

One-dimensional dislocations.

I. Static theory

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The theory of a one-dimensional dislocation model is developed. Besides acting as a pointer to developments of general dislocation theory, it has a variety of direct physical applications, particularly to monolayers on a crystalline substrate and to conditions in the edge row of a terrace of molecules in a growing crystal. Allowance is made in the theory for a difference in natural lattice-spacing between the surface layer or row and the substrate. The form and energy of single dislocations and of regular sequences of dislocations are calculated. Critical conditions for spontaneous generation (or escape) of dislocations are determined, and likewise the activation energies for such processes below the critical limits. Various physical applications of the model are discussed, and the physical parameters are evaluated with the aid of the Lennard-Jones force law for the above-mentioned principal applications.

1. INTRODUCTION

The theory of dislocations is moderately complex even with extensive approximations and unreal restrictions such as that to a simple cubic lattice, and there remain many problems, e.g. of dislocation dynamics, which have only been treated qualitatively even with these simplifications. It has therefore seemed worth while to us to make a more extensive survey of the properties of dislocations in a still more drastically simplified model, the simplest which can display dislocations at all. There are several different mechanical systems, all leading to the same equations. We choose one of them to set up the fundamental equation. It consists of a number of identical balls connected by identical springs and arranged in a straight line to which their motion is constrained, the balls being at the same time acted on by a force which varies periodically along the straight line. In the first instance, we take the periodic field to be sinusoidal. This is realized to a close approximation if the chain of balls and springs rests in a long horizontal frictionless trough with vertical side walls and a sinusoidal corrugation of low amplitude on the bottom of the trough, so that the periodic field is provided by gravity. We may hereafter refer indiscriminately to the balls as 'atoms' and to the source of the periodic field as the 'substrate', though this does not express the only application of the equations to the physics of solids. Certain aspects of this or equivalent systems have been treated by Dehlinger (1939), Frenkel & Kontorowa (1938) and Lennard-Jones (1940), but for brevity we derive the results *ab initio*.

2. THE DIFFERENCE EQUATION

If a is the 'wave-length' of the potential due to the substrate and $\frac{1}{2}W$ its amplitude, b is the spacing between atoms of the chain when their connecting springs are unstrained, μ is the force constant of these springs, and x_n is the displacement of the

n th atom from the n th trough of the substrate potential, each numbered in sequence from an arbitrary commencement, then the potential energy corresponding to N atoms of the chain is

$$V_N = \frac{1}{2}\mu \sum_{n=0}^{N-1} (x_{n+1} - x_n + a - b)^2 + \frac{1}{2}W \sum_{n=0}^{N-1} (1 - \cos 2\pi x_n/a).$$

This may be written

$$V_N = Wl_0^2 \sum_0^{N-1} (\zeta_{n+1} - \zeta_n - 1/P_0)^2 + \frac{1}{2}W \sum_0^{N-1} (1 - \cos 2\pi\zeta_n), \quad (1)$$

if we introduce the abbreviations

$$\zeta_n = x_n/a, \quad P_0 = a/(b-a), \quad l_0 = (\mu a^2/2W)^{\frac{1}{2}}.$$

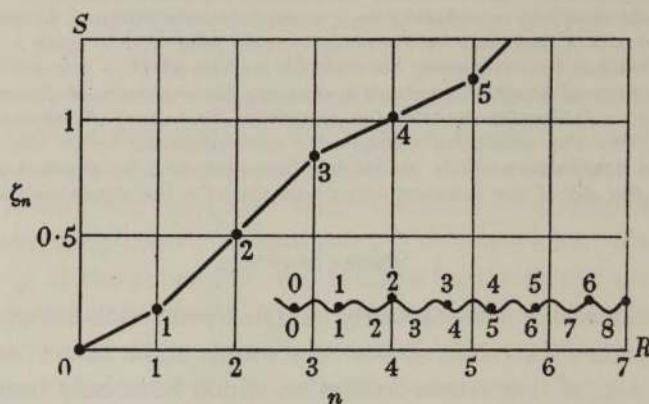


FIGURE 1

ζ is here the displacement measured in units of the substrate spacing; P_0 may be called the vernier period of misfit; the significance of l_0 will become evident later. The condition for equilibrium of the n th atom is $\partial V/\partial\zeta_n = 0$, whence by differentiation of (1)

$$\Delta_n^2 \zeta = (\pi/2l_0^2) \sin 2\pi\zeta_n. \quad (2)$$

Here we employ central difference notation

$$\Delta_n^2 \zeta = \zeta_{n-1} - 2\zeta_n + \zeta_{n+1}.$$

Solutions of equation (2) can be constructed numerically from specified displacements of any two successive atoms. Some simple symmetrical solutions can be found by elementary algebra, e.g. that of figure 1 corresponding to

$$1/l_0^2 = (1 - 4\zeta_1)/\pi \sin 2\pi\zeta_1 \quad (0 < \zeta_1 \leq \frac{1}{4}).$$

3. THE DIFFERENTIAL EQUATION AND ITS SOLUTIONS

When ζ_{n+1} and ζ_{n-1} are expanded in Taylor series about the point n one obtains

$$\Delta_n^2 \zeta = \zeta_{n+1} - 2\zeta_n + \zeta_{n-1} = \frac{d^2\zeta}{dn^2} + \frac{2}{4!} \frac{d^4\zeta}{dn^4} + \frac{2}{6!} \frac{d^6\zeta}{dn^6} + \dots$$

When l_0 is large, i.e. the springs are relatively strong, $\Delta_n^2 \zeta = (\pi/2l_0^2) \sin 2\pi\zeta_n$ will be small, and one is justified to a first approximation in neglecting differential coefficients of higher orders. Hereafter we shall use, for the condition of equilibrium, the differential equation

$$d^2\zeta/dn^2 = (\pi/2l_0^2) \sin 2\pi\zeta, \tag{3}$$

and keep in mind that the greater l_0 the better the approximation.

Integration of (3) gives

$$\begin{aligned} (d\zeta/dn)^2 &= \epsilon^2 + (1 - \cos 2\pi\zeta)/2l_0^2 \\ &= \frac{1 + \epsilon^2 l_0^2}{l_0^2} \left\{ 1 - \frac{\cos^2 \pi\zeta}{1 + \epsilon^2 l_0^2} \right\}, \end{aligned} \tag{4}$$

ϵ^2 being an integration constant. $d\zeta/dn$ is the amount by which the distance between successive atoms, measured in units of a , exceeds unity. ϵ is evidently the value of this excess where $\zeta = 0$, i.e. where successive atoms are in or close to troughs of the substrate potential.

Let us write

$$k^2 = 1/(1 + \epsilon^2 l_0^2) \quad \text{and} \quad \phi = \pi(\zeta - \frac{1}{2}),$$

and choose the zero for n where $\zeta = \frac{1}{2}$, i.e. $\phi = 0$, then (4) becomes

$$d\phi/dn = \pm (\pi/l_0 k) (1 - k^2 \sin^2 \phi)^{\frac{1}{2}}, \tag{5}$$

where the +ve sign refers to expansions of the chain of atoms with respect to the substrate, producing what we shall call negative dislocations. The negative sign corresponds to compression relative to the substrate, and positive dislocations. If we introduce the convention that $l_0 > 0$ for negative dislocations and $l_0 < 0$ for positive ones, we may discard the \pm sign in (5) without loss of generality. It is convenient to consider negative dislocations, which we shall do hereafter, and keep in mind that the results obtained are also valid for positive dislocations.

(i) *Dislocations far apart* ($\epsilon = 0$; $k = 1$)

If $\epsilon = 0$, then $k = 1$. Then from (4)

$$d\zeta/dn = (1/l_0) \sin \pi\zeta,$$

whence

$$\begin{aligned} \pi n/l_0 &= \pi \int_{\frac{1}{2}}^{\zeta} (1/\sin \pi\zeta) d\zeta \\ &= \ln \tan (\pi\zeta/2). \end{aligned}$$

This can be written

$$\zeta = (2/\pi) \arctan e^{\pi n/l_0}, \tag{6}$$

where $n = 0$ when $\zeta = \frac{1}{2}$, and

$$d\zeta/dn = (1/l_0) \sin \pi\zeta. \tag{6a}$$

Figure 2 gives a graphical illustration of (6). It represents a single dislocation infinitely far from any other in the chain. From (6a) and figure 2 one sees that approximately in a distance corresponding to l_0 atoms the displacement ζ changes by 1. In a relatively small region l_0 , therefore, there exists a state of misfit between the atoms and the substrate, while everywhere else there is a nearly perfect degree of fit. In a positive dislocation there is one more and in a negative dislocation there

is one less atom than there are troughs of the substrate potential. l_0 , which is a measure of the magnitude of the region over which misfit extends, may be called the effective length of a dislocation.

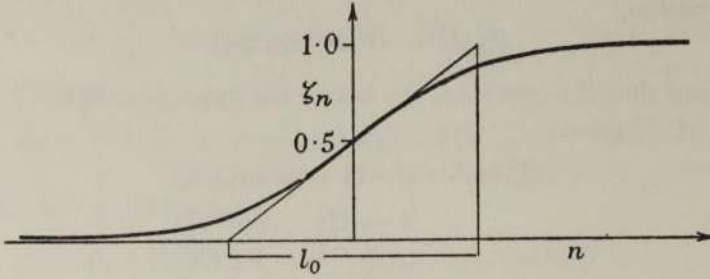


FIGURE 2

(ii) General solution: $k < 1$

From (5) it follows that

$$\begin{aligned} \pi n / l_0 k &= \int_0^\phi (1 - k^2 \sin^2 \psi)^{-1/2} d\psi \\ &= F(k, \phi) = F(k, \pi \zeta - \frac{1}{2} \pi) \end{aligned} \tag{7}$$

in the standard notation for elliptic integrals. This can be written

$$\zeta = \frac{1}{2} + (1/\pi) \operatorname{am} (\pi n / l_0 k)$$

and

$$\begin{aligned} d\zeta / dn &= (1/l_0 k) \operatorname{dn} (\pi n / l_0 k) \\ &= (1/l_0 k) (1 - k^2 \cos^2 \pi \zeta)^{1/2}, \end{aligned} \tag{8}$$

employing the notation of elliptic functions (Jahnke Emde 1938).

Figure 3 illustrates a typical example.

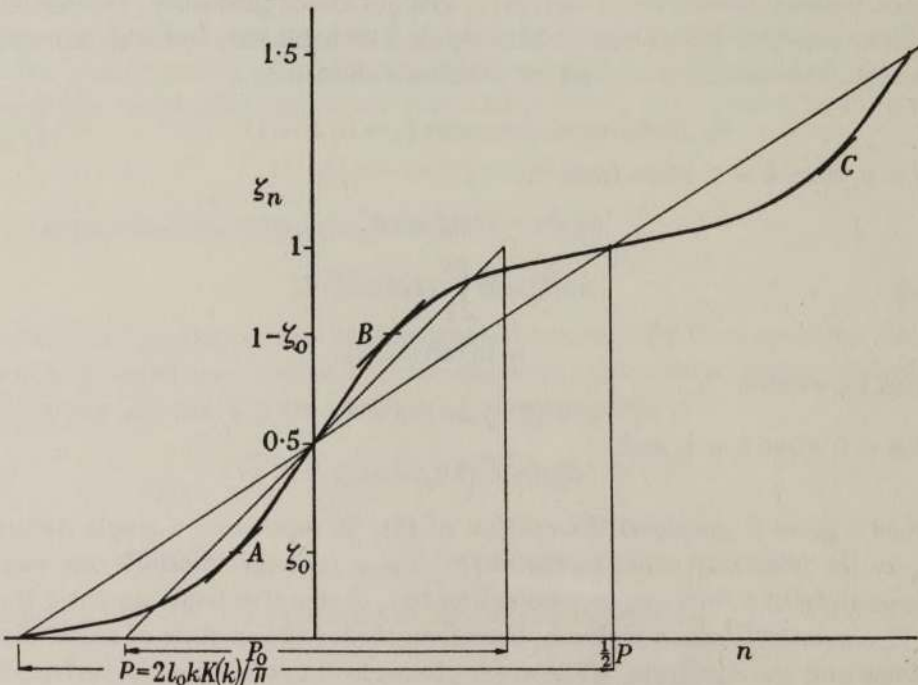


FIGURE 3

We now have a regular sequence of similar dislocations.

From (8) and figure 3 one sees that the effective length of a dislocation is now reduced to kl_0 , and the number of atoms per dislocation is

$$P = 2l_0 kK(k)/\pi, \tag{9}$$

where $K(k)$ is the complete elliptic integral $F(k, \frac{1}{2}\pi)$.

Referring back to figure 1, it is to be observed that even for small values of l_0 , so long as l_0 exceeds unity, there is good qualitative correspondence between solutions of the difference equation (2) and the differential equation (3).

4. EQUILIBRIUM WITH FREE ENDS

On differentiating (1) the term in P_0 , and hence all reference to the natural spring-length b , disappeared. This is only significant in connexion with the boundary conditions. We consider the case in which the chain has a free end whereas the substrate continues.

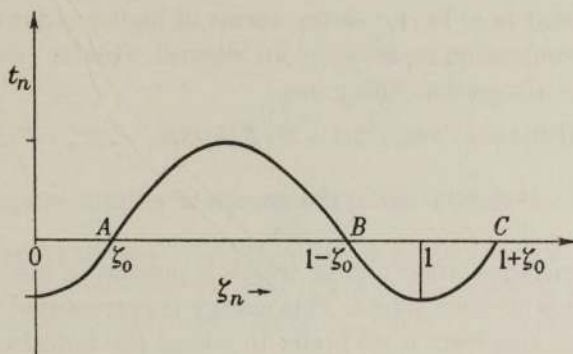


FIGURE 4

For simplicity we speak of tension, which is appropriate for negative dislocations ($l_0 > 0$). The results for positive dislocations are identical.

The tensions in the springs are given by

$$\begin{aligned} t_n &= \mu(x_{n+1} + a - x_n - b) \\ &= \mu a(\zeta_{n+1} - \zeta_n - 1/P_0) \\ &= \mu a \{ d\zeta/dn + (1/2!) d^2\zeta/dn^2 + \dots - 1/P_0 \}. \end{aligned}$$

Neglecting higher terms in the Taylor series, and substituting for $d\zeta/dn$ from (8), we find

$$t_n = (2Wl_0^2/a) \{ (1 - k^2 \cos^2 \pi\zeta)^{1/2} / kl_0 - 1/P_0 \}, \tag{10}$$

and in the special case where $\epsilon = 0, k = 1, P = \infty$,

$$t_n = (2Wl_0^2/a) \{ (1/l_0) \sin \pi\zeta - 1/P_0 \}. \tag{10a}$$

A graphical representation of (10) is shown in figure 4.

If the springs are cut at the points represented by A, B and C in figures 3 and 4, then the separate parts of the chain will remain in equilibrium with their ends free

—cutting it at B , for instance, will leave that part to the right to B in stable and that to the left in unstable equilibrium. The displacements ζ_0 of the free ends ($t_n(\zeta_0) = 0$) follows from (10), i.e.

$$\cos \pi \zeta_0 = \pm (1/k^2 - l_0^2/P_0^2)^{1/2}, \tag{11}$$

and from (10a), at a free end far from any dislocation,

$$\sin \pi \zeta_0 = l_0/P_0. \tag{11a}$$

5. ENERGIES

5.1. Potential energy per dislocation V_D

From (1) the potential energy per dislocation is

$$\begin{aligned} V_D &= Wl_0^2 \sum_{n=0}^{P-1} (\zeta_{n+1} - \zeta_n - 1/P_0)^2 + \frac{1}{2} W \sum_{n=0}^{P-1} (1 - \cos 2\pi \zeta_n) \\ &= Wl_0^2 \int_0^P (d\zeta/dn - 1/P_0)^2 dn + W \int_0^P \sin^2 \pi \zeta dn, \end{aligned}$$

where ζ_{n+1} is expanded in a Taylor series, terms of higher order than the first are neglected, and the summation replaced by an integral. Hence, using (7), (8) and (9), and carrying out the integration, this gives

$$V_D = Wl_0^2 \{ 4E(k)/\pi k l_0 - 2(1 - k^2) K(k)/\pi k l_0 - 2/P_0 + P/P_0^2 \}, \tag{12}$$

where $E(k) = \int_0^{1/2\pi} (1 - k^2 \sin^2 \psi)^{1/2} d\psi$ is the complete elliptic integral of the second kind.

V_D , thus defined, includes strain energy which is present in the chain (unless $1/P_0$ is zero) in the absence of dislocations. This energy is represented by the final term in (12). We may omit this term if we prefer to regard the undislocated state as the zero of potential energy.

5.2. Generation of a dislocation by force on the free end

A dislocation can be generated by pulling the end atom reversibly from its equilibrium displacement ζ_0 (A , figures 3 and 4) to its next stable equilibrium displacement $1 + \zeta_0$ (C , figures 3 and 4). The work done during this process is

$$\begin{aligned} W_D &= a \int_{\zeta_0}^{1+\zeta_0} t d\zeta \\ &= a \int_0^1 t d\zeta \quad \text{as follows from figure 4} \\ &= 2Wl_0^2 \{ 2E(k)/\pi k l_0 - 1/P_0 \}. \end{aligned} \tag{13}$$

The corresponding value for single dislocations then becomes (limit $k = 1$)

$$W_D = 2Wl_0^2 (2/\pi l_0 - 1/P_0). \tag{13a}$$

It may be noted that if Q is the total potential energy of a long chain of atoms containing N dislocations, V_D is the mean potential energy per dislocation, Q/N , while W_D is the differential energy per dislocation, dQ/dN . This relationship may be verified by integration.

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5.3. Activation energies

Consideration of this process, the application of force to the end atom of the chain, enables us to define an activation energy for the introduction of a dislocation, i.e. the work done in pulling the end atom reversibly from its stable equilibrium displacement (*A*, figures 3 and 4) to its unstable equilibrium displacement (*B*, figures 3 and 4) given by

$$U_g = a \int_{\zeta_0}^{1-\zeta_0} t d\zeta = 4Wl_0^2 \{E(k, \frac{1}{2}\pi - \pi\zeta_0)/\pi kl_0 - (\frac{1}{2} - \zeta_0)/P_0\}, \tag{14}$$

where ζ_0 is given by (11). $E(k, \frac{1}{2}\pi - \pi\zeta_0)$ is the incomplete elliptic integral of the second kind.

For dislocations far apart (limit $k = 1$)

$$U_g = 4Wl_0^2 \{(1 - \cos \pi\zeta_0)/\pi l_0 - (\frac{1}{2} - \zeta_0)/P_0\}. \tag{14a}$$

Similarly, the activation energy for the escape of dislocations is

$$U_e = a \int_{1+\zeta_0}^{1-\zeta_0} t d\zeta = U_g - W_D. \tag{15}$$

6. STABILITY LIMITS

The necessary and sufficient condition that a given solution of equation (3) can correspond to equilibrium when the ends of the chain of atoms are free is that there shall exist a real solution ζ_0 of the equation $t(\zeta_0) = 0$, i.e. equation (11). Hence

$$1 - k^2 l_0^2 / P_0^2 \leq k^2 \quad \text{and} \quad 1 - k^2 l_0^2 / P_0^2 \geq 0,$$

i.e.
$$(1/k^2 - 1)^{\frac{1}{2}} \leq l_0/P_0 \leq 1/k. \tag{16}$$

If $1/k < l_0/P_0$ dislocations will be spontaneously generated at the ends, while if $(1/k^2 - 1)^{\frac{1}{2}} > l_0/P_0$ they will spontaneously escape. When dislocations are absent or far apart (16) reduces to

$$0 \leq l_0/P_0 \leq 1. \tag{16a}$$

The state of lowest energy will be that for which the energy remains stationary for generation or escape of dislocations, i.e. that for which $W_D = 0$, so that

$$l_0/P_0 = 2E(k)/\pi k, \tag{17}$$

and the corresponding equation for dislocations far apart is then

$$l_0/P_0 = 2/\pi. \tag{17a}$$

This defines the critical value of misfit, above which the lowest energy state of the system is one containing dislocations. A somewhat larger misfit, as given by (16a), is needed for them to be developed spontaneously (at the absolute zero of temperature).

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7. APPLICATIONS OF THE MODEL

7.1. Imagine a solid crystal with a simple cubic lattice containing one or more straight parallel Taylor (1934) dislocations (all positive or all negative) in a single glide-plane. Suppose the material to be shaved away, parallel to this glide-plane, till there remains only one layer (or a very small number of layers) of atoms above the glide-plane, while the crystal is still thick below it. In the new elastic equilibrium nearly all the strain associated with the dislocation(s) will be in the thin layer above the glide-plane, and the crystal below can be regarded as effectively rigid. Then in each row of atoms immediately above the glide-plane and normal to the dislocation line(s) the conditions are substantially those of our first model, and the equations developed may be applied to the system with reasonably good accuracy. The system may be treated one-dimensionally so long as the dislocation lines remain straight and parallel. In this case b is approximately equal to a , but not exactly, since in general a surface layer of atoms in a crystal has a tendency to expand slightly if held together by homopolar forces, or to contract if they are ionic. Larger differences between b and a arise when we are considering overgrowth or absorption of one substance on a crystal of another.

7.2. Along the edge of an outer layer, or at a place where it is incomplete, ending in a straight terrace edge, we have a row of atoms attracting and repelling each other so as to tend to maintain a natural spacing b and subject to a substantially sinusoidal potential field of wave-length a (not in general exactly equal to b) arising from their neighbours in the rest of the crystal. This is a truly one-dimensional problem, corresponding closely to our first model. We estimate the physical parameters of the model for correspondence with this case from a Lennard-Jones law of forces (1924) between the atoms in § 8, and find that the appropriate value of l_0 , the effective spread of the dislocation, is about 7.

Values of l_0 of similar order of magnitude will apply in case (7.1) when we consider dislocations between a surface monolayer and the remainder of the crystal.

7.3. If in case (7.1) we start with Burgers (1939) 'screw' dislocations in place of the Taylor dislocations, we shall finish with a situation which is again well described by our equations, in which, however, the displacements ζ_n are transverse to the chain of atoms enumerated by n . The atomic positions will in fact correspond directly to the graphs of ζ_n versus n shown in figures 2 and 3. These dislocations, corresponding to screw dislocations in three dimensions, may be called 'transverse': those of case (7.1) corresponding to Taylor dislocations in three dimensions are 'longitudinal'. The longitudinal and transverse dislocations of a surface layer can be of importance in connexion with adsorbed monolayers, oxide layers, and so on. These, and the longitudinal edge dislocations (7.2) all deserve consideration in connexion with the original formation of dislocations in the growth of a crystal.

7.4. A long-chain molecule, say of a normal aliphatic compound, which has some torsional flexibility, and is restrained in twisting by the forces from parallel neighbour chains in the crystal, provides another system to which the same equations are applicable, wherein the displacements ζ_n are angles of rotation.

7.5. A somewhat different physical application is shown in figure 5 which gives a formal two-dimensional description of forced twinning (e.g. as observed in calcite). For the case pictured, an unstrained (two-dimensional) unit cell is supposed to be a 60° rhombus. The state shown, with three or four badly strained unit cells near the centre and around that a rapid asymptotic approach to a strain-free condition, should by its motion translate the twinning surface, causing one twin to grow into the other: and an applied stress should cause it to move. This configuration, however, is not a simple dislocation; its presence does not disturb the continuity of lattice planes. In so far as the twinning plane may be looked upon as a close grid of parallel Taylor dislocations with displacement vectors normal to the plane (Wooster 1940) (which exert forces on each other to hold their neighbours in the same plane, and

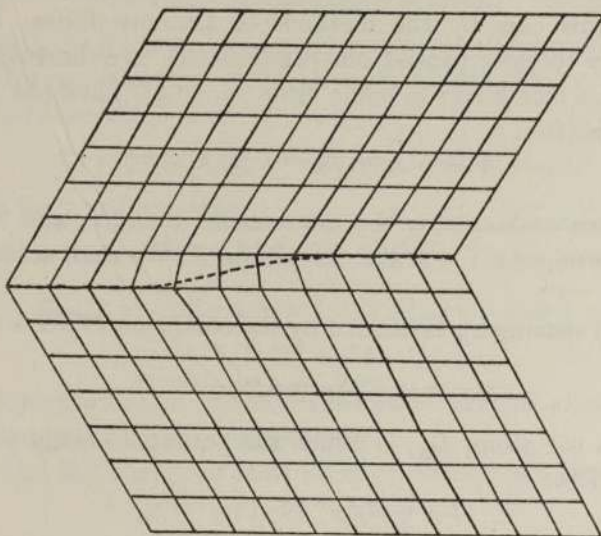


FIGURE 5

are moreover subject to a periodic 'substrate potential' because they are in a crystal), the figure represents a transverse dislocation of the system of dislocations. We may call it a dislocation of second order. Qualitatively, we may describe it by the equations of a one-dimensional dislocatable system developed above, ξ_n representing the displacement of an individual Taylor dislocation. However, at a distance from this second-order dislocation there exists a state of strain similar to that around a single Taylor dislocation; there are $(n + 1)$ unit cells in the same distance, measured parallel to the twinning plane, above it, as contains n below it. On this account these second-order dislocations exert long-range repulsive forces on each other. This agrees with observation; Garber's (1947) elastic twin wedges are only about 1μ thick for a length of the order 1 cm., so that $1/P$, the inclination of the twinning surface to the ideal twinning plane, probably does not exceed about $1/10,000$ to $1/1000$.

There are other second-order dislocations, a sigmoid bend of an ordinary dislocation line from one lattice line on to the next parallel one being the simplest type. These are required to describe the inclined twinning surfaces in a Reusch 'rectangle'

or Garber 'leaf' elastic twin of calcite, as contrasted with the Garber wedges. Being dislocations of a one-dimensional system, they also are qualitatively illustrated by the equations investigated.

8. In order to apply the equations obtained for our model to actual physical systems, it is necessary to assign values to the physical parameters, l_0 and P_0 . The most important applications are to a surface 'island' layer of atoms on a crystal, in which we may have dislocations of the edge row with respect to the rest of the island (§ 7.2) or of the layer with respect to the substrate crystal (§ 7.1). In particular, in the latter case the atoms of the surface layer need not be of the same kind as those of the substrate. In this case P_0 can be estimated approximately from the lattice spacings of the bulk materials. To this approximation it becomes infinite when the atoms are of the same kind, but this is not correct. The values both of P_0 and of l_0 may be estimated in this case by the methods of Lennard-Jones. Let the suffixes $X = \text{I, II, III}$, refer to close-packed one-dimensional, two-dimensional, and three-dimensional lattices (the latter in cubic close packing). Then the potential energy per atom may be written

$$V = -A^m S_X \alpha^{-m} + B^n S_X \alpha^{-n},$$

where A and B are constants, α the interatomic distance, and ${}^m S_X$ signifies the lattice sum for the exponent $-m$ and the lattice X . We shall actually take n to be 12 and m to be 6.

The equilibrium spacing α_X is defined by the condition $\partial V/\partial \alpha = 0$. Thus

$$\alpha_X = (nB^n S_X / m A^m S_X)^{1/(n-m)}.$$

The latent heat per atom, L_X , is minus the potential energy per atom at equilibrium spacing. Thus

$$L_X = A \alpha_X^{-m} m S_X (n-m)/n.$$

The force constant in homogeneous compression is

$$\begin{aligned} \mu_X &= (\partial^2 V / \partial \alpha^2)_{\alpha=\alpha_X} = m(n-m) A^m S_X \alpha_X^{-m-2} \\ &= mn L_X \alpha_X^{-2}. \end{aligned}$$

The lattice sums required are

$$\begin{aligned} {}^6 S_{\text{I}} &= 1.017_3, & {}^6 S_{\text{II}} &= 3 \times 1.063_0, & {}^6 S_{\text{III}} &= 6 \times 1.20433, \\ {}^{12} S_{\text{I}} &= 1.0002_5, & {}^{12} S_{\text{II}} &= 3 \times 1.001_6, & {}^{12} S_{\text{III}} &= 6 \times 1.01097, \end{aligned}$$

the values for ${}^6 S_{\text{III}}$ and ${}^{12} S_{\text{III}}$ being those of Jones & Ingham (1925).

If $\alpha_0 = (2B/A)^{1/2}$ represents the equilibrium spacing of a pair (or triangle or tetrahedron) of atoms, we have

$$\begin{aligned} \alpha_0/\alpha_{\text{I}} &= 1.002_7, & \alpha_0/\alpha_{\text{II}} &= 1.01_0, & \alpha_0/\alpha_{\text{III}} &= 1.029, \\ \alpha_{\text{I}}/\alpha_{\text{II}} &= 1.007, & \alpha_{\text{I}}/\alpha_{\text{III}} &= 1.026, & \alpha_{\text{II}}/\alpha_{\text{III}} &= 1.019. \end{aligned}$$

Accordingly, the natural misfit of a row at the edge of an island layer is given by its vernier period

$$P_0(\text{I, II}) = 144,$$

and correspondingly the natural misfit of a surface layer on the three-dimensional crystal is given by

$$P_0(\text{II, III}) = 53.5.$$

To estimate l_0 for the case of the edge row of a two-dimensional lattice we consider the potential energy of a single atom rolling in contact with the 'straight' edge of a semi-infinite two-dimensional lattice. We take the lattice spacing to be uniform, as though the atoms were hard spheres of diameter α_{II} , and the path of the additional atom to be the same as it would be if it were a hard sphere of the same diameter. Then the highest and lowest energies are obtained at the two symmetrical positions where it makes respectively one and two contacts. These energies are

$$1.019A\alpha_{\text{II}}^{-6} = 0.639L_{\text{II}} = 0.274L_{\text{III}},$$

$$0.784A\alpha_{\text{II}}^{-6} = 0.492L_{\text{II}} = 0.193L_{\text{III}},$$

respectively. Taking the fluctuation to be sinusoidal as an approximation (which we shall refine in a later paper in this series), the appropriate value of W in equation (1) is the difference between these two energies:

$$W_{\text{II}} = 0.325A\alpha_{\text{II}}^{-6} = 0.204L_{\text{II}} = 0.0807L_{\text{III}}.$$

We likewise have the force constant

$$\mu_{\text{I}} = 36A\alpha_{\text{I}}^{-8} \times 1.0173.$$

And hence

$$l_0^2 = \mu_{\text{I}}\alpha_{\text{II}}^2/2W_{\text{II}} = 36 \times 1.0173\alpha_{\text{II}}^8/2 \times 0.325\alpha_{\text{I}}^8.$$

Thus

$$l_0(\text{I, II}) = 7.35.$$

l_0 is naturally larger the harder the atoms. Since W is approximately proportional to L , l_0 is approximately proportional to $(mn)^{\frac{1}{2}}$.

We may now find the energy of such an edge dislocation, from equation (13a).

It is

$$\begin{aligned} W_D &= W(4l_0/\pi - 2l_0^2/P_0) \\ &= 0.0807L_{\text{III}}(9.37 - 0.75) \\ &= 0.688L_{\text{III}}. \end{aligned}$$

Thus it has just the same order of magnitude as the latent heat of evaporation of a single atom. Such edge dislocations should therefore be fairly frequently formed by thermal agitation.

The value of l_0 should be approximately the same for dislocations of the surface layer with respect to the underlying three-dimensional crystal; for the force constant μ should be about the same in both cases (we are not dealing with homogeneous compression in this second case), and the value of W corresponds to the breaking of one atomic contact per atom in both cases. In this case the dislocation is a line and its energy proportional to the line length of the order of magnitude of an atomic latent heat per atomic spacing of length. It is doubtful whether any appreciable number of dislocations will be formed in thermal equilibrium in this case, but it may be noted that the misfit parameter $l_0/P_0 \approx 0.15$ is sufficiently large to give an activation energy hindering the escape of any dislocations which are formed, except when they are very close together (about 15 atomic spacings apart according to equations (16) and (9)).

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One-dimensional dislocations. II. Misfitting monolayers and oriented overgrowth

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The equations derived in part I of this series for a one-dimensional dislocation model are applied in this paper to the case of a monolayer on the surface of a crystalline substrate, particularly when the natural lattice spacing of the monolayer differs from that of the substrate. Justification is given for this extension of the equations to the two-dimensional case. It is shown that the theory predicts a certain critical amount of misfit (9% difference in lattice spacing in a simple case) below which the monolayer in its lowest energy state is deformed into exact fit with the substrate, and above which it is only slightly deformed in the mean, having many dislocations between it and the substrate. The energy of adsorption as a function of misfit is also calculated, becoming almost constant above the critical limit. Up to a larger critical misfit (about 14% in the same simple case) the monolayer can be deposited metastably in exact fit on the substrate, at sufficiently low temperature. Since the dislocated layer is mobile on the surface, completely oriented overgrowth of one crystal on another can only be expected if the first monolayer can be formed over the complete surface under sub-critical conditions. This is in general agreement with observation.

1. PRELIMINARY INVESTIGATION

We propose to apply the equations derived in part I for one-dimensional dislocations to misfitting monolayers on crystalline substrates. Before doing so we examine a little more closely the validity of these equations for a two-dimensional problem. Let us take as a simple first-order representation of the potential energy of a two-dimensional square array of atoms, enumerated by n in the x direction, m in the