

where

$$\zeta_e = \frac{1}{2}h/(1-\nu) \quad (3.8)$$

and α is a constant which determines the core symmetry, with $0 \leq \alpha \leq 1$. The width of the core may be measured by $2\zeta_e$ since for $-\zeta_e < x_1 < \zeta_e$ the disregistry is greater than half its maximum value at $x_1 = 0$. From (3.6) and (3.7) the shear stress in the slip plane is

$$\sigma_{12}(x_1, 0) = B_e z_1 / (z_1^2 + \zeta_e^2) \quad (3.9)$$

where $z_1 = x_1 + \alpha b$. Substituting (3.7) into (3.4) gives

$$\rho_D(x_1) = \zeta_e / \pi(z_1^2 + \zeta_e^2) \quad (3.10)$$

and the stress field is

$$\sigma_{ij}(x_1, x_2) = \int_{-\infty}^{+\infty} \rho_D(x') \sigma_{ij}' dx' \quad (3.11)$$

where σ_{ij}' is the field of an edge dislocation evaluated at $(x_1 - x', x_2)$. This gives for the shear stress components

$$\sigma_{12} = -B_e z_1 \frac{(z_1^2 + z_2^2 - 2x_2 z_2)}{(z_1^2 + z_2^2)^2} \quad (3.12)$$

where $z_2 = x_2 \pm \zeta_e$ for $x_2 > 0$ and $x_2 < 0$ respectively. Equations (3.9) and (3.12) reduce to (2.14) with the dislocation along the line $x_1 = \alpha b$ when $(x_1^2 + x_2^2)^{1/2} \gg \zeta_e$.

The energy in this model consists of the elastic energy stored in the two parts of the crystal plus the misfit energy across the plane $x_2 = 0$, which is the effective core energy. Within a cylinder of radius R , the elastic energy per unit length is

$$E_{\text{el}} = \int_0^R \sigma_{12}(x_1, 0) u_1(x_1) dx_1 = \frac{1}{2} B_e b \ln(R/2\zeta_e) \quad (3.13)$$

but if the work done by the forces on the surface of the cylinder is included this becomes

$$E_{\text{el}} = \frac{1}{2} B_e b \{\ln(R/2\zeta_e) + \frac{1}{2}\}. \quad (3.14)$$

The misfit energy of the ribbon of unit length and width dx_1 is

$$dE_c = - \left\{ \int_0^{\Phi_1} \sigma_{12}(x_1, 0) d\Phi_1 \right\} dx_1 = (\mu b^2 / 4\pi^2 h) \{1 + \cos(4\pi u_1/b)\} dx_1 \quad (3.15)$$

and the total core energy is

$$\int_{x_1=-\infty}^{+\infty} dE_c = \frac{1}{2} B_e b. \quad (3.16)$$

Thus, the total energy of the Peierls–Nabarro dislocation is

$$E_{\text{tot}}^e = \frac{1}{2} B_e b \{\ln(R/2\zeta_e) + \frac{3}{2}\} \quad (3.17)$$

and this is identical with (2.16) if the cut-off parameter is taken as

$$r_0 = 2\zeta_e/e^{3/2}. \quad (3.18)$$

The model may also be applied to a screw dislocation (Eshelby 1949 b), but it is then not clear in which crystallographic plane the misfit energy should be calculated. The displacement is

$$u_s(x_1, 0) = -B_s \tan^{-1}(x_1/\zeta_s) \quad (3.19)$$

where $\zeta_s = \frac{1}{2}h$. The total energy is correspondingly

$$E_{\text{tot}}^s = \frac{1}{2} B_s b \{\ln(R/2\zeta_s) + 1\} \quad (3.20)$$

and the equivalent cut-off radius (from (2.12)) is $2\zeta_s/e$.

The very narrow core of equation (3.8) is a consequence of the sinusoidal force law; more realistic interactions with the same initial slope (fixed by Hooke's law) but lower maxima forces will give greater widths. Foreman *et al.* (1951) examined such laws; in the case that $\alpha = 0$, the displacement becomes

$$u_1(x_1, 0) = \frac{b}{2\pi} \left[\tan^{-1} \left(\frac{x_1}{\zeta} \right) + \frac{((\zeta - \zeta_e)x_1)}{x_1^2 + \zeta^2} \right] \quad (3.21)$$

which does not differ appreciably in form from (3.7) but allows the width ζ to be arbitrary.

Nabarro (1947) and Pearson *et al.* (1957) applied this model to a pair of opposite edge dislocations, and these results are important in the calculation of the stresses needed to create dislocation pairs or a dislocation loop. van der Merwe (1950) and Kochendörfer and Seeger (1950) used the Peierls model to study tilt and twist boundaries and orientated overgrowths, and Jaswon and Foreman (1952) applied it to pile-ups. Leibfried and Dietze (1951) and Seeger and Schoeck (1953) included displacements in both x_1 and x_2 directions in order to calculate the core structure of a dissociated dislocation. The applications of the model to the calculation of the stress needed to move a dislocation and to dislocation dynamics are discussed in §§ 3.4 and 6.3 respectively.

3.2. Dissociation models

When a lattice dislocation dissociates, the separation of the partials varies inversely as the fault energy. If this separation is of the order of the Burgers vector, the partials are not well defined but the dissociation may be taken as a description of a dislocation core in which the displacement undergoes several sharp jumps (see figure 4).

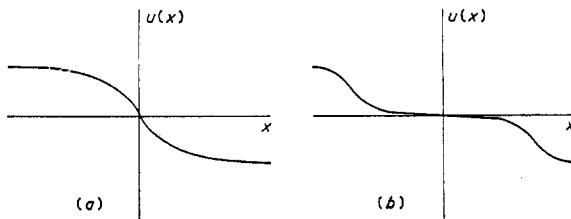


Figure 4. Schematic representation of the dependence of the displacements $u(x)$ on x for (a) an undissociated core, (b) a core dissociated in one plane.

Figure 4(b) represents a core extended in one plane, but dissociation on several nonparallel planes which intersect on the dislocation line is also possible, and the core structure is then three-dimensional. This model has been used extensively for a screw dislocation in the bcc lattice, where three $\{1\bar{1}0\}$ and three $\{11\bar{2}\}$ planes intersect in a $\langle 111 \rangle$ direction, and a more detailed discussion is given in §5.4. In most cases, the separation of the partial dislocations has been obtained by an elastic calculation, but since the expected separations are very small this is clearly unjustified.

As described in §1.3, Vítek (1968) defined a generalized stacking fault by equation (1.2), and he calculated the energy of such faults, $\gamma(x, y)$, by atomic relaxation methods for $\{111\}$ planes in fcc crystals and $\{112\}$ and $\{110\}$ planes in bcc crystals. For the fcc structure, local minima in γ were found corresponding to the expected $1\triangledown$ faults, but no minima were found on either plane of the bcc structure. Fontaine (1968 a, b) obtained a similar result for NaCl type structures.

The absence of minima implies that large stacking faults are unstable, but core dissociations involving 'fault' configurations are still possible. Vítek and Kroupa (1969) introduced the concept of generalized dislocation dissociation, in which the configuration of partials and unstable stacking faults is stabilized by the elastic interaction of the partials. For a selected number of partial dislocations and fault planes, the γ surfaces of which are known, the dislocation energy can be minimized by treating the Burgers vectors of the partials (and correspondingly the fault vectors) as variables. When the γ surfaces have local minima, the generalized splitting of a dislocation is almost identical with the usual assumption that the fault vector is fixed, and the partial dislocations are well defined (e.g. fcc and hcp crystals). When there are no local minima, the Burgers vectors of the partials are not defined in advance but must be calculated. The separation of the partials is then small even for relatively low values of γ because a decrease in γ increases the Burgers vectors of the partials rather than their separation. This generalized splitting can provide a particularly suitable model for a dislocation core if the stacking fault planes and number of partials are known, e.g. from atomic calculations.

An alternative approach is to consider the core as a continuous distribution of partial dislocations as suggested by Fontaine (1968 b). Consider, for example, an

edge dislocation with a planar dissociation, and assume, as in the Peierls–Nabarro model, that all partials also have Burgers vectors parallel to the x_1 -axis. The density of partials is given by $\rho_D(x_1) = (d\Phi/dx)/b$, where Φ as before is the disregistry across the $x_2 = 0$ plane and is a function only of x_1 . The elastic energy of dissociation is

$$E_{el} = -\frac{1}{2}B_e b \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \rho_D(x_1) \rho_D(x') \ln(|x_1 - x'|/r_0) dx_1 dx'. \quad (3.22)$$

The stacking fault energy is

$$E_\gamma = \int_{-\infty}^{+\infty} \gamma(\Phi) dx_1 \quad (3.23)$$

where $\gamma(\Phi)$ is the fault energy for a particular disregistry. The equilibrium configuration is now found by functional minimization of the total energy $E_{el} + E_\gamma$ with respect to Φ , so that

$$\delta E_{tot}(\Phi) = 0 \quad (3.24)$$

and a necessary condition is

$$B_e \int_{-\infty}^{+\infty} \left\{ \frac{1}{|x_1 - x'|} \right\} \left(\frac{d\Phi}{dx'} \right) dx' = -\frac{\partial \gamma}{\partial \Phi}. \quad (3.25)$$

Equation (3.25) is identical with that obtained by equating (3.5) and (3.6) if Φ is expressed as in (3.2) and the shear stress (3.6) is replaced by $-(\partial \gamma / \partial \Phi)$. Thus the assumption of a continuous distribution of partials is identical with the Peierls–Nabarro model if the partial derivatives of the γ surface represent the restoring forces across the cut plane. Hobbart (1968 b, 1969) used this approach to study slightly dissociated dislocations; he assumed a force law similar to equation (3.6) which gives stable infinite stacking faults. A corresponding treatment for a continuous distribution on several crystallographic planes, which would represent a generalization of the Peierls–Nabarro model, has not yet been achieved.

3.3. Atomic models

A full treatment of the atomic structure of a dislocation requires consideration of the interactions between all the individual atoms of a crystal in order to find a stable configuration which reduces to the elastic solution far from the core. Two difficulties arise. Firstly, knowledge of interatomic forces is very limited and rough approximations have to be used. Secondly, the relaxation procedures used in the calculations are very time-consuming, even with high-speed computers.

In early work, a discrete elastic approach was used, and the structure was represented as a series of mass points connected by elastic springs. Fues and Stumpf (1955) and Fues *et al.* (1958) developed a model in which the nonlinear forces between atoms were treated as a perturbation of the linear forces, as in classical nonlinear elasticity. They found a solution for edge and screw dislocations in a simple cubic structure. Babuška *et al.* (1960 a, b) used central interatomic forces of type $f_i = f_{0i} + k(a_i - r_i)$ where a_i is the equilibrium distance of the atoms, r_i their separation in the lattice containing a defect and k is the force constant. The force f_{0i} which occurs at the equilibrium separation represents a prestressing. Periodic Born–Karman boundary conditions were imposed, and the equilibrium equations were solved by application of the discrete Fourier transform. The solution for an edge dislocation in the simple cubic lattice was obtained.

Maradudin (1958) found an exact solution for a discrete elastic model of a screw dislocation in a simple cubic lattice. Only displacements parallel to \mathbf{b} were allowed, and the displacement was assumed to be a function of x_1 and x_2 only. The crystal is thus treated as rows of atoms which move only as solid rods along their length in the x_3 -direction. Each row interacts with its four nearest neighbours through an elastic force proportional to their relative displacements, and the dislocation was introduced as a discontinuity in this displacement across a cut. This method was applied by Celli (1961) to screw dislocations in the diamond structure.

A modification of Maradudin's method was used by Suzuki (1968) who used nonlinear force laws rather than discrete elasticity to calculate the core structure of a $\frac{1}{2}\alpha\langle111\rangle$ screw dislocation in bcc structures. Interactions were considered only between each atomic row and its six nearest neighbours and were of type

$$\phi_{ij} = A \cos \{2\pi(x_3^{(i)} - x_3^{(j)})/b\} \quad (3.26)$$

where ϕ_{ij} is a potential energy and $x_3^{(i)}$ is the coordinate of an atom on the i th row. The potential is thus repulsive for close approach of two atoms, and attractive for large separations; the constant A was adjusted to give the correct shear modulus in $\langle111\rangle$. The atomic rows far from the dislocation centre were fixed in the elastic solution positions, and all other rows were relaxed parallel to x_3 until the force on each was zero. The difference between the relaxed and the elastic positions of the atoms was found to be rather small, even in the core.

Gallina and Omini (1964) and Gallina *et al.* (1965 a, b) considered the dislocation as a perturbation in the phonon field of a perfect crystal. Linear elastic interaction between atoms was assumed, as in the study of lattice vibrations, so that this is again a modification of the discrete elastic model. Dispersion curves with two phase velocities were finally chosen, as in the Debye model; when the Debye radius is allowed to increase to infinity, this model reduces to a pure continuum model (Vitek 1966 b).

Discrete elastic theory has also been extensively used for point defects and their interactions with dislocations (Hardy and Bullough 1967, Bullough and Perrin 1968 a, Englert and Bullough 1969). A detailed account of the method has been given by Flocken and Hardy (1969).

Discrete elastic models cannot be good approximations for very large deviations of the atomic structure from the defect-free equilibrium configuration, and it is just this situation which is expected in a stacking fault or a dislocation core. A more general interatomic interaction, truncated to a reasonable number of neighbours, is therefore required, and this procedure will now be outlined. A finite crystal block is chosen and the surface atoms are given displacements into the positions given by the elastic field (isotropic or anisotropic) of a dislocation somewhere in the centre of the block. The remainder of the crystal is treated as an elastic continuum, and the inner and outer parts are cemented together using either rigid or flexible boundary conditions (Gibson *et al.* 1960). The inner atoms of the block are then relaxed by a static or dynamic method.

In most cases, a central force potential $\phi(r)$ is used to describe the main part of the atomic interactions, and noncentral forces are included only through a 'deformation energy' U_D , which depends only on the total deformation of the lattice, e_{kl} . The lattice energy is then

$$U = \frac{1}{2} \sum_{i,j} \phi(|\mathbf{r}_i - \mathbf{r}_j|) + U_D(\mathbf{e}_{kl}) \quad (3.27)$$

where \mathbf{r}_i is the position vector of the i th atom, and the perfect lattice is defined by $\mathbf{r}_i = \mathbf{r}_i^0$, $e_{kl} = 0$. For small deformations

$$U_D = \frac{1}{2} \sigma_{kl} e_{kl} \quad (3.28)$$

and (Born and Huang 1954)

$$\sigma_{kl} = \frac{1}{2v_a} \sum_{i,j} \frac{x_{ik}^0 x_{jl}^0}{|\mathbf{r}_i^0 - \mathbf{r}_j^0|} \frac{\partial \phi(|\mathbf{r}_i^0 - \mathbf{r}_j^0|)}{\partial (|\mathbf{r}_i^0 - \mathbf{r}_j^0|)} \quad (3.29)$$

where x_{ik}^0 is the k th component of \mathbf{r}_i^0 and v_a is the volume of a unit cell. The summations in (3.27) and (3.29) extend over all the atoms of the crystal.

For cubic symmetry, (3.28) reduces to

$$U_D = p \Delta V \quad (3.30)$$

where ΔV is the total lattice dilatation, and the hydrostatic pressure $p = -\frac{1}{3}\sigma_{kk}$. In the relaxation calculations, U_D can be included either directly or by the application of the stress σ_{kl} on the boundary. However, the total dilatation is negligible for many crystal defects, and U_D may be ignored.

Various calculations (e.g. Harrison 1966, Hodges 1967 a, b, Pick 1967, Meyer *et al.* 1968, Weaire 1968, Duesbery and Taylor 1969) show that for simple metals the part of the energy which depends on atomic positions is equivalent to a central force interaction, and thus provide some justification for (3.27). The remaining part of the lattice energy may be larger but is determined mainly by the average density of the matter, and thus when the number of atoms and the total volume of the crystal are conserved, the change in this energy may again be unimportant, even though the linear approximation (3.28) or (3.30) is not generally valid. In higher approximations, the lattice energy will also contain additional terms, the significance of which it is difficult to assess, especially for more complex metals. Certainly the central force approximation is of doubtful validity for transition metals. Nevertheless it appears that some defect properties are dependent mainly on the crystal structure and not on the details of the interatomic forces (e.g. the 'shape' of the screw dislocation in bcc metals (Vitek *et al.* 1970)). The value of the central force model is that it enables the stability of a particular crystal structure to be ensured, and hence those properties which depend on structure only to be studied. The following potentials have been extensively used in relaxation calculations:

$$(a) \quad \phi(r) = B \exp(-\beta r) \quad (3.31)$$

$$(b) \quad \phi(r) = A \{(r_0/r)^{12} - 2(r_0/r)^6\} \quad (3.32)$$

$$(c) \quad \phi(r) = D [\exp \{-2\alpha(r - r_0)\} - 2 \exp \{-\alpha(r - r_0)\}] \quad (3.33)$$

$$(d) \quad \phi(r) = \sum_{k=0}^n a_k r^k \quad (3.34)$$

(e) oscillating potentials which for larger r have forms such as

$$\phi(r) = A \cos(2k_F r)/r^3 \quad (3.35a)$$

$$\phi(r) = B \sin(2k_F r + \alpha)/(2k_F r)^5. \quad (3.35b)$$

All potentials except (a) are repulsive at small separations and attractive at large r ; r_0 is the equilibrium separation for an isolated pair and k_F is the Fermi wave vector. The Born and Mayer (1932) potential (a) is entirely repulsive and external forces are needed to ensure lattice stability; B and β may be fixed from elastic constants

(Huntington and Seitz 1942, Gibson *et al.* 1960). Potential (*b*) (Lennard-Jones 1937) is a good approximation for solid rare gases. The Morse potential (*d*) is longer-range and is usually truncated; D , α and r_0 may be chosen to give the correct sublimation energy and bulk modulus and zero p in equation (3.30) (Girifalco and Weizer 1959). Equation (3.34) is the general form of the Johnson (1964) potential for iron, which is usually truncated to a given number of neighbours. The constants a_k of a polynomial form are chosen to fit linear and higher order elastic constants (e.g. Chang and Graham 1966 a, Vitek *et al.* 1970) and other physical properties such as phonon dispersion curves. Oscillating potentials were developed from the theory of pseudo-potentials (e.g. Harrison 1966, Pick 1967, Wei-Mei Shyu and Gaspari 1968), model potentials (e.g. Heine and Abarenkov 1964, Animalu and Heine 1965, Hodes 1967 a, b, Weaire 1968) and recently from first-principle calculations (e.g. Duesbery and Taylor 1969). They were also derived from electron-ion scattering amplitudes (Meyer *et al.* 1968) and from neutron scattering data for liquid metals (Johnson *et al.* 1964). These potentials are for large r usually of the form (3.35a) or (3.35b).

The static relaxation method, described in more detail by Doyama and Cotterill (1965), involves gradual shifts of the atoms until the force on each is zero. The dynamical method (Gibson *et al.* 1960) was originally developed for the study of radiation damage and is an iterative integration of the classical equations of motion of the N atoms of the inner block,

$$\begin{aligned} m\dot{v}_{i\alpha}(t) &= F_{i\alpha}\{x_{j\beta}(t)\} \quad i = 1, \dots, n \\ \dot{x}_{i\alpha}(t) &= v_{i\alpha}(t) \quad \alpha = 1, 2, 3 \end{aligned} \quad (3.36)$$

where $x_{i\alpha}$, $v_{i\alpha}$ are the coordinates and velocity components of the i th atom and $F_{i\alpha} = -\partial U/\partial x_{i\alpha}$ is the force acting on it. The derivatives are replaced by differences, and from an initial set of coordinates and velocities, the positions and velocities after successive intervals of time Δt , $2\Delta t$, ..., $n\Delta t$ are calculated until a stable configuration is attained. This may be defined by a maximum kinetic energy, which is equivalent to a minimum potential energy.

An early calculation (Huntington *et al.* 1955, 1959) was made for edge and screw dislocations in NaCl using electrostatic attractions (Madelung 1919) and Born-Mayer repulsions. Rows of ions were treated as solid rods, but not restricted to motion parallel to their length, and the width of the edge dislocation was found to be close to that given by the Peierls-Nabarro model. A similar calculation with varying repulsive potentials has recently been published by Granzer *et al.* (1968).

Englert and Tompa (1961, 1963) computed core structures in a two-dimensional close-packed lattice; they used Lennard-Jones potentials for argon and Morse potentials for copper, silver and gold, and found very narrow cores. Cotterill and Doyama (1966) and Doyama and Cotterill (1966) calculated edge and screw core structures in three-dimensional fcc metals with Morse potentials fitted to the constants of copper and truncated to 179 neighbours. The dislocations had $\frac{1}{2}a\langle 110 \rangle$ Burgers vectors and were undissociated when relaxation was allowed only parallel to \mathbf{b} . With full relaxation, however, the dislocations split into partials on $\{1\bar{1}1\}$ planes (with very narrow cores) as is usually assumed.

Chang and Graham (1966 b) used a Johnson type potential limited to second-nearest neighbours to calculate the core structure of a bcc $\frac{1}{2}a\langle 111 \rangle$ edge dislocation on a $\{10\bar{1}\}$ plane by the static method. No dissociation of the core, of width $1-2b$, was found. Chang (1967) found the width of a screw dislocation also to be about

$2b$, but he interpreted the structure as three partial dislocations of Burgers vector $\frac{1}{3}a\langle 111 \rangle$ on the intersecting $\{10\bar{1}\}$ planes at mutual separations of about b . Bullough and Perrin (1968 b) and Gehlen *et al.* (1969) calculated the structure of the bcc screw dislocation by the dynamical method. These workers also used the Johnson potential for iron truncated to second neighbours, but whereas Bullough and Perrin reported a core dissociated on $\{11\bar{2}\}$ planes, Gehlen *et al.* conclude that the core is very narrow and not dissociated.

These discrepancies illustrate the difficulties of either making the calculations or interpreting the results; some of them may arise from inadequate size of crystal block or incorrect boundary conditions. Recently Vitek *et al.* (1970) have calculated the screw dislocation configuration for several Johnson type potentials and Basinski *et al.* (1970) have made a similar calculation with a potential appropriate to sodium (Duesbery and Taylor 1969). In both cases, two possible configurations of the dislocation, differing slightly in energy, were found (Suzuki 1968), but the differences are only noticeable at the very centre of the dislocation. Figure 5 shows the low-energy ('easy') configuration according to Vitek *et al.* The structure is projected along $[111]$ and the arrows represent the $[111]$ component of the relative displacement of two atoms due to the dislocation, plotted on a scale such that displacement $\frac{1}{3}a[111]$ is just equal to the minimum separation of atoms in the projection. The dislocation centre coincides with a threefold screw axis and the displacements within the core are concentrated on three $\{10\bar{1}\}$ planes radiating from the centre and on three $\{11\bar{2}\}$ planes displaced from the centre. The displacements on $\{10\bar{1}\}$ planes (marked by broken curves in figure 6) extend on only one side of the core and decrease monotonously with distance from the centre. The displacements on $\{11\bar{2}\}$ planes extend in twinning directions only and are interpreted as narrow regions of stacking faults. This interpretation is shown in figure 5.

Basinski *et al.* (1970) also find the structure to have threefold symmetry; however, the concentration of displacement on the $\{10\bar{1}\}$ planes is not so marked, nor is there marked asymmetry between the two sides of a $\{10\bar{1}\}$ plane extending through the core.

The structure of an $a\langle 100 \rangle$ edge dislocation in a bcc structure has been calculated by Bullough and Perrin (1968 b). They conclude that the core is extremely narrow and it forms a micro-crack immediately below the slip plane. The same result has been obtained by Gehlen *et al.* (1968).

3.4. The Peierls barrier or lattice friction stress

The periodic variation of the core energy of a dislocation as the dislocation is displaced represents a barrier to dislocation motion, and the stress needed to move the dislocation over this barrier is called the Peierls stress. The first calculations were made by Peierls (1940) and Nabarro (1947) on the basis of the model described in § 3.1. In equation (3.16) the effects of the discrete lattice are smoothed out by the integration, and to calculate the Peierls barrier the misfit energy has to be summed over the atom rows in the plane of the cut. Nabarro suggested this sum should be made independently over the top and bottom rows, and the energy per row is half that given by (3.15), so that if the width of ribbon dx_1 is equal to b ,

$$\begin{aligned}\Delta E_c(x) &= (\mu b^3/8\pi^2 h) [1 + \cos \{4\pi u_1(x_1)/b\}] \\ &= (\mu b^3/4\pi^2 h) \{\zeta_e^2/(\zeta_e^2 + z_1^2)\}. \end{aligned}\quad (3.37)$$

If the equilibrium position corresponds to $\alpha = 0$, the translation of the dislocation is αb and the coordinates of the rows of atoms are $\frac{1}{2}nb$, so that the misfit energy of the displaced dislocation is

$$E_c(\alpha) = \frac{\mu b \zeta_e^2}{\pi^2 h} \sum_{n=-\infty}^{+\infty} \{(2\zeta_e/b)^2 + (2\alpha + n)^2\}^{-1}. \quad (3.38)$$

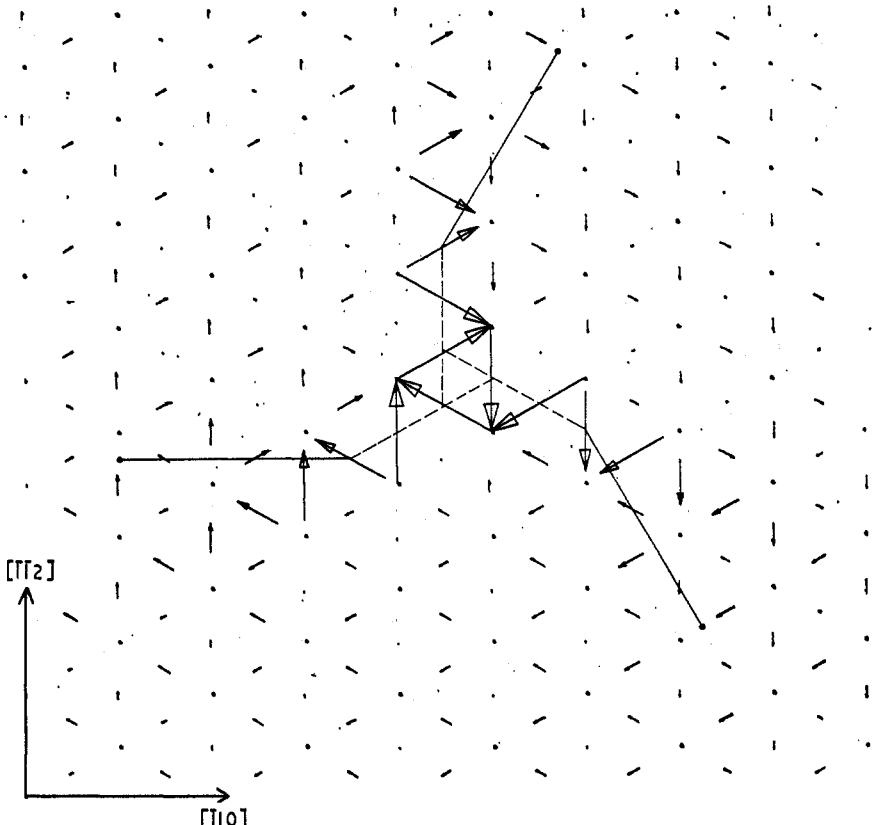


Figure 5. Map of displacements for a $\frac{1}{2}a[111]$ screw dislocation in a bcc crystal according to Vitek *et al.* (1970). The atom positions marked by dots are those of the undislocated lattice, projected along [111]. The arrows joining neighbouring atoms represent the difference in the [111] component of the separation of these atoms in the dislocated and undislocated lattices. The arrows are centred on the mid-points of the dislocated atom pairs, so that (very small) displacements normal to [111] are shown by their deviations from the centre and the direction of the line connecting corresponding atoms. The arrows are scaled so that an arrow of length equal to the smallest projected separation of two atoms represents a displacement of the magnitude $|\frac{1}{2}a[111]|$. The direction of the arrows gives the sign of the displacements.

This sum has been evaluated directly by Cottrell and Nabarro (Cottrell 1953) and gives

$$E_c(\alpha) = \frac{1}{2}B_e b + B_e b \exp(-4\pi\zeta_e/b) \cos 4\pi\alpha. \quad (3.39)$$

This is the Peierls energy barrier expressed as a function of the dislocation displacement, αb . The quantity

$$E_p = 2B_e b \exp(-4\pi\zeta_e/b) \quad (3.40)$$

is the difference between the maximum and minimum values of $E(\alpha)$ and is called the Peierls energy. The corresponding Peierls stress is then

$$\sigma_p = \frac{1}{b^2} \left(\frac{\partial E_c(\alpha)}{\partial \alpha} \right)_{\max} = \frac{2\pi E_p}{b^2}. \quad (3.41)$$

According to (3.40) and (3.41), the Peierls barrier and stress decrease rapidly with increasing width of the core.

Hirth and Lothe (1968 a) point out that according to (3.39) the energy is a maximum for the two symmetrical configurations, $\alpha = 0, \frac{1}{2}$, and a minimum for the asymmetrical configuration, $\alpha = \frac{1}{4}$. Moreover, the barrier has to be surmounted twice as the dislocation moves through b . This occurs because of the independent

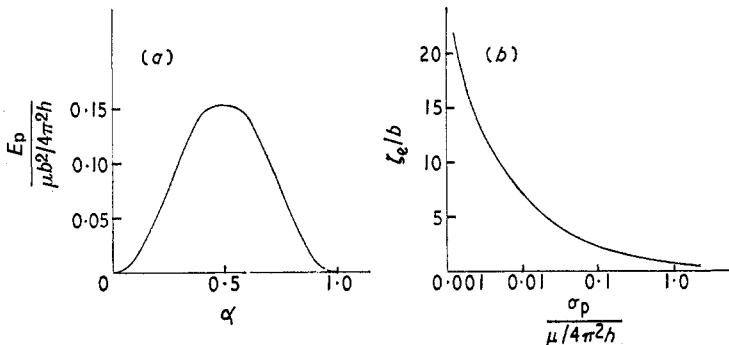


Figure 6. (a) Peierls barrier for $\zeta_e/b = 1$. (b) Peierls stress as a function of ζ_e .

summations in (3.38) and it is physically more reasonable to sum the interaction energy between pairs of atom rows, which is a function of Φ_1 . Assuming interaction only between nearest rows, the energy becomes

$$\begin{aligned} \Delta E_{\text{int}}(\Phi_1) &= (\mu b^2/4\pi^2 h) \{1 - \cos(2\pi\Phi_1/b)\} \quad |\Phi_1| < \frac{1}{2}b \\ \Delta E_{\text{int}}(\Phi_1) &= 0 \quad |\Phi_1| > \frac{1}{2}b \end{aligned} \quad (3.42)$$

which implies the force law (3.6). The Peierls stress can now be found by summing the interaction energy of all rows of atoms adjacent to the cut plane when Φ_1 is given by (3.2) and (3.7) (Vítek, unpublished work). Figures 6(a), (b) show the results of numerical calculations of the Peierls barrier as a function of α , and of the Peierls stress as a function of ζ_e . The minimum and maximum energy configurations now occur at $\alpha = 0$ and $\alpha = \frac{1}{2}$ respectively, and the stress again decreases rapidly with increasing width of the core.

Calculations of the Peierls barrier using the Frenkel-Kontorova model were made by Indenbom (1958 b) and extended by Kratochvíl and Indenbom (1963) and Kratochvíl (1965 a). With the simplest force law, the energy varies exponentially with width, as in (3.40), but with other potentials cases were found when the stress was zero for a finite width. Similar results were obtained for Peierls-Nabarro type models by Kurosawa (1962) and Sanders (1962). However, a detailed analysis of the barrier in the Frenkel-Kontorova model (Hobbart and Celli 1962, Hobbart 1965, 1968 a) has confirmed the exponential dependence on core width.

The mobility of screw dislocations in bcc structures has been extensively studied with the dissociated core model (Escaig 1966, 1967, Vítek and Kroupa

1966, Kroupa and Vitek 1967, Duesbery and Hirsch 1968, Duesbery 1969). The energy barrier to be overcome is represented by the transformation from a sessile to a glissile configuration; this is discussed further in § 6.3.

Several attempts have been made to calculate the Peierls barrier by moving the elastic centre of a dislocation from a stable position and evaluating the energy by atomistic relaxation (Chang and Graham 1966 b, Chang 1967). Suzuki (1968) used the model described in § 3.3, but found that the relaxation always returned the core to the symmetrical configuration. Granzer *et al.* (1968) evaluated the barrier for dislocations in NaCl and Teichler (1967) for dislocations in the diamond structure. However, a correct calculation of the barrier by relaxation procedures requires the application of an external stress to the boundary of the crystal, and this has not yet been accomplished.

4. Dislocation dynamics

4.1. Undamped dislocation motion

The variation of dislocation velocity with stress has been measured by etch pitting to identify the position of a dislocation before and after a stress pulse of known duration (e.g. Johnston and Gilman 1959, Stein and Low 1960, Erickson 1962, Schadler 1964, Stein and Laforce 1965, Prekel and Conrad 1967, Guiu 1968), and has also been derived indirectly from measurements of overall strain rate. The single dislocation results are usually fitted to an empirical equation

$$\dot{x} = (\sigma/\sigma_0)^m \quad (4.1)$$

where \dot{x} is velocity and σ is shear stress, or to

$$\dot{x} = \dot{x}_0 \exp(-\sigma_0/\sigma) \quad (4.2)$$

(Gilman 1960). The parameters in these equations are generally functions of temperature.

The motion of the dislocation is resisted by lattice forces, by interaction with obstacles and internal stress fields arising from other defects, and by energy dissipation through emission of sound waves, phonon scattering, etc. Thermal fluctuations can assist the dislocation to overcome the lattice field or short-range obstacles, and the flow stress is then very sensitive to temperature and strain rate (see § 6). Energy dissipation is important mainly at high velocities; however, it is convenient to consider first undamped dislocation motion.

The equations of motion for an elastic continuum are derived from (2.1) by adding the inertial force $-\rho \ddot{u}_i$, where ρ is material density, to the left-hand side. Thus for a screw dislocation with velocity \dot{x}_1 ,

$$\frac{\partial^2 u_3}{\partial x_1^2} + \frac{\partial^2 u_3}{\partial x_2^2} - \frac{\ddot{u}_3}{c_t^2} = 0 \quad (4.3)$$

where $c_t = (\mu/\rho)^{1/2}$ is the velocity of transverse sound waves (Eshelby 1949 b, Frank 1949, Leibfried and Dietze 1949). The 'relativistic' transformation

$$\beta x_1' = (x_1 - \dot{x}_1 t) \quad \beta = \{1 - (\dot{x}_1^2/c_t^2)\}^{1/2} \quad (4.4)$$

enables equation (4.3) to be written

$$\frac{\partial^2 u_3}{\partial x_1'^2} + \frac{\partial^2 u_3}{\partial x_2^2} = 0 \quad (4.5)$$

and the solution (see equation (2.9)) is

$$u_3 = (b/2\pi) \tan^{-1}(x_2/x_1') \quad (4.6)$$

with corresponding nonzero stresses

$$\sigma_{13} = -\frac{B_s x_2}{\beta(x_1'^2 + x_2^2)} = -\frac{\sigma_{23} x_2}{\beta x_1'}. \quad (4.7)$$

As the velocity increases ($\beta \rightarrow 0$) the stress field contracts and intensifies towards the $x_2 x_3$ plane. In the limit $\dot{x}_1 = c_t$, the stresses vanish everywhere except on the $x_2 x_3$ plane through the dislocation, where they are infinite.

The force between two screw dislocations moving with equal velocity \dot{x}_1 on the same slip plane is $B_s b\beta/d$ where d is the separation, and is thus a factor β lower than the force between stationary dislocations at the same separation; this might cause, for example, a decrease in the width of dissociated, fast-moving dislocations. On parallel slip planes, separation h , the force becomes $B_s b\beta h/(d^2 + \beta^2 h^2)$ in comparison with the stationary force $B_s b h/(d^2 + h^2)$. For small parallel separations d , this force increases with speed, which might assist cross glide in certain circumstances.

The energy U_{sm} of the moving dislocation consists of the strain energy plus the kinetic energy $\frac{1}{2}\rho \int u_3^2 dV$. Applying the transformation (4.4) and noting that u_3 depends only on x_2/x_1'

$$U_{sm} = \frac{\mu}{2\beta} \int \left\{ \left(\frac{\partial u_3}{\partial x_1'} \right)^2 + \left(\frac{\partial u_3}{\partial x_2} \right)^2 \right\} dV. \quad (4.7)$$

Because of (4.6), the integral has the same value as for a stationary dislocation, and the energy per unit length $E_{sm} = U_{sm}/l$ becomes

$$E_{sm} = E_s/\beta \quad (4.8)$$

where E_s is given by (2.12). The energy becomes infinite when $\dot{x}_1 = c_t$, so that the velocity of the screw dislocation cannot exceed the speed of transverse sound waves. An expansion of (4.8) when $\dot{x}_1 \ll c_t$ gives

$$E_{sm} = E_s + \frac{1}{2}m_{0s}\dot{x}_1^2 \quad (4.9)$$

where

$$m_{0s} = \frac{E_s}{c_t^2} = \left(\frac{\rho b^2}{4\pi} \right) \ln \left(\frac{R}{r_0} \right) \quad (4.10)$$

may be regarded as the initial 'rest mass' of unit length of the dislocation. For small velocities and accelerations, the mass m_{0s} may be used in the equation of motion since the force $F_1 = b\tau_{23}$ per unit length does work $F_1 \dot{x}_1 = \dot{E}_{sm}$ as the velocity changes, giving an analogy to Newton's law

$$F_1 = m_{0s} \ddot{x}_1. \quad (4.11)$$

Eshelby (1949 b) showed that c_t is also the limiting velocity for a uniformly moving edge dislocation, but the energy diverges as $1/\beta^3$ rather than as $1/\beta$. Stroh (1962) has shown this is due to a resonance between the moving dislocation and the plane waves propagating in the medium. An interesting result is that the shear stress in the glide plane changes sign for $c_R < \dot{x}_1 < c_t$ where $c_R \approx 0.9c_t$ is the velocity of Rayleigh waves (Love 1920). Thus a very fast edge dislocation attracts other

dislocations of the same sign. The rest mass of an edge dislocation is given by

$$m_{0e} = m_{0s}\{1 + (c_t/c_l)^4\} \quad (4.12)$$

where c_l is the longitudinal sound velocity.

Nabarro (1951 a) developed the dynamic theory of a uniformly moving loop of arbitrary shape, and he and Eshelby (1953 b) treated the non-uniform motion of a screw dislocation. The effective mass is changed so that R in (4.10) no longer represents the external dimension of the crystal, but only the dimension of that part of it to which the elastic disturbance (with velocity c_t) has spread during the acceleration or deceleration. Thus the effective mass of an oscillatory dislocation would involve $R \sim c_t/\omega$ where ω is the frequency of oscillation. The general non-uniform motion of straight dislocations and dislocation loops has been studied by Kosevich (1965), Beltz *et al.* (1968), Malén (1969) and Stenzel (1969 a).

Interactions of free surfaces or other boundaries with moving dislocations may be treated by the image method (Hirth and Lothe 1968 a, Berg *et al.* 1969), and a detailed study of the mutual interactions of moving dislocations was made by Hirth and Lothe (1968 b). The effects of anisotropic elasticity were first considered by Bullough and Bilby (1954) and many calculations have been made for special cases (Teutonico 1961, 1962 a, b, 1963 a, b, Cotner and Weertman 1962, 1963, van Hull and Weertman 1962, Weertman 1962 a, b). The lowest of the three velocities of sound in a given direction varies through a finite range depending on direction, and the critical velocity of a dislocation lies within this range and is usually smaller than the isotropic c_t .

Uniformly moving dislocations may also be described by the Frenkel-Kontorova model or by the Peierls-Nabarro model (Eshelby 1949 b, Leibfried and Dietze 1949, Stenzel, 1969 b). A moving screw dislocation in the latter case is replaced by a density $\partial u_s(x_1, t)/\partial x_1$ of infinitesimal dislocations and with the stress field (4.6) an integral equation is obtained equivalent to that given by (3.5) and (3.6) and the solution (see (3.7)) is

$$u_s(x_1', t) = -(b/2\pi) \tan^{-1}(x_1'/\zeta_s) \quad (4.13)$$

where $\zeta_s = \frac{1}{2}h$ is the width of the stationary dislocation. The width of the moving dislocation is

$$\zeta_s' = \beta \zeta_s \quad (4.14)$$

and decreases with increasing velocity to zero at $\dot{x}_1 = c_t$. Liebfried and Dietze showed that the total energy satisfies the relativistic equation (4.8) with E_s now replaced by E of equation (3.17).

The corresponding width of a moving edge dislocation (Eshelby 1956 b) is

$$\zeta_e' = \zeta_e f(\dot{x}_1) \quad (4.15)$$

where the function $f(\dot{x}_1)$ vanishes at $\dot{x}_1 = c_R$. Weertman (1968) repeated this calculation with force laws different from (3.6) and found that, in contrast to the behaviour of stationary edges, the behaviour of high-speed edge dislocations is sensitive to the force law.

Although the speed of sound appears as a limiting velocity in the above equations, Eshelby (1956 b) investigated the possibility of supersonic dislocations. Equation (4.3) is valid independent of \dot{x}_1 , and the transformation (4.4) is used but with

$$\beta = \{(\dot{x}_1^2/c_t^2) - 1\}^{1/2}. \quad (4.16)$$

Instead of (4.5) there is now a hyperbolic equation

$$\frac{\partial^2 u_3}{\partial x_1'^2} - \frac{\partial^2 u_3}{\partial x_2'^2} = 0 \quad (4.17)$$

with the general solution

$$u_3(x_1, x_2, t) = w_a(x_1' + x_2) + w_b(x_1' - x_2) \quad (4.18)$$

where w_a and w_b are plane waves of velocity c_t inclined to the x_1 -axis at angles of $\tan^{-1}(\pm\beta)$ respectively. Apparently $w_a(x_2 > 0)$ and $w_b(x_2 < 0)$ represent the outward radiation of energy from the disturbance travelling with velocity \dot{x}_1 . This may be compared with a supersonic shock wave or with Cherenkov radiation. A dislocation with $\dot{x}_1 > c_t$ will radiate energy in the form of sound waves.

The stress field of a supersonic screw dislocation may be expressed in terms of the Peierls–Nabarro model where, instead of (3.5),

$$\sigma_{23} = \mu \left(\frac{\partial u_3}{\partial x_2} \right) = \beta \mu \left(\frac{\partial u_3}{\partial x_1} \right) \quad (4.19)$$

and u_3 is given by (4.18). The Peierls integral equation is replaced by the differential equation

$$\beta \mu \left\{ \frac{\partial u_3(x_1, 0, t)}{\partial x_1} \right\} = \frac{B_s}{h} \sin \left\{ \frac{2\pi u_3(x_1, 0, t)}{b} \right\} \quad (4.20)$$

and the solution given by Eshelby is

$$u_3(x_1, 0, t) = \frac{b}{2\pi} \tan^{-1} \left[\exp \left\{ \frac{-2(x_1 - \dot{x}_1 t)}{\beta h} \right\} \right]. \quad (4.21)$$

According to the force law (3.5), this equation implies that the energy of interaction across the cut faces is a maximum before passage of the dislocation and a minimum afterwards. The passage of the supersonic dislocation thus restores the perfect lattice and the driving force to maintain the motion comes from the misfit energy released. In a detailed study, Weertman (1967) and Berg *et al.* (1969) conclude that a dislocation moving on a plane which cannot contribute energy by atomic readjustment is unable to move supersonically.

4.2. Damping by energy dissipation

4.2.1. Acoustic dispersion and radiation damping. In a crystal, the frequency ω of sound waves increases monotonically with wave number k to a maximum value ω_m at k_m . Over the range of k , the velocity decreases from c_t at $k = 0$ to c_m at $k = k_m$. For a dislocation with velocity \dot{x} such that $c_m < \dot{x} < c_t$, a wave number k' exists such that $\omega(k') = \dot{x}k'$. This dislocation is then subsonic with respect to waves of frequency $0 < \omega < \omega(k')$ and supersonic for waves $\omega(k') < \omega < \omega_m$. The supersonic dislocation radiates energy according to (4.18) and its motion is thus damped; the dissipated energy must be supplied, for example, by the work done by an external stress. Eshelby (1956 b) calculated the damping stress σ resulting from this acoustic dispersion and obtained for a screw dislocation according to the Peierls–Nabarro model

$$\frac{\sigma}{\mu} \approx \left(\frac{\dot{x}}{c_m} - 1 \right)^{3/2} \exp \left(\frac{-2\pi \zeta_s}{b} \right). \quad (4.22)$$

Clearly this type of damping occurs only at very high dislocation velocities since c_m is never much smaller than c_t . Even when $\dot{x} > c_m$, both terms in equation (4.22) are small, so that σ is always small.

Next consider an oscillating screw dislocation with the x_1 coordinate of its centre

$$q = d \sin(\omega t + \alpha). \quad (4.23)$$

For small amplitude d , the displacement is

$$u_3 = (b/2\pi) \tan^{-1}\{x_2/(x_1 - q)\}. \quad (4.24)$$

Introduce polar coordinates r, ϕ, z and expand u_3 as a power series, so that for $r \gg q$

$$u_3 = (b\phi/2\pi) + (bq/2\pi r) \sin \phi. \quad (4.25)$$

However, (4.25) is not a solution of the equation of motion (4.3); the correct solution must reduce to (4.25) for small r and represent outgoing waves for large r . Since $(b\phi/2\pi)$ already satisfies (4.3), it is required to find a solution which for $d \ll r \ll c_t/\omega$ approximates to the second term of (4.25). Such a solution is of form (Eshelby 1949 c)

$$u_3^{(1)} = A \sin \phi \{J_1(\omega r/c_t) \cos(\omega t + \alpha) + Y_1(\omega r/c_t) \sin(\omega t + \alpha)\} \quad (4.26)$$

where J_1 and Y_1 are Bessel functions of the first and second type respectively, and $A = b\omega d/4c_t$. For large r , (4.26) represents the outgoing wave

$$u_3 = (\omega b^2 d^2 / 8\pi r c_t)^{1/2} \sin \phi \sin(\omega t + \alpha + \frac{1}{4}\pi - r/c_t). \quad (4.27)$$

The energy flux in the direction of propagation is $\rho \dot{u}_3^2 c_t$ per unit area, so that the energy radiated per cycle per unit length of dislocation is obtained by integration over a cylinder of radius r and over a time $\tau = 2\pi/\omega$ as

$$E_R = \frac{1}{8} \pi \rho b^2 d^2 \omega^2. \quad (4.28)$$

One type of oscillation may be produced by the periodic acceleration and deceleration as a dislocation moves in a periodic lattice field. Hart (1955) investigated this problem for a Peierls–Nabarro edge dislocation where the energy per unit length as a function of the displacement is given by (3.39). The dislocation experiences a force per unit length $F_1 = -dE/dx_1$ given by

$$F_1 = \frac{4\pi E_p}{b} \alpha \sin\left(\frac{4\pi x_1}{b}\right) = \frac{4\pi E_p}{b} \alpha \sin \omega t \quad (4.29)$$

where $x_1 = \dot{x}_1 t$ and $\omega = 4\pi \dot{x}_1/b$. Using the concept of an effective mass, the oscillating motion is defined by

$$m_0 \ddot{q} = (4\pi E_p/b) \alpha \sin \omega t \quad (4.30)$$

where $m_0 \approx (E_p/c_t^2) \ln(c_t/\dot{x}_1)$ (see § 4.1). The solution of (4.30) is

$$q = -d_t \sin \omega t$$

where

$$d_t = \frac{\alpha c_t^2 b}{4\pi \dot{x}_1^2 \ln(c_t/\dot{x}_1)}. \quad (4.31)$$

When $\dot{x}_1 \ll c_t$ then $d_t \gg b$, but for small velocities the motion of the dislocation is not controlled by its inertia, and the amplitude of oscillations cannot exceed half the period of the lattice potentials. Nabarro (1967) therefore suggests that the linear

interpolation

$$\frac{b^2}{d_t^2} = 16\pi^2 \dot{x}_1^{-4} \frac{\{\ln(c_t/\dot{x}_1)\}^2}{\alpha^2 c_t^4} + 16 \quad (4.32)$$

should be used to ensure that $d_t = \frac{1}{4}b$ at small velocities, and d_t tends to the value (4.31) at large velocities.

Now assume that (4.28) is approximately valid for an edge dislocation. The stress σ which maintains velocity \dot{x}_1 does work $\sigma b \dot{x}_1 (2\pi/\omega)$ per period, and this equals the energy dissipated. From (4.28) and (4.32)

$$\frac{\sigma}{\mu} = \frac{1}{4}\pi\alpha^2\gamma_1^{-2} \left\{ (\gamma_1 \ln \gamma_1)^2 + \left(\frac{\alpha}{\pi}\right)^2 \right\}^{-1} \quad (4.33)$$

where $\gamma_1 = \dot{x}_1/c_t$. This stress is always much less than the Peierls stress (3.41).

As the dislocation moves through the lattice, the distance between rows of atoms in the core fluctuates with period \dot{x}_1/b . This leads to energy dissipation by radiation of sound waves. Nabarro (1967) estimates the damping stress from core pulsations as

$$\sigma/\mu = 8\pi\alpha^2(\dot{x}_1/c_t)^2 \quad (4.34)$$

which is also always much less than the Peierls stress. For low speeds the stress (4.34) is less than (4.33), but the stress (4.34) is larger when $\dot{x}_1 \sim c_t$.

4.2.2. Phonon and electron scattering and viscosity. Elastic waves scattered by a dislocation transfer momentum to the dislocation. A sound wave of average energy density W and wave vector \mathbf{k} has a momentum density

$$\mathbf{p} = W\mathbf{k}/c_t k. \quad (4.35)$$

If a plane wave of energy W_0 and wave vector \mathbf{k} at an angle θ to x_1 is scattered during a time t by a stationary dislocation and the scattering cross section is s , the energy scattered per unit length is $sW_0 c_t t$, and the change in the momentum is

$$p_1 = sW_0 \cos \theta t \quad (4.36)$$

corresponding to a shear stress

$$\sigma = (sW_0/b) \cos \theta. \quad (4.37)$$

Evidently if waves impinge from all directions, the average stress is zero.

For a moving dislocation, in a coordinate system x'_1, x'_2, x'_3 , it follows that

$$\begin{aligned} W'_0 &= W_0(1 - 2\gamma_1 \cos \theta) \quad \cos \theta' = \cos \theta - \gamma_1 \sin^2 \theta \\ s' &= s(1 + \gamma_1 \cos \theta) \end{aligned} \quad (4.38)$$

where $\gamma_1 = \dot{x}_1/c_t$ as before and terms in γ_1^2 and higher orders are neglected. The stress now becomes

$$\sigma = W_0 s(\cos \theta - \gamma_1)/b. \quad (4.39)$$

If waves impinge from all directions, the resultant damping stress is

$$\bar{\sigma} = -\frac{1}{2\pi} \int_0^{2\pi} \sigma d\theta = \frac{W_0 s \gamma_1}{b}. \quad (4.40)$$

For an isotropic three-dimensional flux of longitudinal and transverse waves, Leibfried (1950) estimated that the stress is reduced to

$$\bar{\sigma} \approx 0.1 W_0 s \gamma_1 / b. \quad (4.41)$$

A dislocation scatters sound waves firstly because of nonlinear force laws and density changes near the core, and secondly because of forced oscillations caused by the sound waves. These oscillations lead to radiation of elastic waves, and this is sometimes called the 'flutter mechanism'. Both mechanisms have been extensively investigated in relation to the motion of kinks along dislocations. For the flutter mechanism (Leibfried 1950, Nabarro 1951 b, Eshelby 1962, Lothe 1962) the frictional force is proportional to the average kink velocity, and increases linearly with temperature above $\theta_D b/w_k$ where θ_D is the Debye temperature and w_k the kink width. Leibfried assumed the scattering cross section for the core mechanism to be of order b . Seeger and Engelke (1968, 1969) have given a detailed quantum mechanical treatment for the core mechanism of the scattering of phonons by moving kinks in copper, and conclude that the frictional stress is proportional to velocity and increases with temperature; it is at least ten times larger than that given by the flutter mechanism.

Dislocations in metals also scatter electrons and so contribute an additional $P_D \rho_D$ to the resistivity where P_D is a constant (approximately $5 \times 10^{-20} \Omega \text{ cm}^{-3}$) and ρ_D is dislocation density (Lücke 1951, Nabarro 1967). The interaction of a moving dislocation with the electron gas (density of conduction electrons ρ_e) is equivalent to that of a stationary dislocation with a current of density $\rho_e \dot{x}_1$. The energy dissipated in unit volume and time is then $P_D \rho_D \rho_e^2 (\dot{x}_1)^2$ and has to equal the work $\sigma \dot{x}_1 \rho_D / b$ done by an external stress σ . Hence

$$\sigma = P_D \rho_e^2 \dot{x}_1. \quad (4.42)$$

With numerical values for copper, $\sigma \sim 4 \times 10^8 (\dot{x}_1/c_t) \text{ dyn cm}^{-2}$.

A more rigorous treatment of the electric field and current induced by a moving dislocation, and of the associated energy dissipation, requires a solution of the Boltzmann equation (Huffmann and Louat 1968, 1969). The damping stress is found to be proportional to the dislocation velocity divided by the electrical resistivity. Electron scattering always gives a lower stress than phonon scattering, except at very low temperatures where the density of phonons is small.

Since phonons can transfer energy and momentum to each other, with a relaxation time τ , they also behave as a particle fluid with viscosity. Application of a shear stress (an effective extension plus compression) results in a reduction of wave vectors in the compression direction and *vice versa*. The new distribution is not in equilibrium, and if the stress is applied for a time greater than τ an exchange of energy takes place. The effective viscosity (Mason 1960) is

$$\eta = Q_0 K_T / C_v \bar{c}_s^2 \quad (4.43)$$

where Q_0 is the total thermal energy per unit volume, K_T is the thermal conductivity, C_v is the specific heat at constant volume and \bar{c}_s is the average velocity of transverse and longitudinal waves.

For a viscous medium, the shear stress σ is given by

$$\sigma = 2\mu e + \eta \dot{e} \quad (4.44)$$

where e is the shear strain rate. The energy loss rate per unit volume is then

$$d\dot{U}_\eta / dV = \sigma \dot{e} = 2\mu e \dot{e} + \eta \dot{e}^2. \quad (4.45)$$

Consider a screw dislocation with velocity $\dot{x}_1 \ll \bar{c}_s$ and use polar coordinates

$x_1 - \dot{x}_1 t = r \cos \phi$, $x_2 = r \sin \phi$, $x_3 = z$, so that

$$e_{\phi z} = b/2\pi r \quad \dot{e}_{\phi z} = b\dot{x}_1 \cos \phi / 2\pi r^2 \quad (4.46)$$

and from (4.45)

$$\frac{dU_\eta}{dV} = (b^2 \dot{x}_1^2 / 4\pi^2) ((2\mu/r^3) \cos \phi + (\eta/r^4) \cos^2 \phi). \quad (4.47)$$

Integrating from $r = r_0$ to ∞ and $\phi = 0$ to 2π gives the energy loss in unit time for unit length of dislocation as

$$\dot{E}_\eta = (b^2 \eta / 8\pi r_0^2) \dot{x}_1^2 = C b \dot{x}_1^2 \quad (4.48)$$

so that the damping stress is

$$\sigma = C \dot{x}_1. \quad (4.49)$$

For an edge dislocation, Mason (1960) found that (4.49) is still valid with

$$C = \{3b\eta/32\pi(1-\nu)^2 r_0^2\} + \{\mu^2 \chi / 72\pi K^2 (1-\nu)^2 r_0^2\}$$

where K is the bulk modulus and χ the compressional viscosity. A detailed review of theoretical and experimental work on phonon viscosity is given by Mason (1968).

An analogous calculation for the effect of electron viscosity (Mason 1955) again gives (4.49) but with

$$C = (b^2 \eta / 8\pi \lambda_e^2) = (b \rho_e e)^2 / 24\pi \sigma_e \quad (4.50)$$

where λ_e is the mean electron free path, e the electronic charge, σ_e the electron conductivity, and ρ_e the density of conduction electrons, as before.

4.2.3. Thermoelastic damping. The thermoelastic effect (Zener 1940, Päslar 1944, Eshelby 1949 c, Nye 1957) relates the temperature change of an elastic body which expands thermally with the elastic strain (or stress). A change ΔT of temperature produces a dilatation of $\frac{1}{3}\alpha_T \Delta T$ where α_T is the volume coefficient of thermal expansion, and Hooke's law must be modified to

$$e_{ij} = (\sigma_{ij}/2\mu) - \psi \sigma_{kk} \delta_{ij} + (\alpha_T \Delta T / 3) \delta_{ij} \quad (4.51)$$

where $\psi = \lambda/2\mu(3\lambda+2\mu)$. For a change of stress $d\sigma_{ij}$ the entropy change is

$$dS = \left(\frac{\partial S}{\partial T}\right)_\sigma dT + \left(\frac{\partial S}{\partial \sigma_{ij}}\right)_T d\sigma_{ij}. \quad (4.52)$$

The first term in equation (4.52) is C_σ , the specific heat at constant stress, and the second term is equal to $(\partial e_{ij}/\partial T)_\sigma$. Thus it follows from (4.51) and (4.52) that

$$T dS = C_\sigma dT + T \left(\frac{1}{2\mu} \frac{\partial \sigma_{ij}}{\partial T} - \sigma_{kk} \delta_{ij} \frac{\partial \psi}{\partial T} + \frac{1}{3} \alpha_T \delta_{ij} \right) \quad (4.53)$$

in which the term $(\frac{1}{3}\Delta T \delta_{ij})(\partial \alpha_T / \partial T)$ has been neglected since it is generally much smaller than $\frac{1}{3}\alpha_T \delta_{ij}$. If there is no heat conduction, $dS = 0$, and the temperature change dT is related to the change of stress $d\sigma_{ij}$ by (4.53).

Energy dissipation arises from heat flow, which in a time dt is

$$T dS = K_T \nabla^2 T dt \quad (4.54)$$

into unit volume. Neglecting second-order terms in σ_{ij} , (4.53) and (4.54) give

$$K_T \nabla^2 T - C_\sigma \frac{\partial T}{\partial t} = T \alpha_T (3\lambda + 2\mu) \frac{\partial e_{kk}}{\partial t}. \quad (4.55)$$

Weiner (1958) found a steady-state solution of this equation for an edge dislocation moving with velocity \dot{x}_1 . The dilatation e_{kk} was derived from the Peierls–Nabarro model, and for small \dot{x}_1 the dissipation was found to be proportional to \dot{x}_1^2/K_T . For large velocities, the dissipation is proportional to K_T and is independent of \dot{x}_1 .

5. Dislocations in common structures

5.1. Stability criteria

Lattice dislocations of large b are able to lower their energies by spontaneous dissociation, so that the observed dislocations in any structure have a restricted range of Burgers vectors. Equation (2.17) implies that a dislocation b_1 will dissociate into two dislocations, b_2 and b_3 , if $b_1^2 > b_2^2 + b_3^2$, i.e. if $b_2 \cdot b_3 > 0$. Strictly, the energy depends also on the orientation of the dislocation line l , the elastic anisotropy, and the variation of core structure with b and l , but these factors are not normally of sufficient importance to invalidate the b^2 dependence. It follows that the dislocation of lowest energy has b equal to the smallest vector of the Bravais lattice, but that other small values of b may also be stable.

Frank and Nicholas (1953) examined systematically the possible dislocations of some common crystal structures. They classified dislocations for which $b_2 \cdot b_3 = 0$ as doubtfully stable, since the first-order change in elastic energy is zero. They also considered the possibility of further dissociation of lattice dislocations into partials separated by ribbons of stacking fault. Any reduction in elastic energy as the partials separate is then accompanied by increasing fault energy, and the total energy is minimized at some equilibrium separation.

A full description of dislocation stability also involves consideration of the variation of energy with orientation. The concept of line tension shows that in the absence of a stress field a dislocation fixed at two points of an elastically isotropic medium will be a straight line. However, if the energy $E(\theta)$ is a function of the orientation θ , it is possible for a straight line to lower its energy by adopting a zig-zag configuration. Instabilities of this kind may arise from the orientation dependence of either elastic energy or core energy. The core energy effect is difficult to calculate, but is associated with a high Peierls force and may therefore be expected in crystals with covalent bonds and possibly in bcc metals at low temperatures. Elastic instabilities vary with the elastic anisotropy and were first predicted for lithium by de Wit and Koehler (1959).

The equilibrium shape of a closed dislocation loop is given by a Wulff plot construction (Christian 1965) as first pointed out by Mullins (see Friedel 1964). Head (1967) has given a detailed discussion using the inverse Wulff plot (Frank 1963) of $1/E(\theta)$ against θ . If there is any region in which part of this plot lies inside a common tangent to the plot (figure 7), the corresponding orientations of the dislocation line are unstable and may change spontaneously into a V-shaped, Z-shaped or more complex zig-zag in which the directions of the two components correspond to the points of contact of the common tangent. Except for certain simple orientations, the elastic energy $E(\theta)$ must be calculated numerically (see § 2.9). Head shows that in cubic crystals the instability ranges depend on the anisotropy (or Zener's) constant $A = 2c_{44}/(c_{11} - c_{12})$ and on $B = (c_{11} + 2c_{12})/c_{44}$.

5.2. Face-centred cubic structures

In this structure there are twelve stable lattice dislocations with minimum Burgers vectors $\frac{1}{2}a\langle 110 \rangle$ (counting $\pm b$ as distinct), and six doubtfully stable dislocations of type $a\langle 100 \rangle$. Attractive interactions between $\frac{1}{2}a\langle 110 \rangle$ dislocations lead to the formation of low-energy networks and sub-boundaries (Frank 1955), especially when deformed crystals are annealed. Two such dislocations with non-parallel Burgers vectors b_2 and b_3 in the same slip plane have $b_2 \cdot b_3 = \pm \frac{1}{4}a^2$, and with the negative sign they attract to form a single dislocation b_1 . In (111) a typical reaction is

$$\frac{1}{2}a[1\bar{1}0] + \frac{1}{2}a[01\bar{1}] = \frac{1}{2}a[10\bar{1}]. \quad (5.1)$$

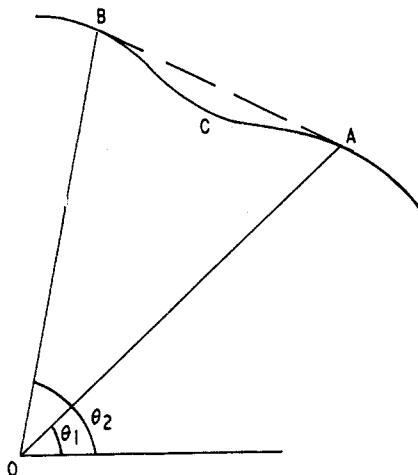


Figure 7. Schematic inverse Wulff plot of $1/E(\theta)$ against θ . A dislocation line in orientation C should be unstable against decomposition into a zig-zag configuration of orientations A and B, represented by angles θ_1 , θ_2 between the line directions and the Burgers vector.

If this reaction occurs over a limited length, a node is formed and (5.1) may be written more symmetrically (see equation (1.1)) as

$$\frac{1}{2}a[1\bar{1}0] + \frac{1}{2}a[01\bar{1}] + \frac{1}{2}a[\bar{1}01] = 0. \quad (5.1a)$$

Nodes of type (5.1a) occur in networks and are very stable when the dislocation lines are mutually at 120° .

The other basic reactions occur between lattice dislocations on different slip planes, and the product dislocation then forms initially along the line of interaction. Equation (5.1) is valid, for example, for dislocations gliding in (111) and (111), in (111) and ($\bar{1}\bar{1}1$), and in (111) and ($\bar{1}11$). The first two cases lead to dislocations which glide in (111), but Lomer (1951) pointed out that in the third case the product dislocation lies along [101] and so is pure edge. The geometrical glide plane of the Lomer dislocation is (010) and since this is not a close-packed plane, the dislocation may be sessile, i.e. unable to glide. Dissociation into partials ensures a completely sessile configuration (see below). Two dislocations on intersecting slip planes may also have perpendicular Burgers vectors. The reaction

$$\frac{1}{2}a[101] + \frac{1}{2}a[10\bar{1}] = a[100] \quad (5.2)$$

produces then no first-order change in elastic energy, and the doubtfully stable [100] dislocation lies along [010] and has a (001) slip plane.

In fcc structures, the possible Burgers vectors of partial dislocations bounding $1\triangledown$ faults are identical with those for $2\triangledown$ faults. Frank and Nicholas (1953) devised a notation in which the positive normal to the (111) plane is directed upwards and the left and right hand edges of $1\triangledown$ and $2\triangledown$ faults are labelled L and R, and λ and ρ respectively. Any vector of the L set is then also a vector of the ρ set, and its negative is a member of the R and λ sets. There are only two types of stable dislocation (Frank partials and Shockley partials) and one doubtfully stable dislocation which can terminate single planar faults. The doubtfully stable partial, of type $\frac{1}{6}a\langle 411 \rangle$, will not be considered further.

With the RH/FS convention, Frank partials on (111) may have Burgers vectors $-\frac{1}{3}a[111]L$, $\frac{1}{3}a[111]R$, $\frac{1}{3}a[111]\lambda$ or $-\frac{1}{3}a[111]\rho$. These dislocations are pure edges and are sessile since they can climb in the (111) plane but cannot glide out of it. A $1\triangledown$ fault is on the tensile side, or a $2\triangledown$ fault on the compressive side, of a Frank partial. Frank and Nicholas also used the notation a, b, c, d for the (111)($\bar{1}\bar{1}\bar{1}$) and (111) planes, and for a full identification the Burgers vector is then followed by a symbol such as L_d or ρ_b .

Shockley partials of the $L-\rho$ set on (111) have Burgers vectors $\frac{1}{6}a[11\bar{2}]$, $\frac{1}{6}a[1\bar{2}1]$ and $\frac{1}{6}a[\bar{2}11]$. Thus there are 12 Shockley partials to each plane, and 48 in all; these dislocations can always glide in the plane of the fault. Heidenreich and Shockley (1948) first pointed out that a lattice dislocation may reduce its energy by dissociation into partials, e.g.

$$\frac{1}{2}a[1\bar{1}0] = \frac{1}{6}a[2\bar{1}\bar{1}]R_d + \frac{1}{6}a[1\bar{2}1]L_d. \quad (5.3)$$

The two partials repel each other and move apart on (111), leaving a layer of $1\triangledown$ fault. The total energy is minimized at an equilibrium separation d given by

$$d = \frac{\mu a^2}{48\pi\gamma} \left(\frac{2 - \nu - 2\nu \cos 2\theta}{1 - \nu} \right) \quad (5.4)$$

where γ is the stacking fault energy and θ is the angle between the direction of the dislocation and of the total Burgers vector (e.g. Friedel 1964). The ratio d/a depends on the value of $\gamma/\mu a$, and in isotropic approximation this is generally the most useful parameter for comparing the properties of different materials.

Equation (5.4) implies that d for an edge dislocation is about twice the value for a screw dislocation, but this difference can be greatly increased when allowance is made for elastic anisotropy (e.g. Seeger and Schoeck 1953, Teutonico 1967). However, equation (5.4) is exact for screw dislocations and '60° dislocations' if the appropriate effective values of μ and ν for {111} planes are used (Aerts *et al.* 1962), and Teutonico shows that the maximum deviation from the correct anisotropic value of d (in edge orientation) is then only about 6%. The measurement of d provides one possible method for the experimental determination of γ , and may soon be possible for a much wider range of metals through a new technique of weak beam, dark field electron microscopy (Cockayne *et al.* 1969).

The alternative dissociation

$$\frac{1}{2}a[1\bar{1}0] = \frac{1}{6}a[2\bar{1}\bar{1}]\lambda_d + \frac{1}{6}a[1\bar{2}1]\rho_d \quad (5.5)$$

also leads to an extended dislocation. Contrary to earlier estimates, it now appears that the energy of a $2\triangledown$ fault is nearly equal to that of a $1\triangledown$ fault in some fcc metals,

so that the equilibrium separations produced by (5.3) and (5.5) should be comparable (e.g. Smallman 1968).

For a lattice dislocation not lying in a glide plane, the dissociation

$$\frac{1}{2}a[\bar{1}\bar{1}0] = \frac{1}{3}a[1\bar{1}\bar{1}] R_a + \frac{1}{6}a[1\bar{1}2] L_a \quad (5.6)$$

produces no change in elastic energy but an increase in total energy because of the fault. This dissociation, first considered by Cottrell and Bilby (1951), should thus not occur spontaneously, but might be effected by an applied stress of magnitude γ/b . Kuhlmann-Wilsdorf (1958) pointed out that since the reverse reaction is energetically favourable, the Shockley partial may be nucleated spontaneously. For example, a closed loop of Frank partial may form by collapse of a planar aggregate of vacancies on $(1\bar{1}\bar{1})$, and may subsequently be converted into a lattice dislocation if a loop of Shockley partial spreads across the stacking fault.

Calculations show that it is energetically favourable to form a faulted loop rather than an unfaulted loop on initial collapse of a small disk, even for relatively high values of γ . If the loop continues to grow by vacancy climb, it becomes metastable relative to the unfaulted loop but the activation energy for nucleation of the Shockley partial in the absence of applied stress is greater than about 10 eV (Saada 1962, Saada and Washburn 1963). Thus, once a faulted loop has formed it is rather difficult to convert it into an unfaulted loop. Electron microscopy reveals both faulted and unfaulted loops in many metals quenched to produce vacancy supersaturations. In the case of aluminium, faulted loops are observed only in very pure specimens quenched from relatively low temperatures. High temperatures or impurities were formerly believed to assist the thermal nucleation of Shockley partials (Cotterill and Segall 1963) but it now appears that the transition depends mainly on stress-assisted nucleation (Edington and Smallman 1965).

The remaining partial dislocations of the fcc structure are the junctions of either two, three or four stacking faults. For two coplanar faults, the Burgers vector of the partial may be written $L_i \rho_i (\equiv \rho_i L_i)$ or $R_i \lambda_i$, whilst the intersections of faults on two different planes have vectors of type $L_i L_j$, $L_i R_j$, etc. where $i \neq j$. The stable dislocations of the $L_i \rho_i$ set have the same Burgers vectors as the sets R_i and λ_i , and similarly the $R_i \lambda_i$ set is equivalent to the L_i and ρ_i sets. However, new Burgers vectors appear when faults on nonparallel $\{111\}$ planes intersect, and the junctions of such faults are called stair-rod dislocations.

In the fcc structure, there are four basic stair-rods, typified by the Burgers vectors $\frac{1}{6}a[\bar{1}10] L_a R_b$, $\frac{1}{3}a[1\bar{1}0] L_a R_b$, $\frac{1}{3}a[00\bar{1}] L_a L_b$ and $\frac{1}{6}a[301] L_a L_b$. The angle between the stacking faults is always obtuse ($109^\circ 28'$) when the stair-rod dislocation is formed from two left-hand or two right-hand edges (e.g. $L_a L_b$, $\lambda_a \lambda_b$, $L_a \lambda_b$, etc.), and acute ($70^\circ 32'$) when left- and right-hand edges combine (e.g. $L_a R_b$, $\lambda_a \rho_b$, $L_a \rho_b$, etc.). The sets $L_a L_b$, $\rho_a \rho_b$, $L_a \rho_b$, $\rho_a L_b$ all have the same Burgers vectors, and these are the negatives of the Burgers vectors of the sets $R_a R_b$, $\lambda_a \lambda_b$, $R_a \lambda_b$, $\lambda_a R_b$. Similarly, the equivalent vectors of the sets $L_a R_b$, $\rho_a \lambda_b$, $L_a \lambda_b$, $\rho_a R_b$ are the negatives of the sets $R_a L_b$, $\lambda_a \rho_b$, $\lambda_a L_b$ and $R_a \rho_b$. Thus there are 12 dislocations of type $\frac{1}{6}a[\bar{1}10] L_a R_b$, 12 dislocations of type $\frac{1}{3}a[1\bar{1}0] L_a R_b$, 12 dislocations of type $\frac{1}{3}a[00\bar{1}] L_a L_b$ and 48 dislocations of type $\frac{1}{6}a[301] L_a L_b$. All except $\frac{1}{6}a[301]$ are pure edges, and this stair-rod is stable only if the $2\bar{\nabla}$ fault has higher energy than the $1\bar{\nabla}$ fault since the dissociation

$$\frac{1}{6}a[301] L_a L_b = \frac{1}{3}a[211] R_a + \frac{1}{6}a[1\bar{1}0] \lambda_a L_b \quad (5.7)$$

gives a small reduction in elastic energy. However, the $\frac{1}{6}\sigma[301]$ dislocation is generally considered a possible stair-rod since it can be formed by combination of two Shockley partials.

Clearly the stair-rod of lowest energy is $\frac{1}{6}\sigma[1\bar{1}0]$, formed when two faults intersect at an acute angle. The interaction of two extended dislocations moving on different glide planes may lead to a configuration containing such a dislocation,

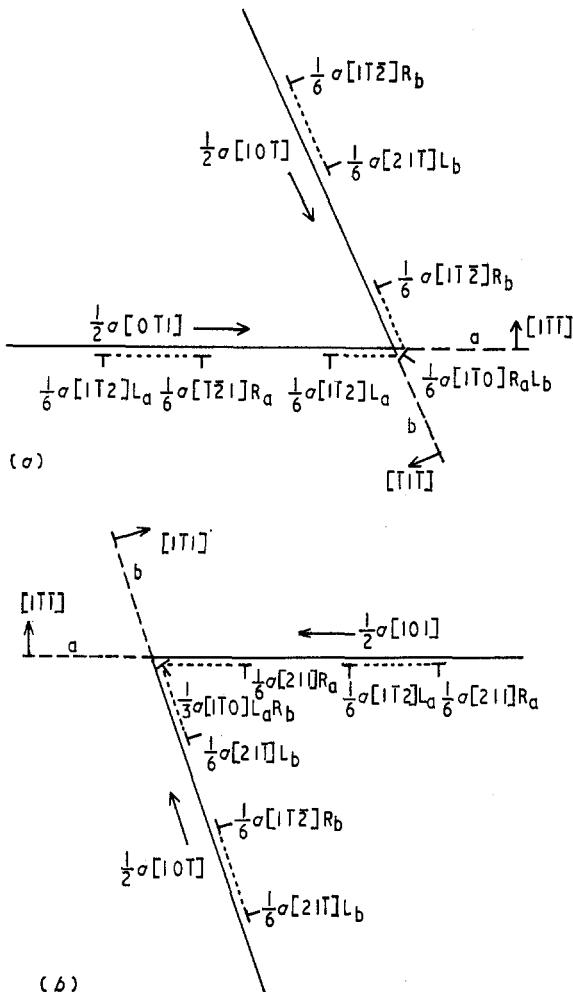


Figure 8. The formation of (a) Lomer-Cottrell locks and (b) Hirth locks by interaction of dissociated dislocations on intersecting {111} planes.

as shown schematically in figure 8. This is generally known as a Lomer-Cottrell lock (Cottrell 1952), and it is the dissociated version of the Lomer dislocation. In general all combinations of Shockley partials into stair-rods of lower energy might be expected during deformation processes; for example, (5.2) can give a combination of a $\frac{1}{3}\sigma[1\bar{1}0]L_aR_b$ stair-rod with $\frac{1}{6}\sigma[211]R_a$ and $\frac{1}{6}\sigma[21\bar{T}]L_b$. This is also shown in figure 8 and is sometimes known as a Hirth lock (Hirth 1961).

All of the stair-rod dislocations are sessile and represent possible barriers to glide dislocations. Some theories of work-hardening (e.g. Seeger 1958) are based

on the assumption that dislocation pile-ups are formed behind such locks, which thereby cause substantial internal stresses to be generated, and possibly other dislocation sources to be activated. The most stable barrier is the Lomer-Cottrell lock, and this is the only type to have been definitely observed by electron microscopy (Basinski 1964).

Stair-rod dislocations may also arise from dissociation of Frank partials when they are parallel to $\langle 110 \rangle$ directions, e.g.

$$\frac{1}{3}a[111] R_d = \frac{1}{6}a[110] R_d L_c + \frac{1}{6}a[112] R_c. \quad (5.8)$$

This gives a smaller elastic energy but additional fault energy, and is important when Frank loops are formed in quenched metals of low fault energy. Detailed comparison of experimental and computed diffraction images (Clarebrough and Morton 1969) has given direct evidence for the dissociation in silver and in copper-aluminium alloys.

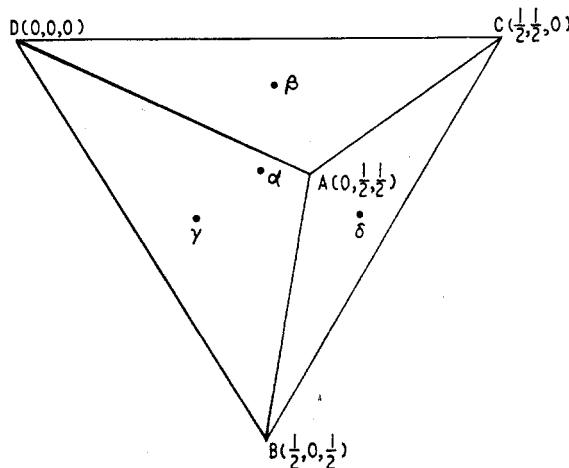


Figure 9. The Thompson tetrahedron.

For completeness, the possible partial dislocations which represent three or four fault interactions (on two $\{111\}$ planes) should be mentioned. The stable three-fault configurations are of types $L_a \rho_a L_b$ and $L_a \rho_a R_b$ and correspond to vectors of the $R_a L_b$ and $R_a R_b$ sets respectively. The four-fault combinations are $L_a \rho_a L_b \rho_b$ and $L_a \rho_a R_b \lambda_b$ and correspond to vectors of the $R_a R_b$ and $R_a L_b$ sets respectively. When stacking faults of a common type on intersecting planes pass through each other, a line of positive or negative dilatation is produced (Ashbee 1967). Other configurations which involve combinations of intersecting stair-rods were studied by Differt (1968).

When all faults are of the same type, the rather complex Frank and Nicholas notation may be replaced by a geometrical representation (Thompson 1953). The faces of a regular tetrahedron (figure 9) represent the $\{111\}$ planes a, b, c, d with centroids $\alpha, \beta, \gamma, \delta$ and opposite vertices A, B, C, D . The Burgers vectors of the stable dislocations are represented in length and direction as follows.

- (i) The 12 lattice dislocations of type $\frac{1}{2}a\langle 110 \rangle$ are given by the edges $AB, BA, BC, etc.$
- (ii) The 8 Frank partials are given by the lines $\alpha A, B\beta, etc.$
- (iii) The 24 Shockley partials have symbols $\alpha B, C\alpha, etc.$

(iv) The 12 stair-rod dislocations of type $\frac{1}{2}a\langle 110 \rangle$ have representations $\alpha\beta, \beta\gamma$, etc.

(v) Doubtfully stable lattice dislocations of type $a\langle 100 \rangle$ are represented by the symbol AB/CD, which means twice the displacement from the midpoint of AB to the midpoint of CD, or (equivalently) is the vector sum AC + BD. Clearly AB/CD = BA/CD = -CD/BA.

(vi) Stair-rod dislocations of type $\frac{1}{2}a\langle 001 \rangle$ are now represented by $\alpha\beta/CD$, etc.

(vii) Stair-rod dislocations of type $\frac{1}{2}a\langle 1\bar{1}0 \rangle$ are represented by $A\alpha/B\beta$, etc.

(viii) Stair-rod dislocations of type $\frac{1}{2}a\langle 301 \rangle$ are represented by $\alpha\beta/BC$, etc.

By assigning to the vertices of the tetrahedron the coordinates shown in figure 9, the previous notation is preserved (except for the fault type) and the order of the letters always gives the correct sign to the Burgers vector. Dislocation reactions are particularly easy to write in this notation; for examples equations (5.1), (5.3) and (5.5) become respectively

$$AB + BC = AC \quad (5.1b)$$

$$AB = A\delta + \delta B \quad (5.3a)$$

$$AB = A\alpha + \alpha B. \quad (5.5a)$$

The Thompson tetrahedron is useful in the discussion of many configurations involving extended dislocations; for example it may be used to show that the nodes of type (5.1a) in a network are alternately extended and constricted if faults of only one type are present. An estimate of the stacking fault energy may be obtained from the radius of curvature of an extended node, which depends also on the self-energies and interaction energies of the Shockley partials. This method was proposed by Whelan (1959) and more accurate calculations of the equilibrium configuration were made by Brown (1964), Siems (1964) and Jøssang, Stowell, Hirth and Lothe (1965). If the extrinsic fault energy is sufficiently low, all threefold nodes are extended, but enclose stacking faults which are alternately of $1\triangledown$ and $2\triangledown$ types with cross-over points (twofold constrictions) between the nodes. The energy of the cross-over points has a considerable effect on the radii of curvature (Gallagher 1966) and makes it difficult to determine the ratio of fault energies. In two silver-indium alloys, Gallagher found the ratio of $2\triangledown$ to $1\triangledown$ fault energies to be 1.09 and 1.03 respectively.

Long jogs in extended dislocations provide another example of the utility of the Thompson tetrahedron. If the jog itself is unextended, the parts of the dislocation lying in the two parallel slip planes must be constricted at each end of the jog. More complex structures arise if the jog is able to lower its energy by dissociating in a {111} plane which is inclined to the slip planes, as discussed in detail by Hirsch (1962). Suppose the dislocation line lies in d and has Burgers vector BC. The important jogs will then be those along the close-packed directions AD, BD and CD, and may be formed, for example, by intersection of other dislocations or (except in the case of AD) by cross-slip of part of the dislocation line.

The equilibrium configuration of an extended jog may be quite complex and depends on the direction of the dislocation line in the plane d, and on whether the jog direction makes an acute or an obtuse angle with each part of the dislocation. The simplest configurations are edge dislocations with acute or obtuse glissile jogs along $\pm BD$ or $\pm CD$, which contain low-energy ($\delta\alpha$ type) stair-rods and higher-energy ($BC/\alpha\delta$ type) stair-rods respectively. (The jogs are glissile because the

motion is parallel to the stair-rods which are simultaneously lengthened at one end and shortened at the other.) The stair-rods are interchanged if the fault on the cross-slip plane is type $2\triangledown$, and Weertman (1963) suggested that obtuse jogs will prefer to adopt this configuration.

More complex configurations are possible when the jog is along AD and is dissociated in planes b and c in relative amounts which depend on the orientation of the dislocation line of vector BC. In screw orientation, the favoured configuration according to Hirsch contains only low-energy stair-rods for both upward and downward jogs, with the main extension in c and b respectively, whilst in edge

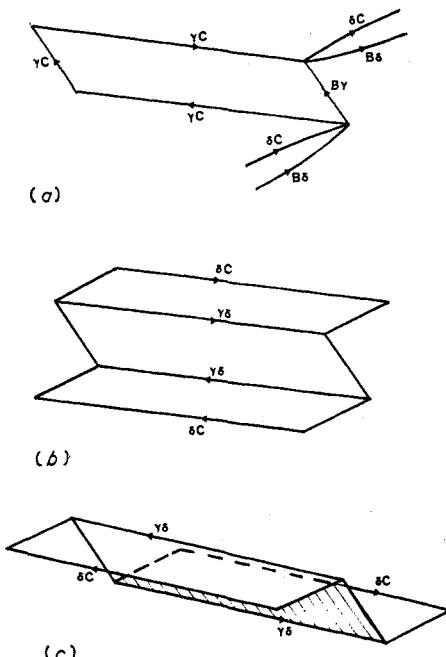


Figure 10. The formation of dissociated dipoles: (a) dipole formed by non-conservative motion of long sessile jog; (b) further dissociation of (a) to give faulted dipole of Z-type; (c) further dissociation of (a) to give faulted dipole of S-type. Extrinsic fault is shown shaded.

orientation the extension is equal on c and b and contains either low- or high-energy stair-rods depending on whether the line is parallel to $A\delta$ or δA . All of these jogs are sessile, and conservative motion is possible only if the jog contracts. Non-conservative motion of sessile jogs involves the trailing of dislocation dipoles which are always of vacancy type if the sessile stair-rod is at the back of the dislocation (figure 10(a)). A consequence of this geometry (Hirsch 1962) is that dislocations with long jogs may trail vacancy-type faulted dipoles when they move in one direction, but either more conservatively or trail unfaulted dipoles in the opposite direction. The asymmetry disappears, of course, if $2\triangledown$ faulted dipoles are produced.

The dipole of figure 10(a) might also be produced by dissociation of an unfaulted dipole Hirsch and Steeds (1963), obtained for example from interaction of dislocations from different sources, provided the dislocations glide until the dipole plane is {111} (c in figure 10(a)). Seeger (1964) pointed out that further dissociation of the opposite Frank partials leads to the configuration shown in figure 10(b),

which is more stable than that shown in figure 10(a). An extended dipole of obtuse type (figure 10(c)) may similarly be obtained if the fault on the inclined plane is $2\sqrt{3}$.

Faulted dipoles form only from the interaction of 60° dislocations, or from the equivalent jog dissociation, i.e. they lie along AB or AC of plane d when the dislocations have Burgers vector BC. They appear in electron micrographs as faint straight lines, and careful contrast experiments are needed to distinguish them from similarly orientated Lomer-Cottrell dislocations. A dipole formed by trapping will remain unfaulted indefinitely unless it is closed at one end because of a large activation barrier between the unfaulted and completely faulted states.

Seeger (1964) first proposed that observations on faulted dipoles provide a method for determining stacking fault energy, and this has been developed by Seeger and Wobser (1966 b), Häussermann and Wilkens (1966) and Steeds (1967 a, b). Steeds used anisotropic theory to investigate four types of transition between the equilibrium configurations of 60° dipoles, dissociated only in the slip plane, and faulted dipoles. Two of these transitions lead to faulted dipoles of the type shown in figure 10(b) (Z dipoles) and two to the type shown in figure 10(c) (S dipoles). A detailed theory of the fault contrast, and especially of the image width of dissociated dipoles in various reflections, was also developed by Steeds (1967 b), and was used in conjunction with the elastic calculations to estimate the stacking fault energy of copper, silver and gold from experimental measurements of the image widths.

In addition to dissociated long jogs, it is important also to consider elementary steps between stacking faults on adjacent close-packed planes. The extended jog then becomes a line defect known as a jog line (Thompson 1955). Jog lines are dipole-like defects corresponding to the overlapping of the cores of two partial dislocations, and there are four basic types, which are equivalent geometrically to lines of one-third or two-thirds vacancies or one-third or two-thirds interstitials. The lowest energy configuration is the one third vacancy line, which corresponds formally to a $\gamma\delta + \delta\gamma$ dipole. Hirsch used arguments similar to those applied to long jogs to discuss the motion of dislocations containing elementary jogs. He estimated the activation energy for conservative motion to be several tenths of an electron volt, and claimed that this may be reduced by stress for interstitial-producing jogs, but not for vacancy jogs. Thus, dislocations with elementary jogs may have different mobilities in opposite directions, and this may lead to the production of more vacancies than interstitials during deformation. However, if each dislocation has equal numbers of jogs there should be no asymmetry in the flow stress.

Planar Frank loops formed by vacancy condensation are frequently observed in quenched fcc metals, but more complex loops which include stepped stacking faults have also been detected (Clarebrough *et al.* 1966, Morton and Clarebrough 1969). A stepped loop could form from two independently nucleated planar loops if these grew until parallel Frank dislocations in $\langle 110 \rangle$ orientation were connected by a common $\{111\}$ plane. Dissociation of the Frank partials according to equation (5.8), followed by glide and mutual annihilation of the Shockley partials on the intersecting $\{111\}$ plane, would then lead to a stepped loop with low-energy ($\alpha\beta$ type) stair-rods along the step edges, and Shockley partial dislocations along the step risers. However, not all of the observed structures are consistent with this mechanism, and it appears that some stepped loops arise from climb processes.

It was originally considered that an extended dislocation must constrict before it can climb, but Escaig (1963) and Schapink and de Jong (1964) showed that a linear row of four vacancies absorbed on a fault may be changed by a simple atomic shift into a triangular array of one-third vacancy jog-lines. Subsequent vacancies can then be absorbed one at a time, each vacancy leading to an increase in length of the triangular fault by one atom distance. When the stacking fault energy is low, the addition of vacancies to the edge of a growing loop will be difficult because of the tendency of the Frank partial to dissociate according to equation (5.8). Thus climb of the stacking fault rather than of the Frank partial will be more probable in materials of low fault energy.

The absorption of vacancies by climb of a stacking fault should be distinguished from the formation of multiple loops by condensation of vacancies on successive {111} planes. Doubly faulted loops were observed by Westmacott *et al.* (1961) and studied by Yoshida and Shimomura (1963) and Edington and Smallman (1965). In quenched aluminium and aluminium alloys, they consist of an outer hexagonal $1\sqrt{3}$ loop and inner triangular $2\sqrt{3}$ loop which is formed by vacancy condensation on the second atomic {111} plane from that of the hexagonal loop. Thus, the extrinsic fault energy is less than twice the intrinsic fault energy. In subsequent work three-layer and four-layer defects have been identified (Edington and West 1966, 1967) and the central area is then unfaulted or has a $1\sqrt{3}$ fault respectively. The observation of four-layer defects suggests heterogeneous nucleation on some impurity.

In metals of low stacking fault energy, characteristic defects of regular or irregular tetrahedron shape have been observed in the electron-microscopic study of specimens quenched from high temperatures. Consider a disk of vacancies on the plane a which collapses to give a triangular-shaped Frank partial with edges parallel to $\langle 110 \rangle$ directions and Burgers vector αA . Each section of this partial can dissociate in the manner of equation (5.8) to give

$$\begin{aligned}\alpha A &= \alpha\beta + \beta A \\ \alpha A &= \alpha\gamma + \gamma A \\ \alpha A &= \alpha\delta + \delta A\end{aligned}\tag{5.9}$$

The Shockley partials bow out on the planes b, c, d , and these dislocations attract each other in pairs to form stair-rods along the intersections AD, AB, AC of the planes $b-c, c-d, b-d$ according to the reactions

$$\begin{aligned}\beta A + A\gamma &= \beta\gamma \\ \gamma A + A\delta &= \gamma\delta \\ \delta A + A\beta &= \delta\beta.\end{aligned}\tag{5.10}$$

The nodes where the pairs of Shockley dislocations meet move away from the original plane a until they meet in a common nodal point. There are then only stair-rod dislocations remaining; these dislocations form the edges of a tetrahedron, the faces of which consist of $1\sqrt{3}$ stacking faults. The tetrahedron may be identified with the Thompson tetrahedron, and the edges AB, BC, CD, BD then have Burgers vectors $\gamma\delta, \delta\alpha, \alpha\beta, \beta\gamma$ which form a tetrahedron inverse to that of the lines themselves.

The above theory is due to Silcox and Hirsch (1959) who also made the first observations of these defects. The final defect is highly symmetrical, and an alternative to the two-stage nucleation process just described is the direct collapse

of small three-dimensional vacancy clusters into tetrahedra which subsequently grow by further vacancy addition (de Jong and Koehler 1963). Experimental evidence exists for both these processes (e.g. Segall and Clarebrough 1964), but in addition it has been established that tetrahedra may be formed by a dislocation reaction during deformation (Loretto *et al.* 1965).

Under conditions of vacancy supersaturation, tetrahedra increase in size by further vacancy condensation. The original mechanism of de Jong and Koehler (1963) requires the nucleation of a high-energy jog line along an edge of the tetrahedron, and it is much more probable (Kimura *et al.* 1963, Kuhlmann-Wilsdorf 1965) that a one third vacancy line is nucleated at an apex. The reverse process of vacancy emission is more difficult to initiate, since the step nucleus is either a short jog line of high energy or a long line of low energy. Tetrahedra formed in quenched metals are indeed very stable against dissolution, and persist in gold, for example, to about 800°C. An alternative mechanism for removing tetrahedra, especially under stress, is the reverse of the Silcox-Hirsch formation mechanism (Meshii and Kaufman 1960).

Observations of coexisting tetrahedra and triangular faults make it important to consider the relative stability of the two defects. The tetrahedron has approximately four times the fault energy and one third the elastic self-energy of the equivalent Frank loop, but a full calculation which includes the interaction energies of the partials is difficult, even in isotropic elasticity. The first treatment by Czjzek *et al.* (1962) was considerably improved by Jøssang and Hirth (1966) and Humble *et al.* (1967). At an intermediate stage, the tetrahedron is truncated parallel to the original fault plane, and figure 11 shows the two models adopted by Humble *et al.* Curves of energy against h were obtained for the one-parameter model with alternative assumptions about the cut-off radii of the dislocations. From these results were calculated curves relating l_c to γ , where l_c is the critical length at which the energy of the Frank loop just equals that of the tetrahedron. The results are rather sensitive to the cut-off radius, since a variation from $\frac{1}{2}b$ to $2b$ was found to change the energy of the defect by up to 13%. Some calculations with the three-parameter model indicate that for given l_c the value of γ is about 5% lower than with the one-parameter model. The results also show that the value of θ is positive, so that the Shockley dislocations bend upwards at the nodes, as shown in figure 11.

Rather similar calculations were made by Jøssang and Hirth, who also proposed an alternative condition for transition which ensures the absence of an energy barrier between initial and final stages. Humble *et al.*, however, show that the equal energy criterion (originally used by Czjzek *et al.*) is likely to be approximately correct in the presence of an applied stress.

Recently the problem has been reformulated by Humble and Forewood (1968 a), who include additional terms such as the kinetic energy of the moving Shockley partials, the energy dissipated to the crystal lattice, and the work done by the applied stress. Using the three-parameter model of figure 11, they calculated curves of potential energy against h for limiting cases of no dissipation of energy to the lattice and complete dissipation of the kinetic energy. The limiting curves were calculated for a cut-off core radius equal to the Burgers vector and for values of applied stress which would produce 0, $\frac{1}{2}$ and 1% plastic strain; they are insensitive to the stress but differ greatly according to the assumption made about energy dissipation, and for given l_c the value of γ obtained from these two assumptions varies by up to 30%. By considering the dissipation processes (lattice friction,

phonon emission) in more detail Humble and Forewood conclude that the critical energy against separation curve which describes the actual process is quite close to the upper limiting curve in which no energy is lost to the lattice. The transformation triangular loop \rightarrow tetrahedron may thus be considered to be conservative, as was simply assumed in the earlier calculations.

Following these calculations, Humble and Forewood (1968 b) conclude that measurements of the size of the largest tetrahedron and smallest Frank loop in a plastically deformed material now give a reliable indication of the stacking fault energy. The energy criterion assumed to govern the transition is that the potential energy of the maximum in the curve equals that of the undissociated Frank loop, so that there is no energy barrier.

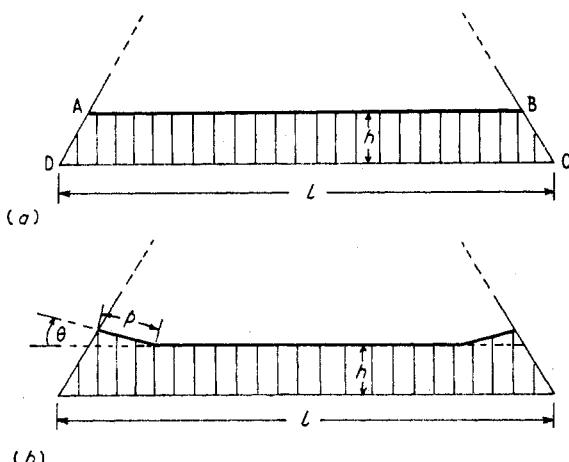


Figure 11. The two models used to consider the stability of a truncated tetrahedral defect: (a) one parameter (h); (b) three parameters (h, p, θ) (after Humble *et al.* 1967).

Many observations have been made of the kinetics of growth or shrinkage of prismatic dislocation loops, faulted loops or tetrahedra in thin foils maintained at constant temperature in the electron microscope. Silcox and Whelan (1960) observed the shrinkage of prismatic loops in aluminium heated to 170–200°C and assumed that the rate-limiting process in climb is the velocity of jogs along the dislocation line. Later experiments (e.g. Dobson *et al.* 1967) showed that dislocation climb in foils is usually limited mainly by point defect diffusion to or from the foil surface, as proposed by Seidman and Balluffi (1966), and the detailed kinetics depend on whether the loop is large (cylindrical diffusion geometry) or small (spherical diffusion geometry).

When both faulted and unfaulted loops are present, they anneal at a different rate, and this is attributed to the dominating effect of the stacking fault energy on the effective climb force for a faulted loop (Edington and Smallman 1965). The force F_c , for the climb of a faulted loop is defined by $2\pi r F_c = dU/dr$ where U is the sum of the elastic self-energy of the loop and the fault energy. Isotropic elastic theory gives

$$F_c = \frac{\mu b^2}{4\pi r(1-\nu)} \left\{ \ln \left(\frac{r}{r_0} \right) + 1 \right\} + \gamma \quad (5.11)$$

and a similar expression is obtained from the more exact expressions for the elastic self-energy of a polyhedral loop given by Bacon and Crocker (1966). The second term on the right-hand side of equation (5.11) is much larger than the first term for all values of $r \gtrsim 10b$.

The kinetics of the loop shrinkage may now be expressed as

$$\frac{dr}{dt} = A_c \left\{ \exp \left(\frac{F_c b^2}{kT} \right) - 1 \right\} \quad (5.12)$$

where b^2 is the area of an atom, and the equation applies independently of whether the process is controlled by jog density and velocity or by vacancy diffusion. The pre-exponential constant A_c involves the diffusion coefficient in all cases, but differs in numerical and geometrical factors. For large faulted loops, $F_c \approx \gamma$ and hence dr/dt is constant, as is observed experimentally. An estimate of γ may thus be obtained if A_c is known (Edington and Smallman 1965), but in the jog-limited case A_c depends on detailed assumptions about the dislocation core, and even in the diffusion-limited case it is difficult to obtain an accurate value of A_c because of uncertainty about the activation energy for diffusion. A better procedure (Dobson and Smallman 1966, Dobson *et al.* 1967) is to compare the shrinkage rates of faulted and prismatic loops.

For a prismatic loop, the second term in (5.11) is zero and the term in brackets in equation (5.12) may be replaced by $\alpha_c b/r$ where α_c (Silcox and Whelan 1960) is essentially constant except for small r/b , and has a numerical value which may be evaluated at each temperature. The annealing rate becomes

$$\frac{dr^2}{dt} = 2A_c \alpha_c b. \quad (5.13)$$

Comparison of equations (5.12) and (5.13) then enables γ to be determined. In a similar way the climb behaviour of doubly faulted loops may be used to obtain an estimate of the extrinsic fault energy.

It remains finally to consider whether any of the dislocations of the fcc structure are unstable in particular orientations. In fcc metals, there is very little directed bonding and the Peierls force is believed to be small. Any marked variation of $E(\theta)$ with θ must thus arise from elastic anisotropy rather than core structure. The calculations of Head (1967) show that for lattice dislocations in this structure, elastic instability only occurs when both elastic coefficients A and B are relatively large, e.g. $A = 6, B = 6$, or $A = 4, B = 10$. These conditions are sufficient to ensure that ordinary lattice dislocations are stable in all orientations for the common fcc metals ($A \lesssim 4$), with the possible exception of lead ($A = 3.9$). Some fcc alloys such as indium-thallium would have appreciable regions of instability because of the large value of A .

The situation is quite different for the individual Shockley partials of an extended dislocation (Clarebrough and Head 1969). For $A = 3.5$ and $B = 6$, for example, the Shockley partial is unstable in an orientation range $78\text{--}102^\circ$ from the screw direction. Experimental evidence for this instability has been found in electron micrographs from a Cu-15.6 at. % Al alloy which has a sufficiently low stacking fault energy for the partials to be readily resolved. The observations show that one partial of a pair is straight, as predicted by theory, whilst the other adopts a Z-shaped or more complex bent form as it passes from one surface of a foil to the other.

The elastic constants of pure fcc metals also indicate instability ranges for Shockley partials—e.g. 79–101° for pure copper—but these have not yet been observed because of the difficulty of resolving the partials in the electron microscope. However, the effect may be important in the calculation of constriction energies, node configurations, etc.

Much of the description in this section has been concerned with stacking faults and partial dislocations. It is evident that in order to discuss the behaviour of a particular fcc metal, the most important parameters are the cell edge, the elastic constants, the core energy (or equivalent cut-off radius) and the stacking fault energy. Core energies and stacking fault energies give particular difficulty, but several methods are available for estimating the latter from experimental measurements. Early indirect methods which depended, for example, on particular theories of the transition from stage II–stage III hardening (see Christian and Swann (1965) for a review) have now been abandoned, and the principal methods currently used for materials of low fault energy are based on the separation of dislocations in an extended dislocation or in a faulted dipole, on the curvature of an extended node, or on the transition from triangular Frank loops to tetrahedra. For materials of high fault energy, the comparison of climb rates of faulted and unfaulted loops appears to be the most reliable technique.

Theoretical calculations of stacking fault energies have been made in recent years by Statz (1962 a) using a tight-binding method, by Harrison (1966), Blandin *et al.* (1966) and Nourtier and Saada (1969) using pseudopotential theory (§ 3.3) and by Hodges (1967 a) using the Heine–Abarenkov model potential. Most of these calculations were combined with attempts to calculate the electrical resistivity of a stacking fault (see also Attree and Plaskett 1956, Seeger 1956 b, Seeger and Statz 1962, Statz 1962 b, Freeman 1965). The results of Blandin *et al.* describe well the stability of various crystal structures and also give energies of reasonable magnitude. For aluminium, they predict a value (about 125 erg cm⁻²) of the 2 ∇ fault energy which is *lower* than the energy (about 150 erg cm⁻²) of the 1 ∇ fault. This is opposite to the conclusion reached from loop annealing experiments, but Nourtier and Saada (1969) believe that these experiments are actually consistent with a lower energy for the 2 ∇ fault.

5.3. Hexagonal close-packed structures

The hexagonal lattice may be defined by a primitive unit cell $a_1 a_2 c$ in which $a_1 \cdot a_2 = -\frac{1}{2}a^2$ and $a_1 \cdot c = a_2 \cdot c = 0$, but directions and planes are often referred to the more symmetrical four-axis system $a_1 a_2 a_3 c$. In the hcp structure, there are two atoms in the primitive cell, and only one-half of the nearest-neighbour interatomic vectors are vectors of the Bravais lattice. There are six stable lattice dislocations with Burgers vectors of type $\frac{1}{3}a\langle 11\bar{2}0 \rangle$ which correspond to nearest-neighbour translations within the close-packed basal planes, two stable dislocations of type $c\langle 0001 \rangle$ which have the smallest Burgers vectors not lying in the (0001) planes, and twelve doubtfully stable dislocations with Burgers vectors $[\frac{1}{3}a, \frac{1}{3}a, -\frac{2}{3}a, c]$. In the three-axis system, dislocations of the first type have Burgers vectors $a\langle 100 \rangle$ and $a\langle 110 \rangle$, and those of the third type have Burgers vectors $\langle a0c \rangle$ and $\langle aac \rangle$.

The basal plane is the main slip plane when $c/a > 1.633$, but in some metals of lower axial ratio, the predominant slip planes are the prismatic or pyramidal planes.

Dislocations in the basal plane interact in exactly the same way as slip plane dislocations in fcc structures, and two-dimensional hexagonal networks may form by reactions of type

$$a[100] + a[010] = a[110] \quad (5.14)$$

which is analogous to (5.1).

Slip dislocations in prismatic and pyramidal planes often have $a\langle 100 \rangle$ Burgers vectors, but if $\langle a0c \rangle$ slip occurs interactions of type

$$[a00] + [00c] = [a0c] \quad (5.15)$$

have to be considered. The $[00c]$ dislocations are sessile but are possibly important in deformation twinning and in phase transformation from fcc to hcp.

Calculations of γ -surfaces (similar to those for bcc crystals, §§ 1.3, 3.2) by Schwartzkopff (1969) using Morse potentials show that metastable stacking faults can exist on basal, prismatic and pyramidal planes of hcp metals. However, the calculated energies are very high for all except basal planes, and there is no convincing experimental evidence for dislocation dissociation on non-basal planes. Thus, there are probably no fault intersections or stair-rod dislocations to be considered. Moreover, the Burgers vector of a partial dislocation in this structure automatically specifies the type of fault to which it is joined. However, a detailed discussion of possible non-planar dissociations in hcp metals has been published by Mendelson (1970).

A $1\triangledown$ fault is produced by a nearest-neighbour displacement between atoms in adjacent basal planes; the magnitude of the displacement is smaller than a when $c/a < 1.633$. There are six sessile partial dislocations of types R($1\triangledown$) or L(1Δ), with Burgers vectors $[\frac{2}{3}a, \frac{1}{3}a, \pm \frac{1}{2}c]$, $[-\frac{1}{3}a, \frac{2}{3}a, \pm \frac{1}{2}c]$ and $(-\frac{1}{3}a, \frac{1}{3}a, \pm \frac{1}{2}c)$, and the negatives of these vectors form the L($1\triangledown$) or R(1Δ) dislocations. The only distinction between the $1\triangledown$ and 1Δ faults is that they occur in alternate planes of the structure, and in terms of configuration symbols all twelve dislocations may form either edge of a C fault. However, the operator notation has the advantage that given the vector of one side of the fault, it specifies which of the remaining vectors may form the other edge.

The $2\triangledown$ (or CC) fault corresponds to partial slip on the basal plane, and the glissile partial dislocations may be compared to Shockley partials of the fcc structure. There are thus three dislocations of the R($2\triangledown$) or L(2Δ) sets with Burgers vectors $[\frac{1}{3}a, -\frac{1}{3}a, 0]$, $[\frac{1}{3}a, \frac{2}{3}a, 0]$, $[-\frac{2}{3}a, -\frac{1}{3}a, 0]$ and the opposite vectors give the L($2\triangledown$) or R(2Δ) dislocations. The extrinsic fault $3\triangledown$ or 3Δ is bounded by sessile edge dislocations with Burgers vectors $[0, 0, \pm \frac{1}{2}c]$ which are normal to the plane of the fault, and these dislocations are thus analogous to Frank partials.

Berghezan *et al.* (1961) used a bipyramid (figure 12) to represent the Burgers vectors of dislocations in the hcp structure, as follows.

- (i) Lattice dislocations with vectors $\langle a00 \rangle$ and $\langle aa0 \rangle$ are given by the sides of the triangle ABC.
- (ii) Lattice vectors normal to the basal plane are $\pm ST$.
- (iii) Lattice dislocations of types $\langle a0c \rangle$ have vectors TA/BS, etc.
- (iv) Partial dislocations bounding 1Δ and $1\triangledown$ faults have vectors AS, SB, etc.
- (v) Shockley type partials bounding 2Δ and $2\triangledown$ faults have vectors A σ , σ B, etc.
- (vi) Partial dislocations bounding extrinsic faults have vectors σS , σT .

Lattice dislocations with basal plane Burgers vectors may dissociate into extended dislocations in a manner analogous to equation (5.3), namely

$$a[100] = \frac{1}{3}a[1\bar{1}0] + \frac{1}{3}a[210] \quad (5.16)$$

or

$$AB = A\sigma + \sigma B. \quad (5.16a)$$

Dislocations of type $\langle 00c \rangle$ may similarly dissociate into partial dislocations separated by $1\triangledown$ faults, e.g.

$$ST = SC + CT. \quad (5.17)$$

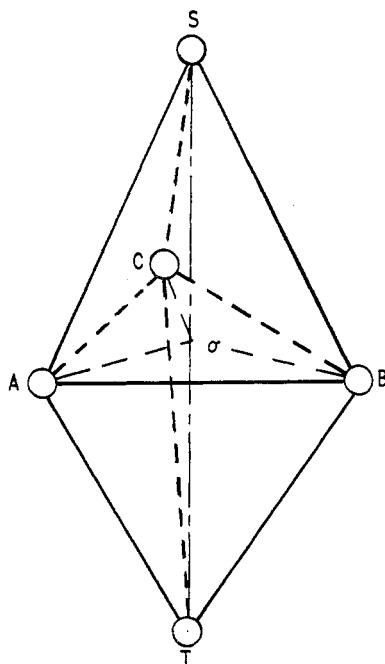


Figure 12. The hexagonal bipyramidal (after Berghezan *et al.* 1961).

Since the partials are sessile, this dissociation could not occur by glide, but it may nevertheless be possible because it only requires climb of atoms over one interplanar distance.

The collapse of a single disk of vacancies on a (001) plane may give either a $3\triangledown$ fault with a low-energy partial σS or a $1\triangledown$ fault with a high-energy partial AS . This is analogous to the formation of Frank loops or prismatic loops in fcc structures, and there should be a critical radius above which the $1\triangledown$ loop is stable. In many metals of moderately high fault energy, direct condensation to $1\triangledown$ loops is probable (Berghezan *et al.* 1961, Price 1963, Lally and Partridge 1966). Conversion of a $3\triangledown$ to a $1\triangledown$ fault requires nucleation of a Shockley partial

$$A\sigma + \sigma S = AS \quad (5.18)$$

as in fcc structures. Exactly equivalent conditions apply to the condensation of interstitials as a single disk.

Vacancies may also precipitate on two successive (001) planes to give prismatic loops of lattice dislocation of Burgers vector [00c] or [a0c]. Loops of type [a0c] may sometimes be formed by pyramidal slip, and can lower their energy by dissociating in accordance with equation (5.15). The [00c] dislocation is sessile, whilst the [a00] loop collapses and disappears. Another possibility is for the loop to dissociate by climb into a faulted loop of twice the original area. Two concentric loops of Burgers vectors TA and AS are produced and one shrinks and disappears whilst the other grows by surface diffusion across the $1\bar{1}$ fault between the two loops. This implies that vacancies may prefer to precipitate as single sheets, despite the energy of the $1\bar{1}$ fault (Price 1963).

In conditions of high vacancy supersaturation, the reverse process occurs by the nucleation of a second layer of vacancies on an already growing $1\bar{1}$ fault, which is thereby removed. There are again two loops separated by an annulus of stacking fault, but both loops are growing outwards. In thin foils, two-, three- or four-layer loops have been observed to form, so that each layer alternately introduces or removes a $1\bar{1}$ fault.

Measurements of the kinetics of loop shrinkage in zinc and magnesium were made by Harris and Masters (1966 a, b) and used to estimate the fault energies. Later work has shown that vacancies are often injected into the specimen by surface oxidation processes (Dobson and Smallman 1966) and the method of comparative climb kinetics of faulted and unfaulted loops has been used to deduce the fault energy. Studies have also been made of the climb kinetics of multiply faulted loops in magnesium (Hales *et al.* 1968). When there is a vacancy supersaturation, both components of a doubly faulted loop increase in size, but the inner dislocation grows more rapidly because it is removing fault. As the loops approach, vacancy transfer across the fault accentuates this difference, and they eventually coalesce to form a prismatic dislocation of Burgers vector TS. The growth rates of inner and outer loops may be written

$$\left(\frac{dr}{dt}\right)_{\text{inner}} = A_c \left(\frac{c_s}{c_0} - \exp\left(\frac{-\gamma b^2}{kT}\right) \right) \quad (5.19)$$

$$\simeq A_c \left(\frac{c_s}{c_0} \right)$$

$$\left(\frac{dr}{dt}\right)_{\text{outer}} = A_c \left(\frac{c_s}{c_0} - \exp\left(\frac{\gamma b^2}{kT}\right) \right) \quad (5.20)$$

where c_s is the concentration of vacancies at the surface and c_0 the equilibrium concentration of vacancies. The growth rate of the combined prismatic loop is

$$\left(\frac{dr}{dt}\right)_{\text{prismatic}} = \frac{1}{2} A_c \left(\frac{c_s}{c_0} - 1 \right) \quad (5.21)$$

where the approximation

$$\exp(F_e b^2/kT) - 1 \simeq A_c b/r \ll 1$$

for large loops has been used. From equations (5.19) and (5.21) the constants A_c and (c_s/c_0) may be determined, and γ may then be found from (5.20). The value obtained for magnesium was 125 ± 25 erg cm $^{-2}$. If both terms in (5.19) are retained, this value is reduced to 102 erg cm $^{-2}$ (Leighly 1970).

5.4. Body-centred cubic structures

In the bcc structure, there are eight stable dislocations with minimum Burgers vectors of type $\frac{1}{2}a\langle 111 \rangle$, and six dislocations of type $a\langle 100 \rangle$, which are also stable according to the Frank approximation. All other lattice dislocations should be unstable against dissociation, although some evidence for the existence of $a\langle 110 \rangle$ dislocations has been claimed (Hale and Henderson-Brown 1969). Lattice dislocations $\frac{1}{2}a\langle 111 \rangle$ glide on $\{10\bar{1}\}$, $\{11\bar{2}\}$ and possibly $\{1\bar{2}3\}$ and other planes of the zone; there is only very indirect evidence for glide motion of $a\langle 100 \rangle$ dislocations (Reid *et al.* 1966). Two dislocations of type $\frac{1}{2}a\langle 111 \rangle$ may attract each other to form the other type of lattice dislocation, e.g.

$$\frac{1}{2}a[111] + \frac{1}{2}a[1\bar{1}\bar{1}] = a[100]. \quad (5.22)$$

This reaction could occur in a single slip plane (e.g. $(01\bar{1})$) or between dislocations moving in different slip planes. When the two slip planes are perpendicular (e.g. $(10\bar{1})$ and (101)), the product dislocation is pure edge in character and has a geometrical slip plane (010) . Cottrell (1958) suggested that the $a\langle 100 \rangle$ dislocation may be so narrow that it is properly regarded as an incipient crack (see § 3.3) and the reaction is then a possible mechanism for crack nucleation.

There is no clear evidence for partial dislocations and associated stacking faults in bcc structures, and calculations based on central force atomic interactions (Vitek 1968) indicate that metastable faults do not exist in this structure. Faulting on $\{112\}$ planes has often been assumed because deformation twinning occurs rather readily, and hard-sphere models of faults on the most usual crystallographic slip plane, $\{110\}$, have also been suggested. Electron microscopic observations of defects with fault-type contrast (Fourdeux and Berghezan 1960–1, Segall 1961, Hirschhorn 1963, Takeyama and Koepel 1963, Lindley and Smallman 1963, Smerd 1968) may all be due to thin precipitates.

The stacking sequence of $\{112\}$ planes has a six-layer repetition ...ABCDEF... and the corresponding twin stacking is ...FEDCBA.... A displacement $\frac{1}{6}a[11\bar{1}]$ on $\{112\}$ produces a stacking of ...ABCDCEFA... which corresponds to a monolayer twin, i.e. a reversal of the correct sequence at only one plane.[†] This intrinsic fault was proposed by Cottrell and Bilby (1951). It may be bounded by glissile partials with Burgers vectors $\frac{1}{6}a[\bar{1}\bar{1}1]L$ or $\frac{1}{3}a[1\bar{1}\bar{1}]L$ or by sessile partials with Burgers vectors $\frac{1}{3}a[112]L$, $\frac{1}{3}a[2\bar{1}\bar{1}]L$ and $\frac{1}{3}a[1\bar{2}\bar{1}]L$ or $\frac{1}{3}a[\bar{1}\bar{1}3]L$, $\frac{1}{6}a[\bar{1}51]L$ and $\frac{1}{6}a[5\bar{1}1]L$, and as usual the negatives of these vectors apply to dislocations at the right-hand edge. A lattice dislocation in $\{112\}$ might then dissociate to form an extended dislocation

$$\frac{1}{2}a[11\bar{1}] = \frac{1}{3}a[11\bar{1}]L + \frac{1}{6}a[11\bar{1}]R \quad (5.23)$$

and many suggested mechanisms for deformation twinning are based on this reaction (figure 13(a)). Further dissociation of the $\frac{1}{3}a[11\bar{1}]L$ dislocation on the $\{112\}$ plane is considered improbable since a different type of fault would be produced, but for a screw dislocation the symmetrical dissociation

$$\frac{1}{2}a[11\bar{1}] = \frac{1}{6}a[11\bar{1}] + \frac{1}{6}a[11\bar{1}] + \frac{1}{6}a[11\bar{1}] \quad (5.24)$$

would be possible if the three partial dislocations moved away on the three $\{112\}$ planes which intersect in the $[11\bar{1}]$ direction. This configuration was proposed by

[†] According to recent calculations (Vitek 1970 a) a monolayer fault is unstable although a three-layer fault can be metastable.

Hirsch (1960) and Mitchell *et al.* (1963), but Sleewyk (1963) showed that it is elastically unstable and should collapse to the asymmetric structure of figure 13(b) which represents a dislocation extended on only two planes. Wasilewski (1965) suggested that the dissociation (5.24) could also take place on {110} planes.

A fault on (101) (Crussard 1961, Cohen *et al.* 1962) is produced by the symmetrical dissociation

$$\frac{1}{2}\alpha[11\bar{1}] = \frac{1}{6}\alpha[10\bar{1}] + \frac{1}{4}\alpha[12\bar{1}] + \frac{1}{8}\alpha[10\bar{1}] \quad (5.25)$$

in which both faults are of the same type. For the particular case of a screw dislocation, Kroupa (1963) and Kroupa and Vítek (1964) suggested the symmetrical dissociation on three {101} planes to produce the configuration of figure 13(c) according to the reaction

$$\frac{1}{2}\alpha[11\bar{1}] = \frac{1}{8}\alpha[10\bar{1}] + \frac{1}{6}\alpha[110] + \frac{1}{8}\alpha[01\bar{1}] + \frac{1}{4}\alpha[11\bar{1}]. \quad (5.26)$$

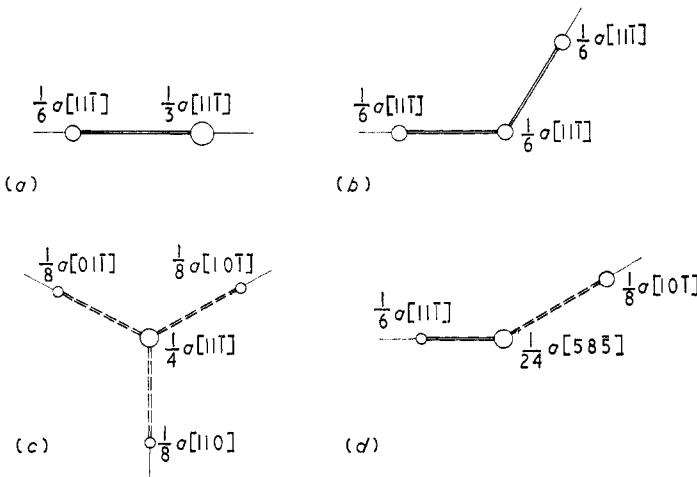


Figure 13. Dissociations proposed for bcc dislocations.

Further possibilities include composite dissociations on {110} and {112} planes (Šesták 1966, Sleeswyk 1966, Duesbery *et al.* 1967, Duesbery and Hirsch 1968, Mitchell 1968 a, Vítek and Kroupa 1968). Figure 13(d) shows the composite dissociation

$$\frac{1}{2}\alpha[11\bar{1}] = \frac{1}{6}\alpha[11\bar{1}] + \frac{1}{24}\alpha[58\bar{5}] + \frac{1}{8}\alpha[10\bar{1}]. \quad (5.27)$$

Mitchell (1968 b) has examined possible dissociations of non-screw dislocations which lie along the intersections of {101} and {112} planes. If the allowed faults are those represented by (5.23) and (5.25), dislocations in {112} planes have lowest energy in the configuration shown in figure 13(a), for all except pure screw orientations. However, dislocations which lie in (101) along [101][131] or [131] may lower their energy by further dissociation of the $\frac{1}{4}\alpha[12\bar{1}]$ component into $\frac{1}{6}\alpha<111>$ type partials on two intersecting {112} planes, leaving a sessile dislocation of type $\frac{1}{12}\alpha[32\bar{3}]$ at the intersection of four faults.

The dissociation of a lattice dislocation in a {112} plane in which it cannot glide, e.g. in (112)

$$\frac{1}{2}\alpha[111] = \frac{1}{3}\alpha[112] L + \frac{1}{6}\alpha[11\bar{1}] R \quad (5.28)$$

is analogous to the fcc reaction (5.6) and has been discussed in connection with deformation twinning (Cottrell and Bilby 1951). There is no first-order change in elastic energy, so a rather high stress would be required to initiate the dissociation.

Interest in the dissociations (5.23)–(5.27) has been stimulated by experimental observations of slip geometry, flow stress asymmetry, predominance of screw dislocations after low-temperature deformation, and by the strong temperature and strain-rate sensitivity of the flow stress. The dissociated screw models are able to provide a single explanation (see § 6.3) for these varied phenomena. As discussed in § 3.2, a generalized splitting of the dislocation core is a better model for the bcc structure than any specific assumption about the type of fault, and the separation of the partials is within the usual core radius. Thus, the general properties of these models are probably of much greater significance than the details of any individual dissociation, although (5.23) and (5.28) may retain their significance for deformation twinning.

Prismatic dislocation loops have been found in zone-refined molybdenum (Meakin *et al.* 1965) but aggregated vacancy defects are not normally observed in quenched bcc metals, either because of strong interactions of vacancies with interstitial impurities or, more probably, because of high formation and low migration energies. Thus, evidence for partial dislocations and stacking faults is not available, apart from some defects seen by field ion microscopy (Smith and Bowkett 1968, D. A. Smith 1969, Smith and Gallot 1969) which have been interpreted as dislocations dissociated on {112} or {110} planes. This dissociation may possibly be a consequence of the strong electrostatic field at the surface of the specimen (Vitek 1970 b).

Some bcc metals are very elastically anisotropic with values of the Zener constant A varying from 0.51 for niobium to 8.15 for sodium and 8.45 for β -brass. In β -brass, [111] dislocations in a (1 $\bar{1}$ 0) plane should be elastically unstable over ranges -26° to $+33^\circ$ and 88° to 116° from pure screw orientation, and there are similarly three instability ranges each for [111] dislocations in (1 $\bar{1}$ 2) and for [001] dislocations in (010) (Head 1967). Electron microscopy reveals many V- or Z-shaped dislocations in this ordered bcc structure.

Head's calculations also show that [001] dislocations in iron have instability ranges of about 30° on (1 $\bar{1}$ 0) and (010) but that [111] dislocations are stable on (1 $\bar{1}$ 0) and (1 $\bar{1}$ 2) in all orientations. Identification of Burgers vectors by electron microscopy is difficult because of complex diffraction conditions (France and Lorretto 1968, Hale and Henderson-Brown 1969) and care is needed to avoid erroneous conclusions. Hale and Henderson-Brown estimate that 5% of the dislocations in deformed iron are $a\langle 100 \rangle$ and 1% are $a\langle 110 \rangle$ type.

5.5. The diamond structure

The diamond structure (figure 14) is based on a fcc lattice with two atoms in the primitive unit cell. When referred to the conventional cubic cell, one atom is at (000) and the other atom at ($\frac{1}{4}\frac{1}{4}\frac{1}{4}$) and equivalent positions. This produces the well known arrangement in which each atom is tetrahedrally bonded to its nearest neighbours, and the binding energy is believed to be expressible mainly in terms of these directional, nearest-neighbour interactions. A comprehensive review of dislocations and plastic flow in the diamond structure has been published recently by Alexander and Haasen (1968).

Lattice dislocations have the same Burgers vectors as in the fcc structure, but this vector no longer represents a nearest-neighbour atom displacement. The structure may also be regarded as a sequence of {111} layers, with a double stacking pattern ...A α B β C γ Atoms in layers A and α , etc. are separated by displacements $\frac{1}{4}a\langle 11\bar{1}\rangle$ which are normal to the layers. Layers α and B have the usual $\frac{1}{4}a\langle 11\bar{2}\rangle$ component of displacement but are separated by a normal vector of only $\frac{1}{2}a\langle 111\rangle$. Possible stacking faults involve the removal or insertion of pairs of layers A α , etc. and they then have the same representations as in the fcc structure, and are bounded by dislocations of the same Burgers vectors. The InSb-type structure is closely related to the diamond structure, except that the planes A, B, C are now occupied by atoms of one type, and the planes α , β , γ by atoms of the other type.

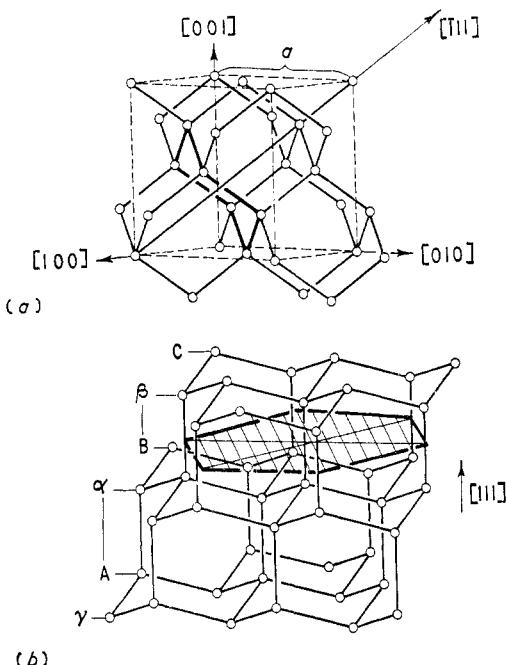


Figure 14. The diamond structure. (a) the relation of the tetrahedral coordination to the cubic unit cell; (b) the stacking sequence ...A α B β C γ ... (after Alexander and Haasen 1968).

Geometrically, the shear produced by dislocation glide could take place between closely spaced planes α -B or widely spaced planes B- β . Since the ratio of nearest-neighbour bonds is 3 : 1, a B- β shear is expected (Shockley 1953). However, a stacking fault can be produced only by a shear between the non-equivalent stacking positions α and B, so that if a lattice dislocation is to dissociate as in equation (5.3) it must be of α -B type. In order to allow for both possibilities, Hirth and Lothe (1968 a) introduce a representation in which two interpenetrating Thompson tetrahedra, ABCD and A'B'C'D' displaced from ABCD in the direction δD , represent dislocations of types α -B and B- β respectively.

Although an extended dislocation may not be formed directly for a dislocation with Burgers vector (say B'C' on d') of the A'B'C'D' set, it is possible for this dislocation to combine with a Shockley partial of the ABCD set on a neighbouring plane d. Thus a stacking fault bounded by δB and B δ could combine with B'C' to

form $\{\delta C + (CB + B'C')\}$ and $B\delta$, and $(CB + B'C')$ then represents a row of vacancies or a row of interstitials depending on which side of d' is taken d . The resulting configuration (Hornstra 1958) is very similar to an extended dislocation in fcc structures. However, it cannot glide unless there is also a local shear or rearrangement of the row of interstitials (vacancies); for this reason, Hirth and Lothe refer to dislocations of type $B-\beta$ as the "shuffle set". On the other hand, Alexander and Haasen (1968) believe that the configuration will split up on application of a stress because of the lower mobility of the Shockley partials, so that glide dislocations are essentially undissociated. It may also be difficult to nucleate this configuration,

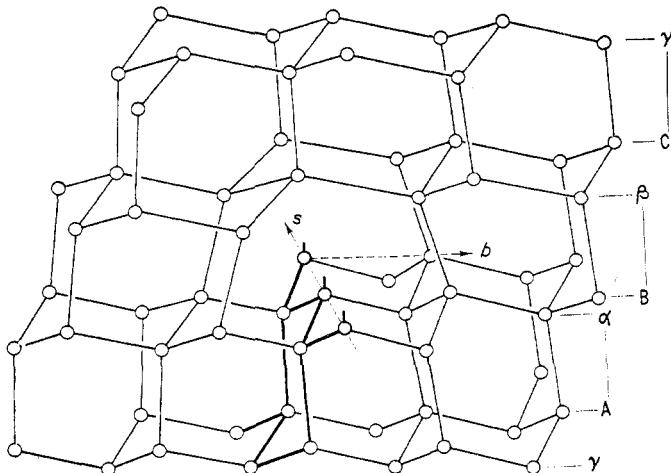


Figure 15. Model of a 60° dislocation in the diamond structure (after Hornstra 1958).

despite the low stacking fault energy. Hirth and Lothe (1968 a) refer to dislocations of type $\alpha-B$ as the glide set, since they are presumably dissociated in the ordinary way, and it is geometrically possible for the Shockley partials to move without shuffling.

Experimental observations of glide dislocations in silicon and other diamond-type structures show that after small deformations they usually lie parallel to the close-packed $\langle 110 \rangle$ directions of the slip plane; that is, they are either 60° dislocations or pure screws. Directed bond models are usually used to depict the structure of these dislocations, and figure 15 shows Hornstra's model for a 60° dislocation of $B-\beta$ type. The 'dangling' bonds are of considerable importance in the electrical properties of dislocations, since they may be regarded as each containing one electron. They may thus act as electron acceptor sites, in order to form electron pairs, or possibly as electron donors. The trapped electrons charge the dislocation negatively and may travel along it; they are shielded by a cylindrical space charge. Thus, p-type channels may be produced in semiconducting materials of diamond structure, even if the bulk of the material is n-type. Heine (1966) has shown that there is a further effect, namely an attraction of electrons to the core of the dislocation because of the dilatation, and he believes this is of greater importance in charging the dislocations. In the InSb structure, 60° dislocations of opposite signs will be terminated by atoms of different types and so may have non-equivalent electrical properties (Haasen 1957).

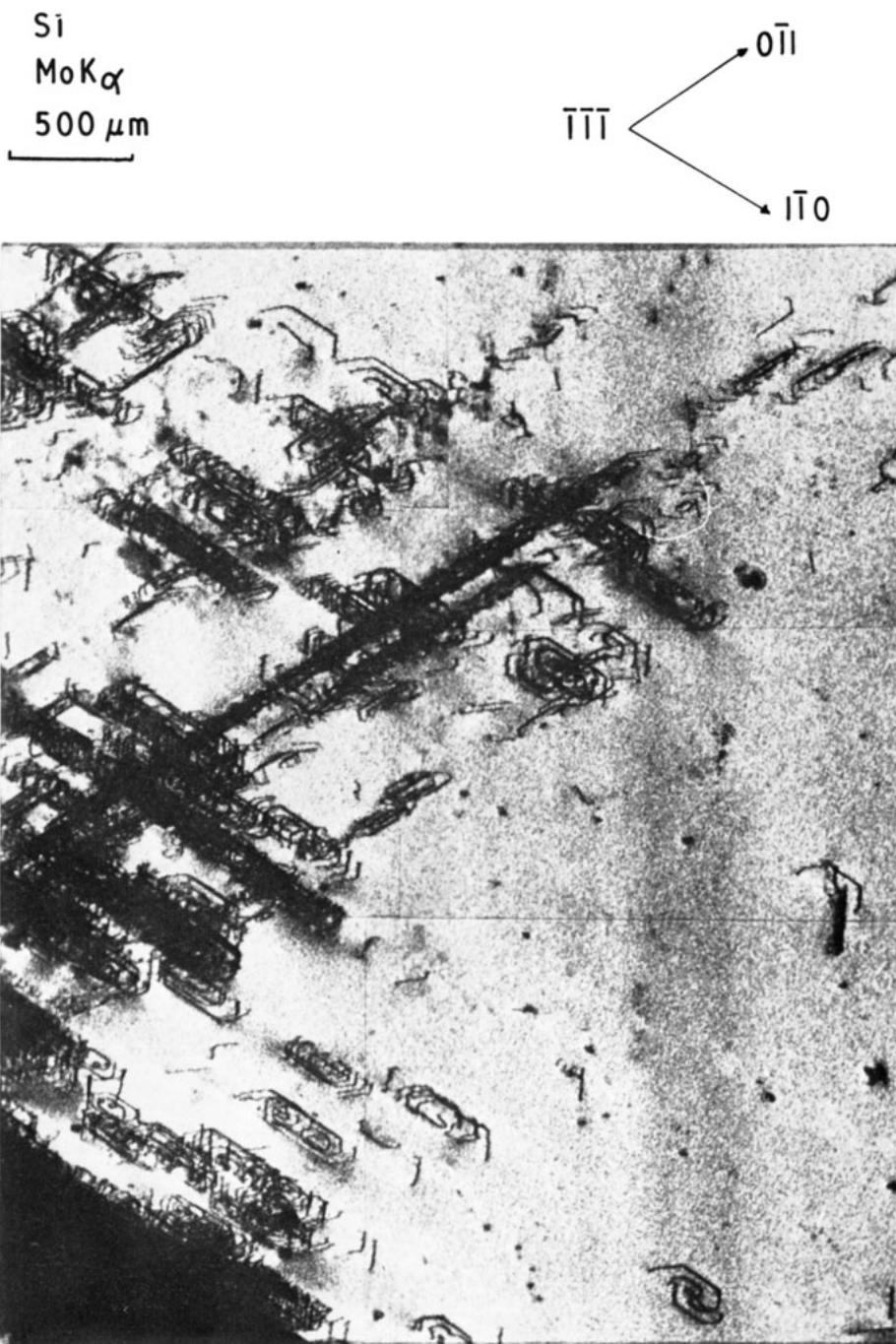


Plate 1. x-ray Lang topograph of (111) silicon slice showing operation of Frank-Read sources and crystallographic orientation of dislocation lines (MoK α radiation) (courtesy of J. Miltat 1970, unpublished).

Alexander and Haasen (1967) and Alexander (1968) have shown by thin-foil electron microscopy that the dislocation structures in plastically deformed germanium are quite similar to those in cold-worked copper; in particular, the tendency of dislocations to follow close-packed directions reported by most early workers is entirely absent. It is not yet known whether silicon deformed at sufficiently high temperatures and to a sufficiently great extent will also show similar structures. Plate 1 shows an x-ray projection topograph of a silicon slice (J. Miltat 1970, unpublished). There are interior and surface sources on three {111} planes, and almost all glide dislocation loops are of screw or 60° type, except where there are strong interactions with neighbouring dislocations. Lomer dislocations have also been observed, both by transmission electron microscopy and by x-ray topography.

Networks of dislocations with extended nodes have been observed in silicon, germanium, InSb and InAs, and have been used to evaluate the stacking fault energies (Aerts *et al.* 1962, Art *et al.* 1963, Holt and Dangor 1963, Siethoff and Alexander 1964). The nodes appear all to be extended, but Booker and Brown (1965) and Shaw and Brown (1967) show that unextended nodes may sometimes appear extended under complex contrast conditions when the separation of the partials is less than half the extinction distance. Thus some uncertainty has existed about the measurements of Aerts *et al.*, but recently Ray and Cockayne (1970) have used the weak beam dark field technique mentioned in § 5.2 to show that dislocations and nodes in silicon are in fact extended. A simple calculation (equation (5.4)) gives a fault energy of $\approx 55 \text{ erg cm}^{-2}$. These observations suggest that dislocations of type α -B exist, since node extension would probably not be expected if all dislocations are of the B- β type.

Dislocation loops formed from point defects do not appear to have been observed in silicon or germanium, and the behaviour of these materials after quenching from high temperatures is difficult to interpret (see Seeger and Chik (1968) for review). Dislocation jogs must be at least two atoms long, so that emission or absorption of point defects by climb or nonconservative dislocation movement presumably must involve pairs of defects. Alexander and Haasen point out, however, that divacancies are less mobile than single vacancies (contrary to most metals) because the nearest neighbours of any atom site are not nearest neighbours of each other.

5.6. Ionic crystals

Crystals with the NaCl structure have a fcc lattice with positive ions M^+ at (000) and negative ions at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ and equivalent positions. The shortest lattice vectors are $\frac{1}{2}a\langle 110 \rangle$ and dislocations with Burgers vectors $a\langle 100 \rangle$ should also be doubtfully stable. The stacking sequence on {111} planes can be expressed as ...AyBaC β ... where A, B and C layers represent (say) positive ions in the usual three stacking positions and α, β, γ represent negative ions in the same positions. Unlike the stacking sequences in the diamond, fluorite or zincblende structures, it is not possible to remove or insert layers on this sequence in such a way that nearest-neighbour relations are preserved. Thus, there are no twins in ionic crystals of this type, and {111} stacking faults and imperfect dislocations are not expected.

Fontaine (1967, 1968 a, b) used Coulomb plus Born-Mayer interactions to calculate the energies of generalized stacking faults on {110} {100} and {111} planes of the NaCl structure. He found no metastable faults, and faults involving large

displacements on $\{100\}$ and $\{111\}$ are mechanically unstable, i.e. they will split the lattice. This suggests that the core may be dissociated on $\{110\}$ planes in agreement with the experimental slip elements $\langle 110 \rangle \{1\bar{1}0\}$. Some crystals of the same structure (e.g. PbTe) are only weakly ionic and extension of the dislocation core on $\{001\}$ is then also possible, in agreement with the observed $\langle 110 \rangle \{001\}$ slip. An earlier theory (Rachinger 1956) considered the possibility of slip in $\langle 100 \rangle$ directions of weakly ionic crystals as the result of coupled pairs of $\frac{1}{2}a\langle 100 \rangle$ dislocations separated by stacking faults of the APB type. However, it now appears improbable that these dislocations glide in any crystal with the rocksalt structure.

Gilman (1959) measured the relative stresses for dislocation motion on $\{1\bar{1}0\}$ and $\{001\}$ for a number of crystals of NaCl type, and found that $\{001\}$ glide is increasingly preferred as the polarizability of the ions increases. Only in PbTe and PbS, however, is $\{001\}$ the primary slip plane. The measured stresses for $\{001\}$ glide in LiF are much higher than for $\{1\bar{1}0\}$ glide and this plastic anisotropy can probably only be explained in terms of core structures.

Dislocation behaviour in ionic crystals is considerably influenced by electrical effects. For example, a $\frac{1}{2}a[110]$ edge dislocation emerging normal to a (001) face introduces a net charge of $\pm \frac{1}{4}e$ at the point of emergence. The charge alternates as successive layers of ions are removed from the surface, or as the dislocation climbs in the $[1\bar{1}0]$ direction. Similarly, elementary jogs in pure edge dislocations have charges $\pm \frac{1}{2}e$, and the charge alternates in sign as the jog moves along the dislocation by climb (Seitz 1950). Double-height jogs, or superjogs which are integral multiples of double-height jogs, are uncharged. This means that there is electrostatic attraction between elementary jogs, and superjogs may be stable against dissociation into elementary jogs (which is not true if only elastic interactions are considered).

Movement of an edge dislocation produces no charge transport parallel to the dislocation line, but this is not true of screw dislocations. Rules for determining the charges of kinks or jogs on screw dislocations are given by Hirth and Lothe (1968 a). They point out that although it has been recognized for some time that edge dislocations may carry a net charge (Bassani and Thomson 1956, Eshelby *et al.* 1958) from a preponderance of jogs of one sign, the corresponding possibility of charged screw dislocations appears to have been neglected. Because of the charge, screw dislocations should interact strongly with point defects at jogs and kinks.

A second important ionic structure is the CsCl type, which is simple cubic with positive ions at (000) and negative ions at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$. The smallest lattice vector is $a\langle 100 \rangle$ and this is the usual Burgers vector, with slip plane (011). The shortest interatomic vector is $\frac{1}{2}a\langle 111 \rangle$, but dislocations of this type would be attached to a stacking fault involving positive-positive and negative-negative bonds. However, there are many examples of this structure where the bonding is predominantly metallic rather than ionic, and slip may then occur in $\langle 111 \rangle$ directions by the glide of coupled $\frac{1}{2}a\langle 111 \rangle$ dislocations separated by antiphase boundary. Rachinger and Cottrell (1956) found $\langle 111 \rangle$ slip for CuZn and AgMg, but $\langle 100 \rangle$ slip for AuCd, AuZn, LiTl, MgTl and thallium halides. They estimated that the fault energy must be less than 250 erg cm^{-2} for $\langle 111 \rangle$ slip, and Fontaine's calculations confirm that the energy is higher than this in CsCl, CsBr and CsI.

5.7. Superlattice structures

The APB faults described in § 1.3 may be formed either by dislocation glide or by the separate nucleation and growth of out-of-phase domains during the ordering

process. Nucleation is generally much easier than in other phase transformations, so that a large number of such domains may form in a relatively small volume. The resultant 'foam' structure will be metastable provided there are at least four different kinds of domain. If there are only two possibilities, the APBs must either cross the original crystal, form closed surfaces or end on dislocation lines. These boundaries can then reduce their energy by contracting to minimum area, leaving only a few straight APBs.

Details of the various types of APBs in the common superlattice structures are given in the extensive review by Marcinkowski (1963) and by Christian and Swann (1965). The most important boundaries associated with dislocations are those of type 1 which are attached to gliding dislocations. Thus, in the ordered β -brass (B2) structure, the copper atoms are at (000) and the zinc atoms at $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of the simple cubic unit cell. The structure is identical with that of CsCl, but Koehler and Seitz (1947) pointed out that because of the relatively low energy of the APB, $\langle 111 \rangle$ slip should result from pairs of $\frac{1}{2}a\langle 111 \rangle$ dislocations, separated by a distance

$$D = \frac{3\mu a^2}{8\pi\gamma_{APB}} \left(\frac{1 - \nu \cos \theta}{1 - \nu} \right) \quad (5.29)$$

(cf. equation (5.4)). The value of γ_{APB} will depend on the plane of splitting, and is expected to be least for the $\{1\bar{1}0\}$ plane which is the observed slip plane. A quasi-chemical approximation for this energy is $kT_c/\sqrt{2a}$, where T_c is the critical disordering temperature. Marcinkowski estimates γ_{APB} for fully ordered CuZn alloys to be 83 erg cm $^{-2}$, and the corresponding widths of dissociated edge and screw dislocations to be 88 Å and 56 Å respectively.

A second important cubic superlattice is the AuCu₃(L₁₂) structure which also has a simple cubic unit cell obtained from the disordered fcc cell by putting Au atoms in sites (000) and Cu atoms in sites $(\frac{1}{2}\frac{1}{2}0)(\frac{1}{2}0\frac{1})(0\frac{1}{2}\frac{1})$. A superlattice dislocation now consists of two ordinary dislocations of the fcc structure with parallel Burgers vectors $\frac{1}{2}a\langle\bar{1}01\rangle$. However, when this dislocation lies in a $\{111\}$ glide plane, each of the $\frac{1}{2}a\langle\bar{1}01\rangle$ dislocations may be further dissociated into Shockley partials, to produce structural stacking faults, and this will also disturb the ordering. A simple approximation is to take the energy of the fault between Shockley partials to be $\gamma_{APB} + \gamma$, where γ is the energy of a $1\bar{\nabla}$ fault in the disordered structure.

The equilibrium configuration now depends on the interactions of all four partials and has to be found by numerical methods. However, if the overall width D' is much greater than the Shockley separations d' , an approximate analytic solution is given by equation (5.4) for d' with γ replaced by $\gamma + \frac{1}{2}\gamma_{APB}$ and by

$$D' - d' = \frac{2}{3}D \quad (5.30)$$

where D is given by (5.29). For Cu₃Au, Marcinkowski assumed $\gamma = 40$ erg cm $^{-2}$ and $\gamma_{APB} = 92$ erg cm $^{-2}$, which gives values of d' and D' as 17 Å, 102 Å for edge dislocations and 8 Å, 65 Å for screw dislocations, whereas the experimental separation is $D' \approx 130$ Å. Similar comparisons for Ni₃Mn suggest a value of 75 erg cm $^{-2}$ for γ_{APB} , rather than the theoretical estimate of 114 erg cm $^{-2}$. The separation D' increases to about 500 Å in a partially ordered Ni₃Mn (order parameter 0.55), and this corresponds to $\gamma_{APB} \approx 24$ erg cm $^{-2}$.

The theory predicts that $d' < d$, the separation of partials in a disordered alloy, but Marcinkowski and Zwell (1963) found d' increases with increasing order. This

implies that the simple additivity of fault energies is incorrect, and γ is itself a function of degree of order.

A similar discussion may be given for other superlattice structures, for example DO_3 and $\text{L}2_1$ which are derived from a disordered bcc structure, $\text{L}1_0$ derived from a disordered fcc structure and DO_{19} derived from a disordered hcp structure. There are also long-period superlattices which may be obtained from simple superlattices by introducing regularly spaced APBs. The stability of such structures must depend on long-range interactions, and true lattice dislocations would have very large Burgers vectors. However, such dislocations are probably completely dissociated into the types discussed above.

6. Thermally activated dislocation motion

6.1. Thermodynamic analysis

Energy barriers to dislocation motion which arise from short-range interactions with discrete obstacles (solute atoms, clusters, point defects, dislocations, etc.) or from alternative low- and high-energy configurations of the dislocation core (Peierls barrier, nonplanar dissociation, etc.) may be overcome with the help of coherent thermal fluctuations. The velocity is then determined mainly by the time of stay at a barrier, $t_1 = 1/\Gamma$, and a quasi-thermodynamical treatment based on chemical reaction rate theory (Eyring 1936) has been used by many authors (e.g. Seeger 1955 b, Basinski 1957, 1959, Conrad and Wiedersich 1960, Christian and Masters 1964, Gibbs 1964, 1965, Schoeck 1965, Li 1965, 1968, Geszti 1967, Hirth and Nix 1969). A recent review is given by Evans and Rawlings (1969).

According to rate theory (Christian 1965) the frequency Γ is given by

$$\Gamma = \nu \exp(-\Delta G/kT) \quad (6.1)$$

where ΔG is the Gibbs free energy of activation and ν for a dislocation process is usually approximated

$$\nu \approx \nu_D b/l \quad (6.2)$$

(Friedel 1964) where ν_D is the Debye frequency and l is the length of dislocation involved in the activation. Let the energy arising from local atomic misfit as the dislocation encounters and overcomes a barrier be $G_B(y)$, where y is the position of the dislocation, so that there is a force $F_B = -dG_B(y)/dy$ or an equivalent 'back stress' $\sigma_B = F_B/b$ acting on the dislocation. The dislocation is held against the barrier by the effective stress $\sigma_e = \sigma - \sigma_\mu$, where σ is the applied shear stress and σ_μ is an internal stress which is locally long range. The free energy of activation (Schoeck 1965) is then

$$\begin{aligned} \Delta G &= G_B(y_2) - G_B(y_1) - \sigma_e bl(y_2 - y_1) \\ &= \int_{y_1}^{y_2} F_B(y) dy - \sigma_e bl \Delta y \end{aligned} \quad (6.3)$$

where y_1 is the equilibrium position of the dislocation before the activation and y_2 is the position when the net force acting on it is again zero. Thus:

$$F_B(y_1) = F_B(y_2) = \sigma_e bl. \quad (6.4)$$

Strictly ΔG should also include a $p\Delta V$ term and a partition function ratio, because of the different effective vibrational frequencies of the dislocation in the critical

position (y_1) and saddle point position (Hirth and Nix 1969), but these terms are usually neglected.

In early work ΔG was treated as a function of σ_e , but Gibbs (1964, 1965) and Schoeck (1965) argued that the entire specimen forms the only acceptable thermodynamic system, so that σ is the correct independent variable. This is formally correct, but Hirth and Nix show that in linear elastic approximation it is equally valid to regard σ_e as the appropriate variable. The two assumptions give

$$d\Delta G = -\Delta V_e d\sigma_e - \Delta S_e dT = -\Delta V_a d\sigma - \Delta S_a dT \quad (6.5)$$

where $\Delta S_e = -(\partial \Delta G / \partial T)_{\sigma_e}$ and $\Delta S_a = -(\partial \Delta G / \partial T)_{\sigma, \mu}$ are alternatively defined entropies of activation, and $\Delta V_e = -(\partial \Delta G / \partial \sigma_e)_T$ and $\Delta V_a = -(\partial \Delta G / \partial \sigma)_T$ are called activation volumes. (This definition of activation volume differs from the pressure derivative of ΔG used in diffusion theory, and some authors prefer the alternative term activation area for $\Delta V_e/b$.) Further parameters may now be introduced:

$$\Delta H_e = \Delta G + T\Delta S_e = \Delta U_e - \sigma_e \Delta V_e \quad (6.6a)$$

$$\Delta H_a = \Delta G + T\Delta S_a = \Delta U_a - \sigma \Delta V_a. \quad (6.6b)$$

If a dislocation moves forward a distance s between obstacles, its mean velocity is $s/(t_1 + t_2)$ where t_2 is the time of flight. For $t_2 \ll t_1$

$$\dot{x} = sv \exp(-\Delta G/kT). \quad (6.7)$$

The experimental variable most often measured is the plastic strain rate $\dot{\epsilon}$ which is given by

$$\dot{\epsilon} = \sum_i \theta_i b_i \rho_{Di} \dot{x}_i = \sum_i \theta_i b_i N_i A_i \dot{x}_i / s_i \quad (6.8)$$

where θ_i is an orientation factor, ρ_{Di} is the density of moving dislocations of Burgers vector b_i , N_i is the effective number of activation sites per unit volume and A_i is the area swept after a successful activation. The summation extends over all obstacles in one slip system, and also over all active slip systems, but it is usually assumed that all quantities may be replaced by average values to give

$$\dot{\epsilon} = \theta b N A \exp\left(\frac{-\Delta G}{kT}\right) = \dot{\epsilon}_0 \exp\left(\frac{-\Delta G}{kT}\right). \quad (6.9)$$

By differentiating, it now follows (Hirth and Nix 1969) that

$$\Delta H_a = kT^2 \left(\frac{\partial \ln(\dot{\epsilon}/\dot{\epsilon}_0)}{\partial T} \right)_\sigma \quad (6.10a)$$

$$\Delta H_a = -kT^2 \left(\frac{\partial \ln(\dot{\epsilon}/\dot{\epsilon}_0)}{\partial \sigma} \right)_T \left(\frac{\partial \sigma}{\partial T} \right)_{\dot{\epsilon}/\dot{\epsilon}_0} \quad (6.10b)$$

$$\Delta V_a = kT \left(\frac{\partial \ln(\dot{\epsilon}/\dot{\epsilon}_0)}{\partial \sigma} \right)_T \quad (6.11a)$$

$$\Delta V_a = -kT \left(\frac{\partial \ln(\dot{\epsilon}/\dot{\epsilon}_0)}{\partial T} \right)_\sigma \left(\frac{\partial T}{\partial \sigma} \right)_{\dot{\epsilon}/\dot{\epsilon}_0}. \quad (6.11b)$$

and

$$\Delta V_e = \Delta V_a = bl\Delta y \quad (6.12)$$

$$\Delta H_e = \Delta H_a - T\Delta V_a \left(\frac{\partial \sigma_e}{\partial T} \right)_\sigma. \quad (6.13)$$

Equation (6.12) is derived under the assumption that the back stress σ_B provided by the obstacle is not itself a function of the effective stress; Hirth and Nix (1969) give a more general formulation in which this assumption is not made, and it may then be necessary to distinguish between the measured activation volume and $b\Delta y$.

Provided \dot{e}_0 is independent of temperature and stress, the parameters in equations (6.10)–(6.13) may be determined from experimental measurements of reversible changes of flow stress σ with temperature and strain rate, from changes of creep rate with temperature and stress, and from stress relaxation experiments. Possible variations of \dot{e}_0 arise from ν , ρ_D and s . For discrete obstacles of average separation λ in the slip plane, Friedel (1956, 1964) assumed a steady state in which the dislocation loop which has overcome one obstacle is stopped by a new single obstacle and the area swept, $A = \lambda^2 = ls$, is constant. This gives

$$l^3 = 2\tau \frac{\lambda^2}{\sigma_e b} \simeq \mu b \frac{\lambda^2}{\sigma_e} \quad (6.14)$$

where τ is the line tension. Equation (6.14) applies to weak obstacles which yield when $\sigma_e \ll \mu b/\lambda$; for strong obstacles

$$l \simeq 1.25\lambda \quad (6.15)$$

where the numerical factor arises from the non-uniform distribution (Kocks 1966 a, b, Foreman and Makin 1966). It follows from equations (6.2), (6.9) and (6.14) that

$$\dot{e}_0 \simeq \theta \nu_D b^{4/3} \lambda^{2/3} \rho_D (\sigma_e/\mu)^{2/3} \quad (6.16)$$

at low stresses, but at high stresses

$$\dot{e}_0 \simeq \theta \nu_D b^2 \rho_D. \quad (6.17)$$

In nonfixed obstacle models, other functional dependences are observed, e.g.

$$\dot{e}_0 = B \sigma_e^r \quad (6.18)$$

where $r = 1$ for the double kink mechanism for activation over the Peierls barrier (Hirth 1969).

Variations of \dot{e}_0 can also arise from changes of ρ_D with stress or temperature. However, the reversibility of changes of flow stress with increments of temperature and strain rate, together with other indirect arguments, all suggest that $\Delta\rho_D$ may be neglected during such increments, except perhaps during discontinuous yielding (Christian 1964). In general, of course, ρ_D varies with dislocation structure, i.e. with strain.

The effect of changes in \dot{e}_0 with stress (equations (6.16) or (6.18)) appears, for example, as an extra term $r k T / \sigma_e$ in the measured activation volume. Hirth (1969) uses the example of the double kink model to show that the additional term can be larger than the activation volume itself, and this possibility must clearly be recognized in any attempt to correlate theory with experiment. However, the difficulty probably exists only at high temperatures and low effective stresses, since the extra contribution may be neglected if

$$\sigma_e \Delta V_e \gg r k T. \quad (6.19)$$

It is reasonable to assume that $\sigma_\mu = C\mu$, and equation (6.13) then becomes

$$\Delta H_e = \Delta H_a + T \Delta V_a \sigma_\mu (d \ln \mu / dT) \quad (6.20)$$

which is a form given by Conrad and Wiedersich (1960). The additional assumption that F_B (equations (6.3) and (6.4)) is proportional to μ leads to an expression for the free energy (Schoeck 1965)

$$\Delta G = \frac{\Delta H_a + T\Delta V_a \sigma(d \ln \mu / dT)}{1 - T(d \ln \mu / dT)} \quad (6.21)$$

which contains only measurable quantities.

Comparison of experimental results with theoretical models in order to identify mechanisms is not easy, and it is not always clear which parameters are most useful. Although the parameters ΔH_a , ΔV_a and (with the assumption above) ΔG may be measured without knowledge of σ_e , theory gives the relation $G_B(y)$ or $F_B(y)$ and hence the variations of the measured parameters with σ_e are required for comparison. Various methods for separating σ into σ_e and σ_μ depend on the assumption that ΔG becomes effectively zero when $\sigma = \sigma_\mu$.

A further difficulty in correlating theory with experiment arises from the double averaging which leads to (6.9), which makes the relation of the measured parameters to those of a model more tenuous. In particular, when several slip systems are operative, or several types of obstacle are involved, an analysis based directly on (6.8) seems preferable (W. Frank 1968 a, Duesbery 1969).

In experimental results from crystals of varying substructure, two limiting types of behaviour may be distinguished. At one extreme, typified by bcc metals or some dilute alloys, the strain-rate sensitivity $(\partial \sigma / \partial \ln \dot{\epsilon})_T$ and the temperature sensitivity $(\partial \sigma / \partial T)_\dot{\epsilon}$ are constant with strain, so that the obstacles are fixed in density. For fcc metals, on the other hand, the Cottrell-Stokes law expressed in the form $(\partial \ln \sigma / \partial T)_\dot{\epsilon} = \text{constant}$ (Adams and Cottrell 1955, Cottrell and Stokes 1955) or $(\partial \ln \sigma / \partial \ln \dot{\epsilon})_T = \text{constant}$ (Basinski 1959) is observed, and shows that the obstacles (e.g. dislocations) are created during deformation. When the temperature and strain rate dependence of the flow stress is large, so that at low temperatures or high strain-rates $\sigma_e \gg \sigma_\mu$, interpretation of the results is less likely to be in error through neglect of entropy terms or because of wrong corrections for the temperature dependence of σ_μ ; this applies to bcc metals. A linear relation between ΔG and temperature, or approximately between ΔH and temperature, at constant $\dot{\epsilon}$ indicates constancy of $\dot{\epsilon}_0$ and also that ΔH is a function of stress only, but these two conclusions cannot be established directly. Although there is no direct test for constancy of $\dot{\epsilon}_0$ (Hirth and Nix 1969), the experimental ΔH and ΔV may be at least tested for self-consistency if they are determined by various techniques. Moreover, if these quantities, and more especially the experimental pre-exponential factor, are found to be independent of structure, it is a reasonable conclusion that $\dot{\epsilon}_0$ is not strongly dependent on either structure or stress.

Experiments on individual dislocations have usually been interpreted in terms of a modified form of equation (4.1), namely

$$\dot{x} = (\sigma_e / \sigma_0)^{m^*}. \quad (6.22)$$

Analysis of experimental data in this way, and comparison with rate theory, has been discussed by Li and Michalak (1964), Christian (1964), Michalak (1965), Altshuler and Christian (1967) and Yada (1967). The parameter m^* is related to the activation volume by

$$m^* = \sigma_e \Delta V_e / kT \quad (6.23)$$

(Christian 1967). Yada claimed m^* varies as $1/T$, but this is only valid for certain

assumptions about the stress dependence of ΔV_e . Application of the third law of thermodynamics (Li 1965) suggests, however, that $m^* T$ should be constant as $T \rightarrow 0$, and there is some experimental support for this (Altshuler and Christian 1967). In terms of equation (6.22), this implies that $\sigma_e \Delta V_e$ tends to a constant value.

6.2. Discrete obstacles

Two kinds of discrete obstacles will be discussed briefly as examples of the treatment in § 6.1, namely solute atoms or other point defects, and ‘forest’ dislocations which intersect the glide plane. The interaction energy $G_B(y)$ of equation (6.3) is given for solute atoms by equations such as (2.68) or (2.70)–(2.74). Maximum interaction occurs with obstacles immediately adjacent to the glide plane, so it is usual to transfer to Cartesian coordinates and to put $x_2 = \pm b$ and $x_1 = y$. The curve of $F_B(y)$ obtained by differentiation of the appropriate elastic expression is clearly invalid very close to the solute atom, and this fact is troublesome since one basis for the comparison of mechanisms depends on the maximum value of the back force F_B .

A theory for the temperature dependence of flow stress controlled by impurity interactions has been developed by Fleischer (1962 a, b), and W. Frank (1966, 1967 a, b, c). For tetragonal defects in LiF, the calculated elastic force-distance curve has a flat maximum value of about $0.35 F_0$ at $x_1 \sim 1.5x_2$ (i.e. $y \sim 1.5b$), where F_0 is an elastic parameter. Fleischer replaced this with a simpler expression designed to match the calculated curve except at very small y and to give the same total energy of interaction. This approximation

$$F_B(y) = F_0 b^2 (y + b)^{-2} \quad y \geq 0 \quad (6.24)$$

has a cusped maximum at $y = 0$ which corresponds to a value $\sigma_0 = F_0/bL$ for the effective stress at 0 K. The separation of obstacles of concentration c is $\lambda \simeq (2c)^{-1/2}$ and for strong obstacles $l \sim \lambda$ (see equation (6.15)). Equation (6.3) becomes

$$G = F_0 b \{1 - (\sigma_e/\sigma_0)^{1/2}\}^2 \quad (6.25)$$

and from (6.9) the temperature dependence of the flow stress at constant strain rate is

$$\left(\frac{\sigma_e}{\sigma_0}\right)^{1/2} = 1 - \left(\frac{T}{T_c}\right)^{1/2} \quad T < T_c \quad (6.26)$$

where T_c is the temperature at which $\sigma_e = 0$. The corresponding activation volume is

$$\Delta V_e = b^3 (2c)^{-1/2} \left(\frac{\sigma_0}{\sigma} - 1\right)^{1/2}. \quad (6.27)$$

Equation (6.27) agrees well with experimental results for LiF, but the true force-distance curve must presumably be flattened at the top rather than sharply peaked. It is difficult to decide how this will affect the maximum force (although it should presumably be lower than its elastic value) or the slope of the curve of stress against temperature. Mott and Nabarro (1948) considered activation over a parabolic barrier, and if any smooth-topped barrier can be represented in this way their result that for small $\sigma_0 - \sigma_e$

$$\sigma_0 - \sigma_e = CT^{2/3} \quad (6.28)$$

should be valid at very low temperatures. With a smooth barrier the activation

volume tends to zero as $\sigma_e \rightarrow \sigma_0$, but if the barrier is flat-topped, there is some minimum value of Δy (equation (6.3)) and the activation volume can then be rather large for discrete obstacles, even at low temperatures.

W. Frank (1966, 1967 c, 1968 a, b) has given a more complete theory and applied it to dumb-bell shaped interstitial defects produced by irradiation of fcc metals to interstitial solutes in bcc metals, and to alkali halides containing divalent cations. The calculated temperature dependence is more complex than (6.26), and fits several sets of experimental data for carbon in iron. Frank concludes that the rate-determining process is interaction with single carbon atoms for atomic concentrations $c \leq 10^{-3}$ and with small precipitates for higher concentrations. However, flow stress-temperature curves are rather insensitive tests of particular mechanisms, especially if the very-low-temperature region is not included. Other tests include measurements of ΔG and ΔV_e and their variation with stress and with solute content. The mechanism of the large σ_e found in quite pure bcc metals is still in dispute both because of conflicting experimental evidence and different interpretations of the experimental results. A recent review of dislocation-point defect interactions and of their influence on thermally activated glide is given by Christian (1968).

A dislocation moving in a glide plane must necessarily encounter other dislocations which cross the glide plane and with which in general it may have either attractive or repulsive interactions. These interactions increase the flow stress at given strain rate and may give contributions to both σ_μ and σ_e . When an extended glide dislocation cuts through the forest dislocation, the energy of constriction and of the two jogs (or kinks) has also to be supplied, and this is a part of σ_e ; the subsequent motion of the glide dislocation may also be hindered if a sessile jog is produced but this situation will not be considered here.

The theory of thermally assisted motion through a dislocation forest has been considered by many workers (e.g. Seeger 1955 b, Basinski 1959, Hirsch 1959, Carrington *et al.* 1960, Saada 1960, 1961, Friedel 1964). The simplest case is the intersection of undissociated dislocations which have perpendicular Burgers vectors and have no long-range interaction. In equation (6.3) Δy is assumed constant and approximately equal to b , and $G_B(y_2) - G_B(y_1) = 2U_j$, where U_j is the jog energy (about $\mu b^3/4\pi$). If the forest density is $\rho_D = \lambda^{-2}$ and l is given by (6.14), the temperature dependence obtained from (6.9) may be written in the form

$$\sigma_e = \sigma_0 \left(1 - \frac{T}{T_c}\right)^{3/2} \quad (6.29)$$

where

$$\frac{\sigma_0}{\mu} = \left(\frac{2U_j}{\mu\Delta y}\right)^{3/2} (b^2 \lambda)^{-1} \quad (6.30)$$

and

$$kT_c \ln \left(\frac{\dot{e}_0}{\dot{e}}\right) = 2U_j \quad (6.31)$$

with \dot{e}_0 given by (6.16). The parameter T_c is not constant but increases with decreasing stress, so that σ_e approaches zero only asymptotically at high temperatures. However, the variation in T_c is small except when σ_e is very small, so it is a sufficient approximation to replace σ_e in equation (6.16) by σ_0 and thus to define a critical temperature T'_c by

$$kT'_c \ln \left(\frac{2\theta\nu\rho U_j}{\mu\Delta y \dot{e}}\right) = 2U_j \quad (6.32)$$

and σ_e is now given by writing T'_c for T_c in equation (6.29) when $T < T'_c$, and is effectively zero for $T > T'_c$.

When the glide and forest dislocation have an attractive interaction, there need be no thermal activation required to create the jog (Saada 1960). For repulsive trees, the mechanism is similar to that above, except that it may now be more reasonable to assume that $l \approx \lambda$, a constant. This gives

$$\sigma_e = \{1 - (T/T_c)\} \sigma_0 \quad (6.33)$$

where

$$\sigma_0 = 2U_j/b\lambda\Delta y \quad (6.34)$$

and T_c is now a constant given by (6.31) and (6.17).

Equations (6.29)–(6.34) are derived on the assumption that Δy is constant. However, an extended dislocation must form a constriction before it can cut through the forest dislocation, and even for nominally unextended dislocations the configurations of the cores will change as they approach closely. Thus the form of the $\Delta G(y)$ curve is much more complex than the square shape treated above, and constriction energies also contribute to ΔG . A fuller discussion is given by Basinski (1959).

In general, the thermal stresses resulting from intersection processes are smaller than the σ_μ contributions, and thus the temperature dependence observed for fcc metals and basal slip in hcp metals is relatively small. During work hardening of pure materials, the Cottrell–Stokes law is obeyed, and two explanations have been offered. One is that dislocation distributions produced by different treatments differ only in scale but not in pattern (Adams and Cottrell 1955, Kuhlmann-Wilsdorf 1962 a, b), whilst the other which is due to Mott (see Cottrell and Stokes 1955) is that the elastic forces giving σ_μ are of the same origin as the short-range forces σ_e . This latter view has been especially emphasized by Basinski in the forest theory of work hardening; it is supported by experiments which show that the Cottrell–Stokes ratio is unchanged so long as the forest density increases in proportion to the primary density, but that the ratio may be changed considerably when this balance is disturbed (Basinski and Basinski 1964, Jackson and Basinski 1967). A review of work-hardening theories, which cannot be discussed here, is given by Nabarro *et al.* (1964).

6.3. Changes in dislocation configuration

An undissociated screw dislocation may cross-slip freely from one plane of the glide zone to another, but an extended dislocation is likely to cross-slip only if it is stopped in the primary plane by some obstacle. Before cross-slip can occur, the dislocation must be constricted over part of its length and this process may be thermally assisted. Large stresses are needed to constrict widely dissociated dislocations, and may be provided, for example, by dislocation pile-ups (Seeger *et al.* 1959).

The cross-slip involves constriction along a length l of the dislocation, the re-dissociation of this length on the cross-slip plane when this is possible, and the bowing out of the redissociated dislocation (Friedel 1957, 1964). The energy of the configuration may be divided into (i) the energy of the two constrictions which is independent of l provided $l \gg d$ where d is the width of splitting (calculated e.g. by

Stroh 1954 b), (ii) the difference in energy of the length l of dislocation dissociated in the cross-slip and initial slip planes, and (iii) the negative work done by the external stress. No bowing in the cross-slip plane is required if the dislocation has a lower energy in this plane than in the primary plane, for example if the external stress tends to widen the dislocation in the cross-slip plane and compress it in the primary plane (Escaig 1968 a, b); the contribution (iii) then arises from work done in changing the positions of partials. However, if the dislocation energy is unchanged or larger in the cross-slip plane, as for slip on to prismatic or pyramidal hcp planes (Friedel 1959) where dissociation is not observed, the contribution (iii) includes the work done by the external stress in bowing to the critical configuration. In both cases, the saddle-point configuration involves a critical length l_0 obtained by maximizing the energy change with respect to l .

For the hcp case, Friedel defined the critical configuration in terms of the angle θ between the original screw dislocation and the critical direction of the circular loop on the cross-slip plane and found a critical condition

$$\theta_c = \{2E_{\text{rec}}/(\tau + E_{\text{rec}})\}^{1/2} \quad (6.35)$$

where E_{rec} is the recombination energy of the partials per unit length. This gives

$$\Delta G \simeq U_{\text{cs}} + \frac{4\tau E_{\text{rec}} \theta_c}{3\sigma_e b} \quad (6.36)$$

where U_{cs} is the energy of a single constriction.

A treatment of cross-slip which did not include the bowing of the dislocation was given by Schock and Seeger (1955) and Wolf (1960). An alternative mechanism (Fleischer 1959) does not require constriction, but involves further dissociation and the formation of stair-rod dislocations with high activation energy. It does not appear that the true saddle point is obtained in either of these theories. Cross-slip mechanisms have been studied by many workers with different assumptions about the type of dissociation or the driving force from external stress or internal stress. A recent calculation (Duesbery and Hirsch 1969) considers cross-slip caused by precipitates.

Another thermally activated process which has attracted much attention is the overcoming of a Peierls barrier by formation of a double kink. Dislocations not parallel to a close-packed direction may consist of straight sections in Peierls valleys and kinks which cross Peierls hills; these dislocations can readily move by migration of the geometrical kinks which are thus eliminated. Thus, with a little strain, most dislocations are straightened and then move only by the thermally assisted production of a kink pair (Seeger and Schiller 1962). With zero applied stress, production of thermal kink pairs of both signs occurs at the same rate, but in the presence of an applied stress pairs of one sign are favoured and there is a resultant dislocation velocity.

Seeger (1956 a) and Seeger and Schiller (1962) developed a model for double kink formation under very small applied stress, and applied it to the low-temperature internal friction phenomena (Bordoni peaks) observed in fcc metals (Seeger 1956 a, Donth 1957, Seeger *et al.* 1957, Lothe 1959, Jøssang *et al.* 1963). In the original model, the critical configuration was assumed to be a length l_c of dislocation in the maximum energy position, and the energy consisted in the additional Peierls energy of this length plus the energy of a single kink (equated by two half-kinks).

The length l_c was calculated by balancing the applied stress to the elastic interaction of the half-kinks. This gives a dependence of activation energy on stress

$$\Delta G = U_k \left(1 + \frac{1}{4} \ln \left(\frac{16\sigma_p}{\pi\sigma_e} \right) \right) \quad (6.37a)$$

where U_k is the kink energy and σ_p is the Peierls stress. In the later papers, Seeger and Schiller (1962, 1966) made a detailed statistical study of the motion of the double kinks and also showed that for large separations of kinks the activation energy is

$$\Delta G \approx 2U_k \left(1 - \left(\frac{\sigma_e}{10\sigma_p} \right)^{1/2} \right). \quad (6.37b)$$

Theories of double kink production when the Peierls barrier is much larger than the thermal energy, i.e. at high values of σ_e , were first developed by Celli *et al.* (1963) and Dorn and Rajnak (1964). They assume that the major factor is the additional dislocation line energy resulting from the Peierls barrier (Friedel 1963); this is valid if the curvature is small. If the straight dislocation throws forward a loop of shape $y = y(x_3)$ where x_3 is the coordinate along its line, the configuration has additional energy

$$U = \int_{-\infty}^{+\infty} \left[\left\{ E(y) \left(1 + \left(\frac{dy}{dx_3} \right)^2 \right)^{1/2} - E(y_0) \right\} - \sigma_e b(y - y_0) \right] dy \quad (6.38)$$

where $E(y)$ is the energy per unit length as a function of position (e.g. in the Peierls–Nabarro model $E(y)$ is given by $E_c(\alpha)$ of equation (3.39)) and $y = y_0$ is a minimum energy position. Solution of the variational problem $\delta U = 0$ enables the critical shape to be found by Euler's equation to give

$$\frac{dy}{dx_3} = \pm \left\{ \frac{E(y)}{E(y_0) + \sigma_e b(y - y_0)} - 1 \right\}^{1/2} \quad (6.39)$$

but further integration then has to be carried out numerically. Dorn and Rajnak computed numerical curves for the variation with stress of the critical value of U for a sinusoidal barrier and barriers of modified shape. From these results for the activation energy, they plotted curves of (σ_e/σ_0) against (T/T_c) , where σ_0 and T_c have the meanings previously given. Suitable choice of parameters gives good agreement with results for slip in bcc metals (e.g. Christian and Masters 1964, Arsenault 1967, 1968, Guyot and Dorn 1967) and for prismatic slip in hcp metals (Mukherjee and Dorn 1964, Rosen *et al.* 1964). Recently the model has been modified to include asymmetric Peierls barriers (Dorn and Mukherjee 1969, Kroupa and Hull 1969).

As a final example of activated processes, consider the sessile–glissile transitions in screw dislocations discussed in §§ 3.2 and 5.4. It is probable that the low-energy configuration of a screw dislocation in a bcc metal cannot move through the lattice unless an undissociated core, or a core dissociated in a single plane, is first produced. The motion of the dislocation then consists of alternate sessile–glissile and glissile–sessile transitions.

Escaig (1966, 1967) considered the temperature variation of stress which results from thermally activated sessile–glissile transitions, and Vitek (1966 c), Vitek and Kroupa (1966), Kroupa and Vitek (1967), Duesbery and Hirsch (1968) and Duesbery (1969) discussed also on this mechanism the effects of the crystal orientation on the slip behaviour, i.e. the slip geometry. Vitek and Kroupa supposed that screw dislocations dissociated on three {110} planes (equation (5.26)) or two {112} planes

(equation (5.24)) have equal probability, and the sessile–glissile transformation then proceeds in a manner formally identical with that required for cross-slip. In the critical configuration, the dislocation must be bowed in the slip plane, and the activation energy has the form

$$\Delta G = A + B/\sigma_e \quad (6.40)$$

(see equation (6.36)), where A and B are functions of the stacking fault energy. It is supposed that when the critical configuration is reached the dislocation stops by redissociation into the sessile form. The distance s (equation (6.7)) is, therefore, equal to the critical distance of bowing. It is assumed that the dislocation can transfer into glissile configurations in different planes of the slip zone with different frequencies, and that the average path consists of short segments of these planes. The observed slip geometry can then be explained by suitable choice of the stacking fault energies on $\{110\}$ and $\{112\}$. However, the activation energy becomes very large for small stresses, and the explanation of the temperature dependence of the flow stress is not very satisfactory.

Duesbery and Hirsch (1968) and Duesbery (1969) suggested that the mechanism of motion is different in different stress ranges. They suggest that s of equation (6.7) is always the distance from one lattice position in which the dislocation can dissociate into sessile form to the next such position. For small and intermediate stresses this dissociation begins before the saddle point for bowing out is reached, so that a double kink is formed. For very small stresses, the double-kink mechanism is similar to that discussed by Seeger and the saddle point is determined by the elastic interaction of the kinks. For intermediate stress, the saddle point depends on the extra line energy of the dislocation and the kink pair. At large stresses, the critical bowing out distance is smaller than s , and the cross-slip type mechanism outlined above is then operative. In this way, the activation energy does not increase indefinitely as $\sigma_e \rightarrow 0$.

As an illustration of this theory, it is applied to mixed splitting on $\{110\}$ and $\{112\}$ (equation (5.27)), but the model is actually not sensitive to the detailed dissociation mechanism (Vítek 1967, Duesbery 1969). However, all calculations necessarily use isotropic elasticity, and the computed dislocation separations are only of order b , so that they may only be regarded as an extrapolation from a region where linear elasticity is valid. A detailed study of this process, as indeed of most of the activation processes discussed in this section, requires calculation with atomic models.

7. Interface dislocations

7.1. Coherent interfaces: twinning and transformation dislocations

Boundaries between crystals of different structure and/or orientation may usefully be classified into coherent, semicoherent and incoherent types (see e.g. Christian 1965), and the corresponding dislocation descriptions are of zero dislocation content, physically separable interface dislocations and overlapping interface dislocations. Twin crystals are often separated by fully coherent boundaries, but such boundaries can be formed between crystals of different structures only in some special cases. Burgers (1939) and Bragg (1940) first demonstrated that some special semicoherent boundaries may be regarded as arrays of dislocations, and much further work was due to Read and Shockley (see Read 1955). The concept

of a dislocation boundary was generalized by F. C. Frank (1950) who showed how to define the net dislocation content of an arbitrary grain boundary, and by Bilby (1955) who similarly developed the dislocation description of a boundary between arbitrary lattices.

The dislocation description may be applied formally to any boundary, but loses its physical significance when the separation of individual dislocations is less than the core diameter. If two lattices have a common origin and interpenetrate, the array of coincident points of the two lattices is called the coincident site lattice (Kronberg and Wilson 1949). For lattices differing only in orientation, there are systematic relations specifying those special orientations for which the fraction of coincident sites, $1/\Sigma$, is comparatively large (Ranganathan 1966), and a closely packed plane of the coincident site lattice will then represent an interface of relatively good fit of the two lattices, with a lower energy than other high-angle boundaries. For slightly different misorientations, the lattices near the interface may be distorted into exact coincidence site relationships in local regions (Brandon 1966) but the accumulating misfit must be periodically corrected, and the regions of misfit are then effectively dislocations of the coincident site lattice. Thus there is a close analogy to the ordinary low-angle grain boundary, which contains misfit regions between two lattices which differ slightly from the exact coincident site relation $\Sigma = 1$.

Two lattices may be connected by an affine transformation $\mathbf{S} = [S_{ij}]$ such that a vector \mathbf{u} of one lattice is changed into a vector \mathbf{v} of the other lattice by the operation

$$v_i = S_{ij} u_j. \quad (7.1)$$

When \mathbf{S} is fixed, directions, planes and unit cells of one lattice are uniquely related to corresponding directions, planes and cells of the other lattice. In a basis A in which all lattice vectors \mathbf{u} have rational components $[u_i]_A$, the components $[v_i]_A$ will generally be irrational. Introduce a new basis B, defined by vectors of the second lattice, such that the components $[v_i]_B = J_{ij}[v_j]_A$ are rational. Then $[v_i]_B = C_{ij}[u_j]_A$, where $\mathbf{C} = \mathbf{JS}$ is called the correspondence matrix, and has components which are small integers or rational fractions, depending on the chosen bases A and B; the determinant of \mathbf{C} equals the ratio of the numbers of atoms or molecules in the two basic unit cells.

For any lattice relation there are many possible choices of \mathbf{S} , but in some cases one choice has physical significance inasmuch as there is an associated lattice correspondence which is preserved as one crystal grows from the other. This means that a labelled set of lattice points defining a direction in one structure would continue to define a direction (the corresponding direction) after incorporation into the other structure. When this happens, for example in deformation twinning or martensite formation, \mathbf{S} may be regarded as a homogeneous lattice deformation by which one lattice is carried into another, and it is sometimes convenient to factorize \mathbf{S} into a pure deformation \mathbf{P} and a pure rotation \mathbf{R} . In such cases, \mathbf{C} is often chosen by inspection, and this fixes \mathbf{P} but not \mathbf{R} .

If the lattices match exactly along a common plane of unit normal \mathbf{n} , \mathbf{S} has the form

$$S_{ij} = \delta_{ij} + g e_i n_j \quad (7.2)$$

where g is a scalar, e_i are the components of any vector and n_i are the components of \mathbf{n} referred to the reciprocal basis. In the case of deformation twinning, $e_i n_i = 0$ and g specifies the magnitude of the twinning shear; in conventional notation (see

Christian 1965) \mathbf{n} and e then define the K_1 plane and η_2 direction respectively. For two arbitrary lattices, it is improbable that a matching plane \mathbf{n} can be found; the necessary condition (Bilby and Christian 1956) is that one eigenvalue of \mathbf{S} (referred to an orthonormal basis) is unity and the other two are respectively greater and smaller than unity. This implies a relation between lattice parameters which can be satisfied only coincidentally, and the only known examples of fully coherent interphase boundaries are between hcp and fcc structures.

Figure 16 shows a virtual process in which a planar interface with a step P is

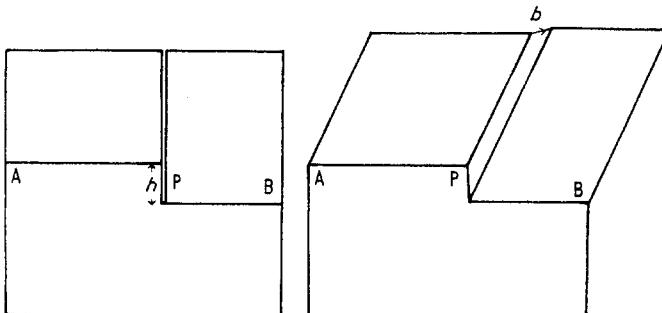


Figure 16. The formation of a transformation dislocation.

produced by applying a deformation \mathbf{S} to part of an original single crystal. If the flat portions AP, PB are to have identical configurations, the step height h must be an integral multiple of the spacing of the lattice planes \mathbf{n} . A stress-free condition is obtained only by cutting the crystal over a surface which ends on P, and the deformation \mathbf{S} then gives the two cut faces a relative displacement as shown. When these faces are rewelded, the whole assembly is left in a self-stressed state, and the elastic field is similar to that of a lattice dislocation.

Steps of this kind are quite distinct from interface dislocations which allow two structures to meet at a planar interface and were called second-order dislocations by Frank and van der Merwe (1949). The more usual term is transformation dislocations or twinning dislocations if \mathbf{S} represents a twinning shear. The equivalent Burgers vector is equal to the relative displacement of the cut surfaces, and from (7.2)

$$\mathbf{b} = h\mathbf{e}. \quad (7.3)$$

A formal definition of \mathbf{b} requires a reference system consisting of the two interpenetrating lattices, and the closure failure of the Burgers circuit connects a point of one lattice to a point of the other.

A twinning dislocation may be edge or screw in character, but the equivalent of a screw transformation dislocation has a direction parallel to the component of \mathbf{b} resolved in the plane \mathbf{n} . By definition, dislocations of this type must remain in the plane \mathbf{n} and they glide conservatively in this plane, even though it need not contain \mathbf{b} . In some lattices a monolayer twin corresponds to a metastable fault of low energy, and the twinning dislocation then has the same Burgers vector as a glissile partial dislocation bounding the fault. However, as already emphasized for bcc structures, the existence of a twin and of twinning dislocations need not imply the stability of the corresponding faults and partial dislocations.

A low-energy fault may also be equivalent to a monolayer of another structure, and the transformation dislocation then corresponds to a partial dislocation of the

lattice. Faults in fcc and hcp structures satisfy this condition only if the change in spacing of the close-packed layers is ignored. This model suggests that there may be a real change of spacing at a fault, with the corresponding partial dislocation having a Burgers vector approximating to a transformation dislocation. Howie and Jouffrey (1966) examined cadmium, where the hexagonal structure has an axial ratio much larger than ideal, but concluded that despite the 'fcc' arrangement of layers at the fault, the layer spacing is unchanged to within about 1%.

If a lattice dislocation with Burgers vector \mathbf{b}_A intersects a coherent interface, it will produce a step of height $\mathbf{b}_A \cdot \mathbf{n}$ which will run from the point of intersection to the edge of the interface, or to another dislocation line. Hence, a similar step must be produced in the interface plane of the other crystal by introducing a dislocation into that structure. This means that a lattice dislocation cannot end on a coherent interface but must pass through it. There is now a dislocation node of (at least) two lattice dislocations and one transformation dislocation. Only when \mathbf{b}_A is parallel to the interface is there no step, and the dislocation then simply bends on passing from one structure to the other.

An alternative way of introducing this configuration, called by Bilby (1953) a generating node, is to imagine the lattice dislocation to be present in a single crystal, part of which is then transformed to a product crystal. In the transformed region, the Burgers vector \mathbf{b}_A becomes

$$\mathbf{b}_B = \mathbf{S}\mathbf{b}_A = \mathbf{b}_A + g(\mathbf{b}_A \cdot \mathbf{n})\mathbf{e}. \quad (7.4)$$

Hence, if the positive directions of the dislocation lines are defined by looking inwards or outwards from the node, the Burgers vectors in parent, product and interface are respectively \mathbf{b}_A , $-\mathbf{b}_B$ and $g(\mathbf{b}_A \cdot \mathbf{n})\mathbf{e}$.

Suppose now that the lattice dislocations are fixed and that the transformation dislocation glides in the interface plane, and so rotates about the lattice dislocations. Each complete rotation displaces the node through a distance $\mathbf{b}_A \cdot \mathbf{n}$ (or $\mathbf{b}_B \cdot \mathbf{n}$ if measured in the other structure) in the direction $\pm \mathbf{n}$, and the direction of displacement depends on the sense of motion. Thus, either structure may grow progressively from the other and the region through which the transformation dislocation sweeps is automatically given a change of shape corresponding to \mathbf{S} . This is usually known as the pole mechanism, and is topologically similar to the operation of a single-ended Frank-Read source, or to Frank's mechanism of crystal growth. Clearly a double-ended pole could operate if a step runs between generating nodes arising from lattice dislocations with opposite Burgers vectors.

The above description is entirely in terms of lattices, and the transformation \mathbf{S} does not necessarily relate all the atomic positions in the two structures. Atomic displacements additional to those specified by \mathbf{S} are called 'shuffles'. Considerable progress has been made in classifying the shuffles in deformation twinning (Bilby and Crocker 1965, Christian 1965) but only general descriptions are possible for phase transformations. This work will not be described here, but has relevance to atomic models of the interface.

Suppose that \mathbf{n} is rational and \mathbf{S} relates all lattice points of the two structures. Twinning or transformation dislocations then have minimum vector $\mathbf{b} = h_1\mathbf{e}$, where h_1 is the spacing of lattice planes \mathbf{n} , and any shuffles required because the spacing of atomic planes \mathbf{n} is less than h_1 are accomplished automatically as the interface moves; these are structure shuffles. However, \mathbf{S} may relate only some fraction of the lattice points, and lattice shuffles are then also required. The

direction e of equation (7.2) is the zone axis of planes of invariant normals; it is also possible to find the conjugate zone axis \bar{e} of planes of normals of unchanging length (Christian 1969). (In deformation twinning, \bar{e} is the η_2 direction.) Now let the smallest lattice vector in the e direction cross q lattice planes of type n . The minimum translation of the interface from one position to an equivalent parallel position is then $\frac{1}{2}qh_1$ or qh_1 , depending on whether q is odd or even, and steps of this height probably represent the smallest glissile steps. For the particular case of twinning, such steps have been called zonal twinning dislocations (Westlake 1961, Kronberg 1959, 1961). Because of the lattice shuffles, atoms in equivalent lattice positions do not suffer identical displacements during the motion of a zonal dislocation, but the net displacement may be factorized into that given by the Burgers vector plus the appropriate shuffle.

7.2. Dislocation models of interfaces

Let two real lattices be produced from a reference lattice by deformations \mathbf{S}_+ and \mathbf{S}_- , which would act upon an interface vector $OA = \mathbf{p}$ to produce vectors $OA_+ = \mathbf{S}_+ \mathbf{p}$ and $OA_- = \mathbf{S}_- \mathbf{p}$. If a closed circuit $AA_+ OA_- A$ is described in the real crystals, the corresponding path in the reference crystal has a closure failure

$$\mathbf{b} = (\mathbf{D}_+ - \mathbf{D}_-) \mathbf{p} \quad (7.5)$$

where \mathbf{D}_+ and \mathbf{D}_- are the deformations inverse to \mathbf{S}_+ and \mathbf{S}_- . In particular, if the reference lattice is identical with the $(-)$ lattice, equation (7.5) becomes

$$\mathbf{b} = (\mathbf{D} - \mathbf{I}) \mathbf{p} = (\mathbf{P}^{-1} \mathbf{R}^{-1} - \mathbf{I}) \mathbf{p} \quad (7.6)$$

where \mathbf{I} is the unit matrix and $\mathbf{S} = \mathbf{RP}$ is now the deformation carrying one lattice into the other and has been factorized for convenience into a pure deformation \mathbf{P} and a pure rotation \mathbf{R} . The general grain boundary is a special case where $\mathbf{S} = \mathbf{R}$ and

$$\mathbf{b} = (\mathbf{R}_+^{-1} - \mathbf{R}_-^{-1}) \mathbf{p} = (\mathbf{R}^{-1} - \mathbf{I}) \mathbf{p}. \quad (7.7)$$

Equations (7.5)–(7.7) give the total or net Burgers vector of all the dislocations which cross a vector \mathbf{p} in the interface between the crystals. The resolution of this net vector into individual dislocation lines may not be unique, and may also be without physical significance. The derivation just given follows that of F. C. Frank (1950) for a grain boundary, but he expressed the result in vector form. If \mathbf{R}_+ , \mathbf{R}_- correspond to rotations θ_+ , θ_- about unit vectors \mathbf{r}_+ , \mathbf{r}_- , equation (7.7) is equivalent to

$$\begin{aligned} \mathbf{b} = & (\cos \theta_- - \cos \theta_+) \mathbf{p} + \mathbf{p} \times (\sin \theta_+ \mathbf{r}_+ - \sin \theta_- \mathbf{r}_-) \\ & + (\mathbf{r}_+ \cdot \mathbf{p})(1 - \cos \theta_+) \mathbf{r}_+ - (\mathbf{r}_- \cdot \mathbf{p})(1 - \cos \theta_-) \mathbf{r}_-. \end{aligned} \quad (7.8)$$

In a median reference lattice from which the real lattices are obtained by rotations of $\theta_+ = -\theta_- = \frac{1}{2}\theta$ about a common direction \mathbf{r} , (7.8) assumes the simple form

$$\mathbf{b} = 2 \sin \frac{1}{2}\theta \mathbf{p} \times \mathbf{r}. \quad (7.9)$$

Equation (7.5) is a particular example of the relation of the dislocation distribution to the deformation of lattice lines and the macroscopic change of shape, and it may also be derived from the theory of continuous distributions of dislocations (Bilby 1955). Suppose that dislocations are confined to a layer of thickness t which separates two dislocation-free lattices, and let the tensor dislocation density α_{ij} increase as t decreases in such a way that the product remains finite and tends to

a limit β_{ij} , which Bilby called the surface dislocation tensor. If equations (2.76) and (2.84) are applied to a small loop passing through the dislocation layer, it follows that

$$\beta_{ij} = -\epsilon_{jkl}(D_{+il} - D_{-il})n_k \quad (7.10)$$

where n_i are the components of the unit normal to the layer, referred to the reciprocal basis, and \mathbf{D} changes discontinuously from \mathbf{D}_+ to \mathbf{D}_- on crossing the layer. (Note that in this section the homogeneous deformation \mathbf{S} corresponds to the general deformation \mathbf{Q} of §2.8, but \mathbf{D} is used for the inverse deformation in both cases.) A small area of the boundary layer of dislocations is defined by the vectors $t\mathbf{n}$ and \mathbf{p} , and the normal to this area thus has vector components $t\epsilon_{jmn}p_m n_n$. From (2.76) the resultant Burgers vector of the dislocations passing through this area is

$$b_i = \beta_{ij}\epsilon_{jmn}p_m n_n$$

and after substituting from (7.10) and writing

$$\epsilon_{jkl}\epsilon_{jmn} = \delta_{km}\delta_{ln} - \delta_{kn}\delta_{lm}$$

it follows that

$$b_i = (D_{+il} - D_{-il})p_l \quad (7.5a)$$

which is identical with (7.5).

When \mathbf{S} has form (7.2) and \mathbf{n} is normal to the boundary, $\mathbf{b} = 0$ for all \mathbf{p} , as may be verified from (7.5). However, a new description, \mathbf{S}_1 , may be obtained by combining \mathbf{S} with a symmetry operation of either lattice, and the net Burgers vector given by (7.5) is then not necessarily zero. Thus, more generally, alternative descriptions of the relation between two lattices may lead to different \mathbf{b} for any \mathbf{p} ; the most likely description to have physical significance is that corresponding to minimum density of discrete dislocations. For grain boundaries, this is generally equivalent to minimum rotation θ (Bilby *et al.* 1964), and for interphase boundaries an intuitive choice of the lattice correspondence (based on minimum principal strains) specifies \mathbf{P} which should then be combined with a minimum rotation.

The simplest dislocation boundary is the symmetrical low-angle tilt boundary (Bragg 1940) in which \mathbf{r} is contained in the boundary, and there is a single set of edge dislocations parallel to \mathbf{r} and with \mathbf{b} parallel to \mathbf{n} (equation 7.9). Another simple low-angle boundary is the pure twist boundary with \mathbf{r} parallel to \mathbf{n} and the net Burgers vector is then normal to \mathbf{p} and of fixed magnitude for all interface vectors \mathbf{p} of constant length. This may be achieved by two perpendicular sets of equally spaced screw dislocations, or by equivalent arrangements which will vary with the symmetry of the interface plane.

More generally, interface dislocations are of two types. Pure screws and dislocations with a Burgers vector not in the interface can move conservatively with the interface, and some arrays of this kind are thus glissile. When the Burgers vector is parallel to the interface (except for screws) the density of lattice points in planes parallel to the interface differs in the two structures, and the motion is then non-conservative. Such interfaces can move only by dislocation climb, and are sometimes called epitaxial (Christian 1962).

A martensitic interface must be glissile, and the simplest structure is a single array of parallel dislocations with a common Burgers vector. The motion of these dislocations produces a simple shear \mathbf{G} , which is called the lattice-invariant shear (Bilby and Christian 1956). During transformation, large vectors undergo the

macroscopic or shape deformation \mathbf{E} , which is a combination of lattice and lattice-invariant deformations, so that $\mathbf{E} = \mathbf{RPG}$. The interface must be an invariant plane of the shape deformation, which implies that $\mathbf{Ep} = \mathbf{p}$ for any interface vector \mathbf{p} which is larger than the dislocation spacing. In terms of the dislocation description, the new vector formed from \mathbf{p} by \mathbf{G} is $\mathbf{p} + \mathbf{b} = \mathbf{P}^{-1} \mathbf{R}^{-1} \mathbf{p}$, from equation (7.6). Hence $\mathbf{RP}(\mathbf{p} + \mathbf{b}) = \mathbf{p}$.

The glide planes of the interface dislocations are the invariant planes of \mathbf{G} and intersect edge-to-edge in the (possibly irrational) interface. The dislocations are parallel to this intersection, which must be an invariant line of \mathbf{S} . With an array of pure edge dislocations, the lattice deformation reduces to a pure rotation and the boundary becomes the symmetrical tilt boundary, which may thus be regarded as a prototype martensitic boundary.

For a single array of parallel dislocations, the Burgers vector must coincide with a rational lattice direction, since otherwise faults will be produced by the interface motion. (If the fault energy is sufficiently low, the individual dislocations may correspond to partial dislocations of the product lattice, and the product structure is then an array of parallel faults; this is observed, for example, in copper-aluminium alloys (Swann and Warlimont 1963).) However, the net direction of \mathbf{b} may be irrational if two or more sets of dislocations are present in the interface. In general, a glissile interface is obtained if all dislocations have either the same glide plane or the same Burgers vector. The separate shears then combine to give a lattice-invariant deformation \mathbf{G} which is still a simple shear, but in which either the invariant plane or the shear direction is irrational. Recently, attempts have been made to extend still further the formal theory of martensite to include two independent lattice-invariant shears which do not reduce to a single shear (Acton and Bevis 1969–70, Ross and Crocker 1970), but there are unsolved problems connected with the glide geometry and the mobility of such an interface.

7.3. Glide of dislocations across a coherent interface

Incoherent interfaces act as efficient obstacles to glide dislocations and to deformation twins, but slip or twinning may propagate across coherent boundaries if the corresponding planes in which the dislocation glides meet edge-to-edge. The Burgers vector of the part of the dislocation which crosses the interface is related to its original Burgers vector by the lattice deformation, or if expressed in terms of the new basis by the correspondence matrix. This also applies to a dislocation crossing a semicoherent interface, but lattice planes meet edge-to-edge only along a single direction, the invariant line of the lattice deformation. For other intersections of a dislocation with the boundary, the glide planes meet, if at all, only macroscopically and it is not evident that the dislocation can cross the interface.

Unless the dislocation crosses the interface in pure screw orientation, it must leave a step of height equal to the component of its Burgers vector normal to the interface along the line over which it crosses. At each end of the step there is a node which is exactly of the type discussed in § 7.1; the topological configuration is independent of whether the dislocation glides into the product or the product grows and incorporates the dislocation (Saxl 1968).

If the correspondence relates all the lattice points, a parent dislocation will become a lattice dislocation of the product. In other cases, the new dislocation will have a lattice Burgers vector if the interface plane \mathbf{n} is rational, provided the

step height $b_A \cdot n$ is an integral multiple of $\frac{1}{2}qh_1$ (q even) or of qh_1 (q odd). This means that the step must be a zonal twinning or transformation dislocation (Saxl 1968). Elementary steps cannot be defined when n is irrational (e.g. in type II twinning) since $h_1 \rightarrow 0$, but there is an analogous condition that $b_A \cdot n$ equals $\frac{1}{2}\bar{q}$ or \bar{q} interplanar spacings of the conjugate undistorted planes \bar{n} , where \bar{q} is defined as the number of rational \bar{n} planes crossed by an elementary lattice vector in the e direction.

If the new Burgers vector b_B is not a lattice vector, the dislocation cannot glide into the second lattice without leaving a fault, but a group of parent dislocations may form a single dislocation which can glide into the product. In the case of $\{10\bar{1}2\}$ twins in hcp structures, for example, only one of the three lattice dislocations of type $\langle 11\bar{2}0 \rangle$ can glide across the twin boundary, and experimental evidence has been obtained that a moving twin boundary pushes dislocations of the other two types ahead of itself (Price 1961, Cooper and Washburn 1967). In principle, however, pairs of dislocations may glide together from parent basal or prism planes to give $\frac{1}{2}a\langle 1\bar{2}13 \rangle$ type dislocations which move into the twin on $\{10\bar{1}0\}$ or $\{1\bar{2}\bar{1}2\}$ planes respectively (Yoo and Wei 1966). Experimental evidence for the two types of basal plane dislocation interaction in zinc crystals has been obtained by electron microscopy (Tomsett and Bevis 1969); in particular the formation of a zonal twinning dislocation and the operation of the previously unreported $\{10\bar{1}0\}\langle 1\bar{2}13 \rangle$ slip system in the twin has been confirmed.

Obviously the geometrical continuity of the slip systems is not in itself sufficient to ensure that dislocations will glide across coherent boundaries. The new slip plane may not be a usual slip plane of the product lattice, or the resolved shear stress acting on the product system may be too low. Calculations of appropriate Schmid factors for corresponding slip planes in parent and product have been made for $\{10\bar{1}2\}$ twins in titanium (Partridge and Peel 1968) and for bcc $\{112\}$ twins (Kelly and Pollard 1969). It should be noted that if the boundary plane can contain a screw dislocation line of the lattices, it may possibly propagate across the interface into a noncorresponding slip plane which has a more favourable Schmid factor.

Acknowledgements

The authors wish to thank Professor P. B. Hirsch, F.R.S., Dr. F. Kroupa and Dr. I. Saxl for their very helpful comments on the manuscript. V. V. also wishes to acknowledge the award of an I.C.I. Research Fellowship.

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