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Fifty-year study of the Peierls–Nabarro stress

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Abstract

The origin of the Peierls model and its relation to that of Frenkel and Kontorova are described. Within this model there are three essentially different formulae for the stress required to move a dislocation rigidly through a perfect lattice, associated with the names of Peierls, Nabarro and Huntington. There are also three distinct approaches to experimental estimates of the Peierls stress, depending on the Bordoni internal friction peak, the flow stress at low temperatures and Harper–Dorn creep. The results in the case of close-packed metals can be reconciled with the aid of ideas due to Benoit et al. and to Schoeck. The analytical elegance of Peierls's solution depends on the assumption of a sinusoidal law of force across the glide plane. This is physically unrealistic. Foreman et al. and others have obtained interesting results using other laws of force, while still operating in the framework of the Peierls model. The locking-unlocking model extends the ideas to the case in which the dislocation core has two mechanically stable configurations. © 1997 Elsevier Science S.A.

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1. The early history

The idea that dislocations of the crystal lattice provided the principal mechanism of crystal plasticity was introduced simultaneously by Orowan [1], Polanyi [2] and Taylor [3] in 1934. Orowan considered the motion of dislocations to be thermally activated, the applied stress combining with the internal stress produced by the dislocation to reduce the activation energy for motion of the dislocation in the direction favoured by the applied stress. Taylor assumed that dislocations were free to move through the lattice under the influence of the applied stress, their mutual elastic interactions and the obstacles presented by the boundaries between crystallites, 'mosaic blocks.' Only Polanyi considered the stress required to move a dislocation through an otherwise perfect lattice.

We are really concerned with two separate, but related, problems.

First, what is the configuration of the atoms in the core of an isolated dislocation in a crystal otherwise free from stress? Fig. 1 shows the result of Peierls's calculations [4] for a simple rectangular lattice. Here, we have taken the spacing a between slip planes to be different from the unit slip distance, the Burgers vector b. The early calculations were made for a simple square or cubic lattice with $a = b$. It seems to have been Cottrell [5] who first recognized that the physically significant cases with $a \neq b$ could be treated by a mathematically trivial extension of the theory for the case $a = b$. The second problem is more difficult. As the dislocation moves through the lattice, its energy fluctuates with period b (Fig. 2). It will not be able to move unless the applied stress exceeds a value which was estimated first by Polanyi [2] and then by Peierls, and is usually denoted by σ_p. The estimation of σ_p may be made on two levels of approximation. In the first, which can be carried out analytically, the displacement field which has been calculated for a dislocation in a stress-free lattice is assumed to be displaced rigidly as the dislocation moves through the lattice. In the second, the configuration of the dislocation core is recalculated for increasing values of the applied stress σ_a until a value $\sigma_a = \sigma_p$ is attained for which no stable configuration can be found. This calculation can only be carried out numerically and is technically difficult.

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Polanyi's model of the core of an edge dislocation was a simple vernier in which $n+1=11$ atoms on one side of the glide plane face $n=10$ atoms on the other side (Fig. 3).

If the material above the glide plane is displaced by $1/n$ of an interatomic spacing, the configuration of the core is restored, but displaced by one interatomic spacing. The elementary calculation of the shear strength of a perfect lattice (e.g. Frenkel [6]) shows that the lattice will yield at a shear strain of order 0.5 under a stress of under 0.1–0.2 of the shear modulus. Since, in Polanyi's model, the core configuration of the dislocation is restored after a shear of order $1/n$, the critical shear stress should be of the order of $1/n$ of the Frenkel value. Polanyi remarked that the observed low shear strengths of good metal crystals could only be explained if they contained dislocations with cores some 1000 atoms wide.

2. Peierls's model and the Frenkel–Kontorova model

Peierls's model combines Frenkel's model of the interaction of the atoms on opposite sides of the glide plane with the solution for the elastic field of a dislocation in a continuum. Following Cottrell's generalization, we shall consider two glide planes separated by a distance h, in a rectangular lattice with unit glide distance b as in Fig. 1, but with a replaced by h. An edge dislocation is travelling in the $+x$ direction, and the atoms above the glide plane at a point x' are displaced with respect to those below the glide plane by $u(x')$. Then $u(-\infty)=b$, $u(+\infty)=0$. Between x' and $x'+\mathrm{d}x'$ there is an infinitesimal dislocation of strength $(\mathrm{d}u/\mathrm{d}x')\mathrm{d}x'$. From the elastic theory, this produces at a point x in the glide plane a shear stress

$$p_{yx}=\frac{\mu}{\pi(1-v)}\frac{\mathrm{d}u(x')}{\mathrm{d}x'}\frac{\mathrm{d}x'}{x-x'}, \tag{1}$$

where μ is the shear modulus and v is Poisson's ratio.

According to the Frenkel model, the shear stress across the glide plane at the point x is given by

$$p_{yx}=\frac{\mu b}{2\pi h}\sin\frac{2\pi u}{b}, \tag{2}$$

Equating these, we obtain Peierls's equation

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}u(x')}{\mathrm{d}x'}\frac{\mathrm{d}x'}{x-x'}=\frac{(1-v)b}{2h}\sin\frac{2\pi u}{b}, \tag{3}$$

where the Cauchy principal value of the integral is taken.

In fact, the elastic solution shows that the dislocation causes displacements in the y direction as well as in the x direction, and the coefficient on the right of Eq. (3) is slightly modified [7,8].

The history of this problem and its solution has been recorded by the protagonists. Orowan wrote [9] "the equations...led to an integral equation which was the solution of the problem. It would have taken me days or weeks of study to solve it; fortunately I was a daily guest in the hospitable house of the brilliant theoretical physicist Rudolf Peierls. He solved the equation, if I remember well, within a few hours and he also drove me to a conference in Bristol University in 1939 where I gave a paper, and he gave another [4] on the problem he had just solved".

Peierls's version [10] is similar. He adds "I was greatly surprised to find that the simplest function with the expected qualitative behaviour turned out to be an

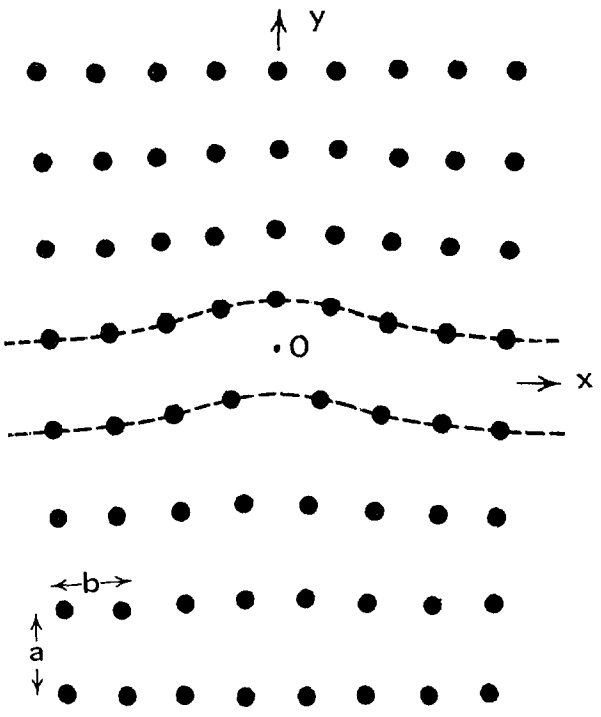

Fig. 1. Atomic positions in Peierls's model of the core of a dislocation in a simple rectangular lattice.

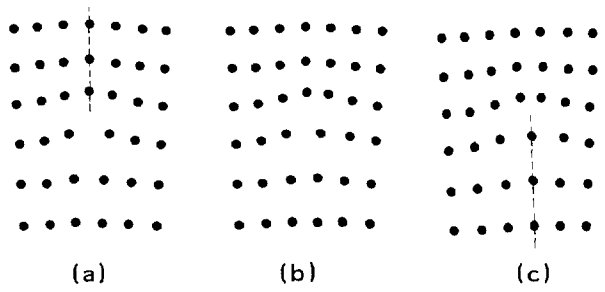

Fig. 2. Change in the atomic displacements of Fig. 1 as the dislocation moves through the lattice from one symmetrical configuration to another inequivalent symmetrical configuration.

exact solution of this integral equation. Orowan says that it would have taken him 'days or weeks' to study this problem, and this may be a generous estimate; in any event there is no doubt he could have found the solution without difficulty".

Here, Peierls was too modest. He not only found "the size of a dislocation", as the title of his Bristol paper implies, but also solved the much more difficult problem of determining the stress required to move the dislocation, although with the simplifying assumption that the displacement field moved rigidly through the lattice.

All of this was happening on the brink of the second World War. Peierls was busy establishing the feasibility of a nuclear bomb, and, by the time his paper was published, we were all absorbed in matters other than the theory of crystal dislocations. It was not until the war was over that I attempted to reproduce Peierls's results (which he gave without proof) and to extend them to the case of a pair of dislocations of opposite sign lying on the same glide plane and in unstable equilibrium under their mutual attraction and the action of an external stress. There seemed to be a discrepancy of a factor of 2 between my formulae and Peierls's. I was not happy about my derivation, which involved the use of infinitesimals and singular integrals which my mathematics teachers had taught me to avoid, so I travelled from Bristol to Birmingham to consult Peierls. He guided me through his calculation and I went back to Bristol to sort things out. The factor of 2 was still there and my results [11] were published in 1947. The results, in the present notation, were

$$u(x)=\frac{b}{2}-\frac{b}{2\pi}\tan^{-1}\frac{x}{\zeta}, \tag{4}$$

where

$$\zeta=h/2(1-\nu), \tag{5}$$

and

$$\sigma_{\mathrm{p}}=\frac{2\mu}{1-\nu}\exp\left(-\frac{4\pi\zeta}{b}\right) \tag{6}$$

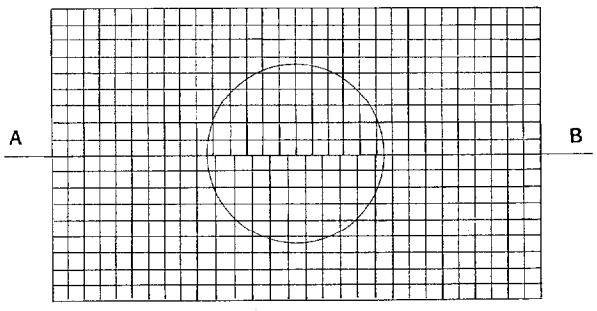

Fig. 3. Polanyi's model of a dislocation core as a simple vernier [2].

Peierls's result, with a somewhat different coefficient, had an exponential factor $\exp(-8\pi\zeta/b)$.

Orowan commented "the width calculated by Nabarro amounted to a few atomic spacings while Peierls obtained an order of magnitude of thousands of spacings... Peierls checked it and found that a factor of 2π was accidentally omitted in an exponent, which amounted to a factor of about 1000 in the result". Peierls's later comment was "Orowan mentions a factor 2π, but in the interest of historical accuracy, I must point out that this is an exaggeration. Actually, this error occurs in a large exponent, so that even the factor 2 changes the magnitude of the critical stress by several orders of magnitude". It is worth while to point out that the width of the dislocation was in error by a factor of 2, while the Peierls stress was of the wrong order of magnitude. This emphasizes the great sensitivity of estimates of the Peierls stress.

As is well known, the calculation is barely self-consistent even for the largest practical values of h/b. The basic Eq. (3) is derived on the assumption that the core of the dislocation is many atoms wide, while the solution shows that the core is only a few atoms wide. Since Peierls's original estimate of the critical stress was about $10^{-7}\,\mu$, he did not think that it was worth while to refine the calculation.

The one-dimensional model of Frenkel and Kontorova [12–14] reproduces the topological properties of dislocations and, because of its relative mathematical simplicity, is often used to illustrate the properties of dislocations. It consists of a chain of atoms linked by nearest-neighbour harmonic forces, and interacting with a substrate with a potential which is a sinusoidal function of position (Fig. 4). The period of the interaction potential may or may not be equal to the equilibrium separation of the atoms in the chain. If $n\pm1$ atoms occupy n potential troughs, we have the analogue of a positive or a negative edge dislocation. The analogy is sometimes useful, but it can be misleading. Peierls wrote to me on 7 August 1989 saying "I am surprised that people are still playing with the Frenkel–Kontorova model, which is a little too simple—now unnecessarily simple." The essential difference between the Peierls model and the Frenkel–Kontorova model is that, in the former, the force between two well-separated dislocations varies inversely as the distance between them, while, in the latter, the force decays exponentially with the distance. There is a case in which the two models lead to contrary predictions, and, as we shall see, the predictions are each correct for the case in which the model applies. We consider a sample of wide but finite extent in the glide direction. The equilibrium lattice parameters above and below the glide plane are different, but the lattices are coherent. Elastic stresses are present, which could be removed by an array of misfit dislocations. Following Olson and Cohen [15], we

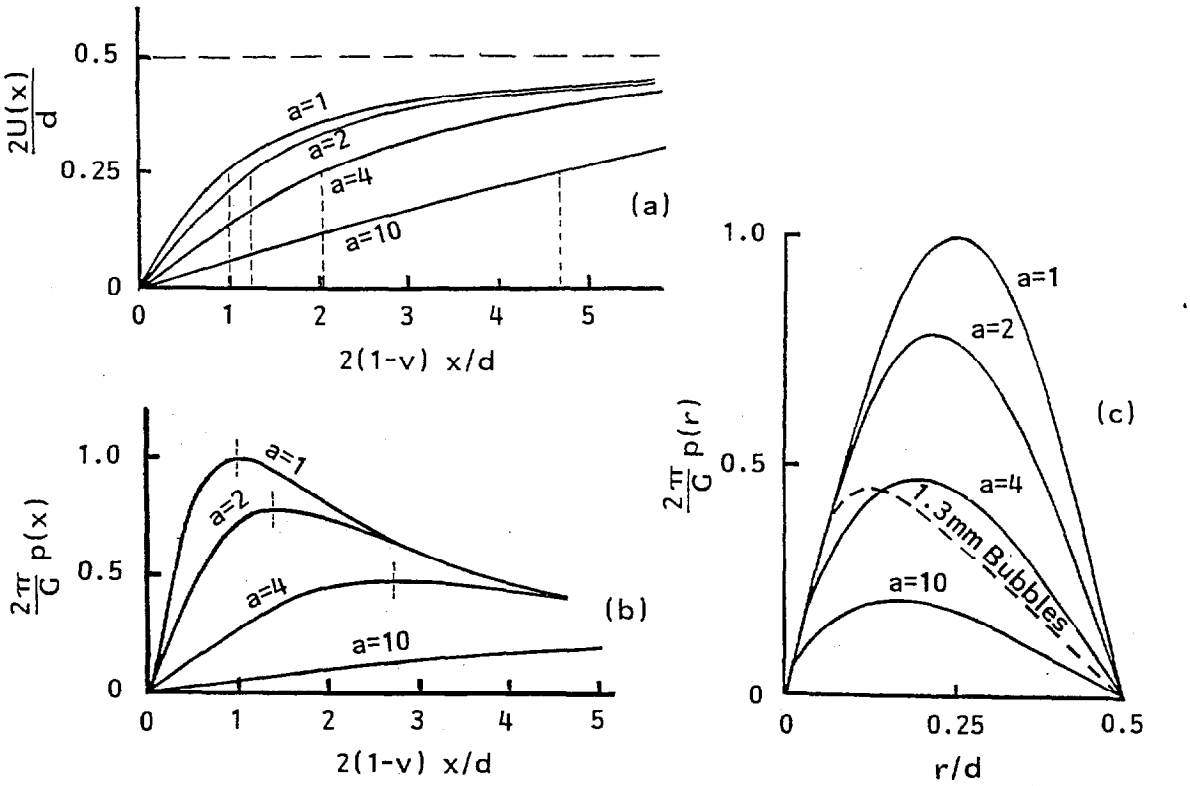

Fig. 4. (a) The relative displacement u of atoms above and below the glide plane from their position of maximum displacement in the core of the dislocation as a function of distance x along the glide plane. (b) The corresponding shear stress distributions. (c) The corresponding stress-displacement curves (after Foreman et al. [17].)

imagine that these misfit dislocations are present, but are compensated by an array of anti-misfit 'coherency' dislocations. If these coherency dislocations run out of the glide plane under their mutual repulsion, coherency is destroyed and the strain energy is released. The outermost coherency dislocations are held in by the Peierls stress. If we use the Peierls model, the outward force exerted on an outermost coherency dislocation by all the other coherency dislocations is given by the sum of a series of the form $1+\frac{1}{2}+\frac{1}{3}+\frac{1}{4}+\ldots$, and diverges logarithmically as the width of the glide plane increases. The outward force will always exceed the Peierls force and coherency will always be destroyed. However, if we use the Frenkel–Kontorova model, the series is of the form $\alpha+\alpha^2+\alpha^3+(\alpha<1)$ and converges. The total outward force on an outermost dislocation may or may not exceed the Peierls force and coherency may or may not be maintained. In fact, the Frenkel–Kontorova model is appropriate to the case of a thin epitaxial layer, while the Peierls model is appropriate to the case of a thick deposit and their predictions are each correct in the appropriate case.

3. The contributions of Huntington

Peierls's model shows a surprising property. The two symmetrical configurations of the dislocation core shown in Fig. 2 (a) and (c) have the same energy. If the energy of unit length of the dislocation when its core is at $x=\zeta$ is expressed as a Fourier series

$$U(\xi)=U_0+U_1\cos(2\pi\xi/b)+U_2\cos(4\pi\xi/b)+U_3\cos(6\pi\xi/b)+\ldots, \quad (7)$$

then the coefficient U_1 vanishes. The mathematical structure of the analysis shows that

$$U_n\propto\exp(-2n\pi\zeta/b), \quad (8)$$

so that the unexpected vanishing of U_1 implies that the Peierls stress is much smaller than it would be if the stress had the expected period of b rather than the calculated period of $\frac{1}{2}b$.

Huntington [16] first showed that the equality of the energies of the two symmetrical configurations arose from an accidental symmetry of the model. If the model of a rectangular lattice is replaced by the physically more realistic one of a distorted hexagonal lattice,

Table 1

a	1	2	3	4	5	10	∞
$(1-v)w/d$	1.000	1.255	1.653	2.076	2.507	4.697	$0.422a$
$(2\pi/G)p_{max}$	1.000	0.787	0.594	0.471	0.389	0.207	$2.202/a$
$2\pi(1-v)wp_{max}/Gd$	1.000	0.988	0.982	0.978	0.975	0.973	0.973

The width w of a dislocation normalized to the width in Peierls's model, and the maximum shear stress p_{max} normalized to that in Peierls's model as functions of the parameter a, showing that their product is almost independent of a (after Foreman et al. [17]).

representing the close packing of parallel ellipses in a plane, this symmetry is destroyed, the energy has the expected period b and the Peierls stress is of order

$$\sigma_P = \frac{1}{1-v}\exp(-\frac{2\pi\zeta}{b}), \quad (9)$$

much greater than the value of Eq. (6).

Huntington then made a more fundamental advance. In Peierls's calculation, the interaction energy across the glide plane is calculated by summing the contributions from atoms lying on both sides of the glide plane in the positions they had before the final displacements which establish equilibrium across the glide plane. Since these displacements can be of the order $\frac{1}{4}b$, it is physically more reasonable to estimate the contribution of each atom if it is placed in its final displaced position rather than in its position before the final displacement. The calculation then becomes mathematically ugly, but it leads to the physically satisfactory result that the Peierls stress is given by Eq. (9) whether the equilibrium lattice is rectangular or distorted hexagonal.

4. Beyond the sinusoidal force law

Foreman et al. [17] showed that the Peierls model could be solved for a specific class of interaction potentials across the glide plane. Their method consists essentially in choosing a distribution $\rho(x)$ of dislocation density along the glide plane which is characterized by a parameter a. Then the displacement function $u(x)$ is determined by direct integration, while the shear stress $p_{yx}(x)$ follows from Eq. (1). The distribution $\rho(x)$ is chosen so that the total displacement is b, while the relation between $p_{yx}(x)$ and $du(x)/dx$ is given by Hooke's Law when $|x|$ is large. The distribution when $a=1$ corresponds to Peierls's model with a sinusoidal law of force, while larger values of a correspond to laws of force in which the stress initially increases with displacement according to Hooke's Law, but then rises more slowly than in the sinusoidal approximation. Fig. 4(a–c) show respectively, the relative displacements of the atoms facing one another across the glide plane from their positions of unstable equilibrium, as functions of the distance from the core of the dislocation ($d \equiv b$), the corresponding shear stresses and the stress as a function of the displacement. An important result (Table 1) is that the width w of the core is very closely inversely proportional to the ratio of the maximum shear stress p_{max} across the glide plane to the shear modulus. The authors state that "this relation has been found to hold approximately for several families of dislocations of the same type as that described here." The dominant influence of the ratio μ/p_{max} on the properties of the dislocation has been recognized by several authors [18,19], but it has proved difficult to incorporate this idea into a coherent theory.

The calculated Peierls stress decreases very rapidly with increasing width of the dislocation (Table 2). As Sanders [20] seems to have been the first to notice, the dependence of the Peierls stress on the dislocation width is different in Cottrell's modification of Peierls's model and in the modification by Foreman et al. In Cottrell's modification the dislocation core is widened by increasing the separation of the atomic layers facing one another across the glide plane while retaining the sinusoidal law of force and the Peierls stress follows Eq. (6). In the model of Foreman et al. the dislocation core is widened by softening the law of force while retaining a separation between atomic layers equal to the Burgers vector and the Peierls stress varies roughly as $\exp(-4\pi w/d)$. Since w is defined as the full width to half height of the dislocation density distribution, while ζ is the half width to half height and d is taken equal to b, this corresponds to $\exp(-8\pi\zeta/b)$.

Lejček [21] pointed out that the results of the calculation of Foreman et al. retain a formal significance when the parameter a is less than unity. The model tends towards one of snapping bonds, and the dislocation density becomes two-humped when $a < \frac{3}{4}$. However, the core is then very narrow and the assumptions of the Peierls model are no longer meaningful.

Table 2

	a	1	2	4	10
$v=1/3$	w	$1.5d$	$1.9d$	$3.1d$	$7.1d$
	T	$2\times10^{-4}G$	$5\times10^{-7}G$	$2\times10^{-14}G$	$4\times10^{-36}G$
$v=1/4$	w	$1.3d$	$1.7d$	$2.8d$	$6.3d$
	T	$6\times10^{-4}G$	$3\times10^{-6}G$	$1\times10^{-12}G$	$1\times10^{-33}G$

The width w of a dislocation in units of the spacing d between glide planes and the corresponding Peierls stress T as a function of the parameter a, for two values of Poisson's ratio v (after Foreman et al. [17]).

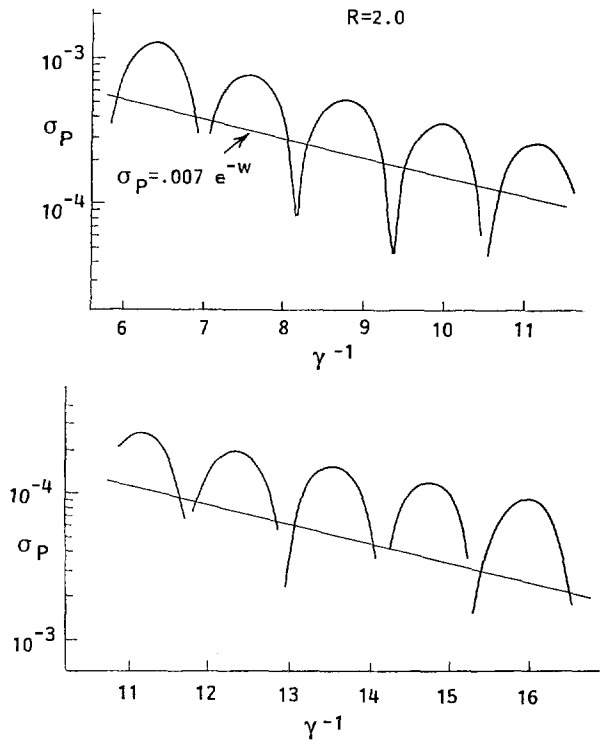

Fig. 5. Peierls stress as a function of the quality $\gamma^{-1} = \mu/p_{max}$ in the model of Sanders [20].

The calculations of Foreman et al. also remove an interesting anomaly. The elastic solution for a screw dislocation in an isotropic continuum has rotational symmetry. If Peierls's model is applied to a screw dislocation which is allowed to spread along a specified glide plane, the rotational symmetry of the problem is destroyed. Surprisingly, the solution still displays rotational symmetry. This symmetry is removed as soon as the parameter a differs from unity.

Sanders's own model goes beyond that of Peierls in that the matrix itself is treated atomistically, though on the very simple model of Rosenstock and Newell, for which displacements parallel and perpendicular to the slide plane are uncoupled, but both central and non-central linear forces are considered. The law of force across the glide plane is piecewise linear. While the overall dependence of the Peierls stress is again exponential, though only as $\exp(-2\zeta/b)$, there is a strong periodic variation in σ_p as a parameter is varied to vary the dislocation width. This is illustrated in Fig. 5. In Fig. 5, the ratio γ^{-1} of the shear modulus to the maximum shear stress across the glide plane p_{max} is according to the calculations of Foreman et al. and of Sanders, a close measure of the width of the dislocation core. The Peierls stress fluctuates by about a factor of 10 in any cycle. Similar fluctuations were found in various other models [22–25].

Some understanding of the reason for the minima of the Peierls stress for certain values of the width of the dislocation core may be obtained [26] from a consideration of the work of Kratochvíl and Indenbom [22]. Their model was the linear chain of Frenkel and Kontorova, modified to show piecewise linear forces. Fig. 6 shows the potential, the force and the positions of the atoms in a dislocation which is moving to the right. As long as no atom crosses a kink in the force-distance curve, the response of the system to the applied stress is strictly linear. Where, as shown, atom no. 0 crosses a kink, the force exerted on it by the substrate suddenly changes from one which increases numerically with increasing displacement to the right to one which decreases numerically. The configuration undergoes a sudden rearrangement, which dissipates energy. However, if the dislocation core is slightly narrower, so that atom no. -2 crosses an upward spike just as atom no. 0 crosses a downward spike, the response remains linear.

5. Dislocations between close-packed planes

A dislocation with Burgers vector

$$b = \tfrac{1}{2}a[1\bar{1}0] \tag{10}$$

lying on a close packed plane (111) in a face-centred cubic lattice dissociates into partial dislocations according to the scheme

$$\tfrac{1}{2}a[1\bar{1}0] = \tfrac{1}{6}a[21\bar{1}] + \text{stacking fault} + \tfrac{1}{6}a[1\bar{2}1](111) \tag{11}$$

The Burgers vectors of the two partial dislocations make angles of $\pm 30°$ with the resultant slip direction, and we shall neglect the difference between $\cos 30° = 0.866$ and unity. A similar dissociation occurs on the basal plane of hexagonal close-packed crystals. The distance d between the cores of the two partial disloca-

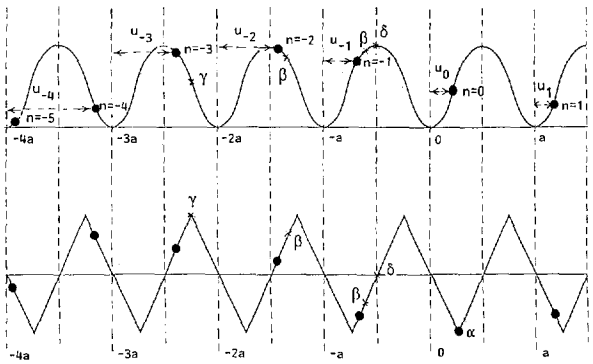

Fig. 6. Location of the atoms in the potential and force fields in the core of a dislocation in the model of Kratochvíl and Indenbom [22]. Atom no. 0 is about to meet a discontinuity in the dependence of force on displacement.

tions is often so large that they may be regarded as separate, though coupled, entities. The equilibrium separation is governed by the balance between the force of repulsion between the cores, which varies inversely as their separation and the surface tension of the stacking fault, which is independent of the separation. The Burgers vector of each partial dislocation has magnitude $b' = a/\sqrt{6}$ and a separation between glide planes of $h = a/\sqrt{3}$, giving the unusually high value $h/b' = \sqrt{2}$, for which the approximations of the Peierls model should be tolerable.

We consider first the situation in which the configuration represented by Eq. (11) moves rigidly through the lattice. Then, if the equilibrium separation of the partial dislocations is an integral or half integral multiple of $\frac{1}{2}a\langle 110\rangle$, so that the two partials reach troughs or crests of the Peierls potential simultaneously, the Peierls stress required to move the configuration is simply the stress required to move an isolated partial dislocation. However, as was pointed out by Benoit et al. [27], if the two partials are rigidly separated by $\frac{1}{4}$ or $\frac{3}{4}$ times $\frac{1}{2}a\langle 110\rangle$, the Peierls forces on them are always equal and opposite, and the applied stress required to move the rigid configuration vanishes.

More interesting problems arise when we recognize that the separation of the partials is not rigidly determined, but may be altered if the two partials lie along inequivalent lines in the Peierls potential. If the Peierls stress is large and the coupling of the partials is weak, the Peierls stress can alter the spacing between the partials by $\frac{1}{4}$ of $\frac{1}{2}a\langle 110\rangle$ or more and the partials move independently through the lattice. Schoeck [28] considered the limiting case in which the equilibrium spacing is $\frac{1}{4}$ or $\frac{3}{4}$ of $\frac{1}{2}a\langle 110\rangle$, so that the first-order perturbation of the energy of a rigid dissociated dislocation by its interaction with the lattice potential is independent of its position. When one partial is on top of a Peierls hill and one is at the bottom of a trough, the lattice exerts no force on either. But when one partial is moving up a hill and the other is moving down, the lattice exerts opposite forces on them and their separation is either increased or decreased. This relaxation reduces the energy, so that the total energy fluctuates between top–bottom and middle–middle configurations. For weak Peierls stresses, the distortion of the configuration of the dissociated dislocation is proportional to the Peierls stress, the energy relaxation is proportional to the square of the Peierls stress, and so the minimum observable flow stress is proportional to the square of the Peierls stress in a single partial.

It is not easy to modify the Peierls model to treat dislocations in close-packed structures, because their dissociation involves coupled displacements in two directions. However, a simple modification of the model of Foreman, Jaswon and Wood considers a dislocation entirely of edge character lying between two planes which have a mechanically stable (thermodynamically metastable) stacking position midway between each two thermodynamically stable stacking positions. Fig. 7(a) shows the dislocation density along the glide plane as a function of ψ for various values of a parameter a. Here x is proportional to $a \tan \psi$ and the dislocation in this model divides into two distinct partials separated by a distance proportional to a as b becomes large. Fig. 7(b) shows the normalized stress across the glide plane as a function of ψ, while Fig. 7(c) shows this normalized stress as a function of the relative displacement $y(\psi)$ from the metastable configuration, verifying that the model obeys Hooke's Law for displacements which are close to odd multiples of $\frac{1}{2}b$. The calculation of the Peierls stress in this model is in progress.

6. Comparison with experiment

There are three main experimental methods of estimating the Peierls stress. We give here only a brief summary of them and of the comparison of their results with theory, referring the reader to [29] for references and more details.

The first method is the analysis of the Bordoni internal friction peaks. These peaks are caused by the generation and annihilation of double-kink pairs under the combined influence of the applied stress and thermal activation. The values of σ_p/μ found for copper and aluminium are 1.2×10^{-3} and 8×10^{-3}, respectively, in general agreement with Huntington's calculations. Since the Bordoni mechanism samples the whole dislocation array, this is to be expected.

An interesting effect occurs (Caillard et al. [30]) if the applied stress is constant rather than alternating. As kink pairs are formed and migrate along the dislocation, the dislocation drifts forward under the influence of the applied stress. Since the number of sites at which kink pairs can be nucleated is proportional to the length of the dislocation segment, the drift velocity of a dislocation segment is proportional to its length.

The second method is the measurement of the flow stress of a good single crystal at a low temperature, where the thermal nucleation of double kinks can be neglected. This has been done for a range of materials, from the hard and brittle to soft close-packed metals. The results assembled by Ohsawa et al. [31] are shown in Fig. 8 to fit closely the Peierls–Nabarro line. Here, the partial dislocations in the soft metals are assumed to move independently. The physical model for these soft metals is that they contain internal stresses sufficient to cause the partial dislocations in some 'soft' regions to lie $\frac{1}{4}$ or $\frac{3}{4}$ of $\frac{1}{2}a\langle 110\rangle$ apart, so that Schoeck's argument applies and these dislocations will move under a stress which contains the square of Huntington's exponential factor; this square is the Peierls–Nabarro

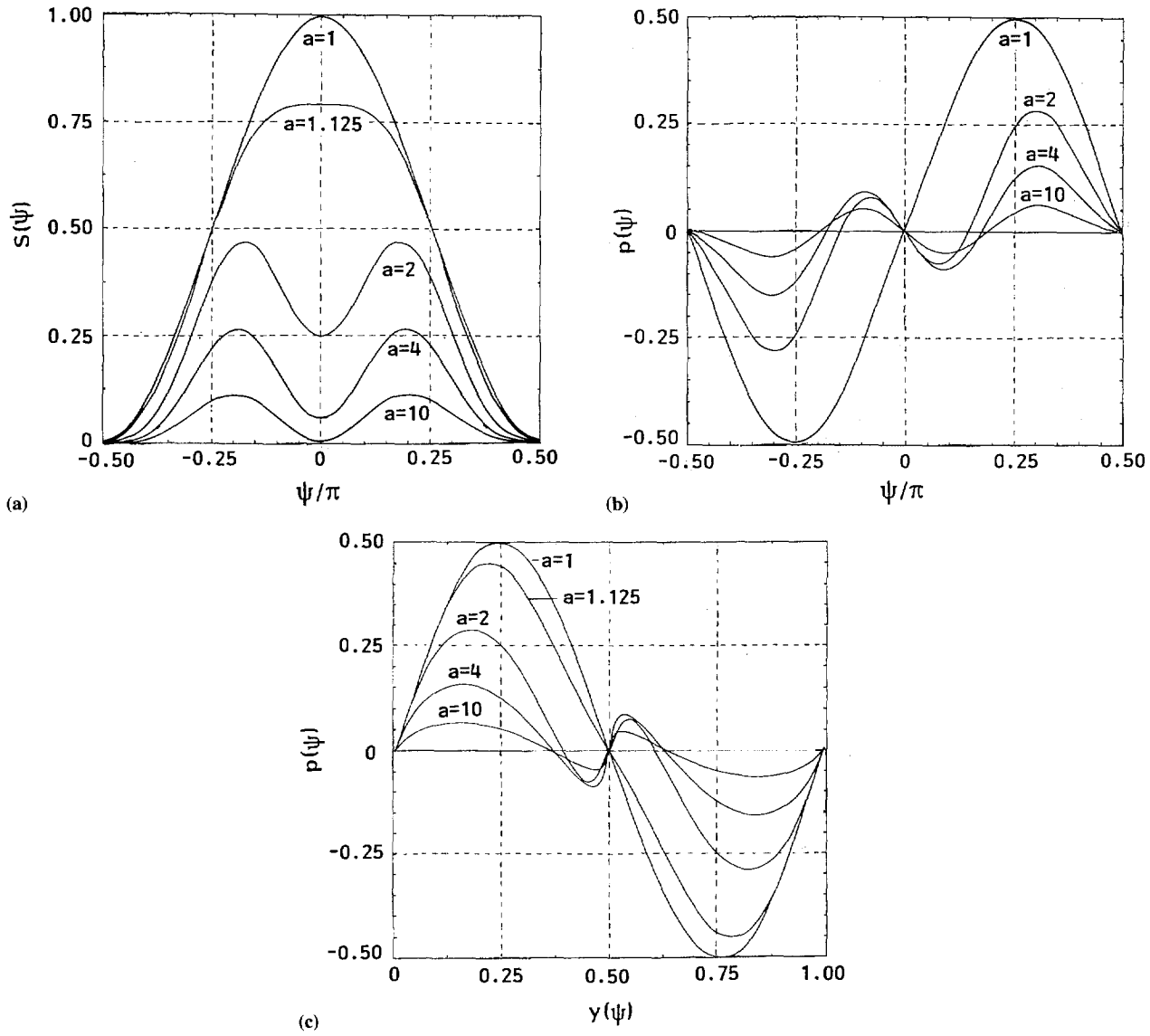

Fig. 7. (a) The dislocation density in a modification of the model of Foreman et al. [17] for different values of the parameter a. The distance along the glide plane is proportional to $a \tan \psi$. (b) The normalized stress as a function of position. (c) The normalized stress as a function of the relative displacement of the atomic surfaces above and below the glide plane, measured from the position of maximum misfit in the core of the dislocation. Hooke's Law is obeyed for small displacements from the stable equilibrium position.

factor. Once these dislocations have escaped from their Peierls troughs, they act as sources for extensive plastic flow. The calculation fails for dislocations of intermediate width, but for hard crystals all models give a flow stress of order $\mu/30$ as is observed, while the rest of the curve is determined adequately by the values for small and large h/b and the slope for large h/b.

The third method is the measurement of the rate of Harper–Dorn creep, or, equivalently, of the dislocation density during Harper–Dorn creep (Fig. 9). The data assembled by Wang [32] (Fig. 8) are again fitted to a (slightly modified) Peierls–Nabarro line. Again the argument is that the annihilation of an edge dipole will be initiated under the conditions considered by Schoeck and will then spread until the whole dipole has been annihilated.

7. The locking–unlocking mechanism

Couret, Caillard and their colleagues [33,34] have developed an extension of the Peierls model which they call the locking–unlocking mechanism. Until now, we have considered the structure of the core of the dislocation to be rigid as it moves through the lattice, or, in atomistic calculations, to be modified slightly with period b as the dislocation moves through the lattice. In the locking-unlocking mechanism, the dislocation has

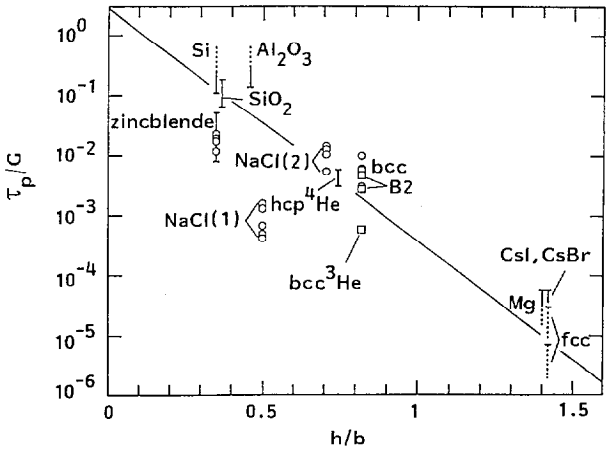

Fig. 8. The observed flow stresses of a wide range of materials show the dependence on the ratio h/b of interplanar spacing to Burgers vector predicted by the Peierls–Nabarro formula (from Ohsawa et al. [31]).

an internal coordinate i. In the state of lowest energy when the core is at $x=0$, we have $i=0$, and the configuration is sessile. Specifically, we may think of it as dissociated off the glide plane. To move it through the lattice in this configuration requires a large Peierls energy U_{Ps} (Fig. 10) with a corresponding Peierls stress comparable with the theoretical strength of the perfect crystal. There is also, at $x=0$, a glissile configuration with $i=1$ and energy exceeding that of the sessile configuration by U_{sg}. This glissile configuration can glide through the lattice with a small Peierls energy U_{Pg}, and a correspondingly small Peierls stress. If we assume

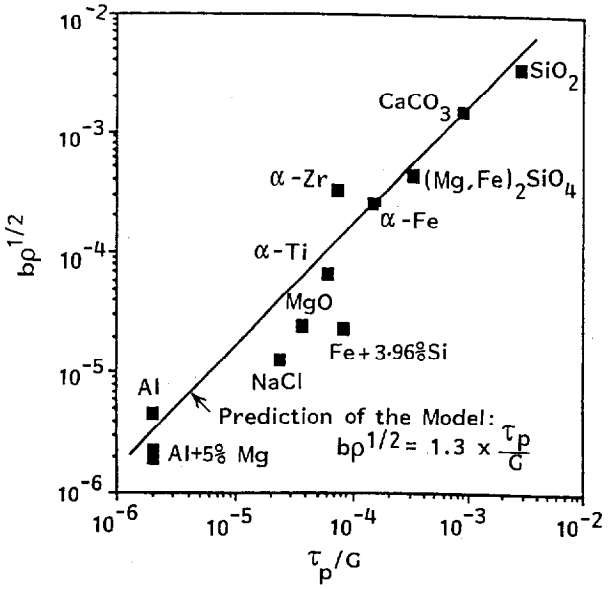

Fig. 9. The observed dislocation densities during Harper–Dorn creep of a wide range of materials fit closely to those predicted by a slight modification of the Peierls–Nabarro formula.

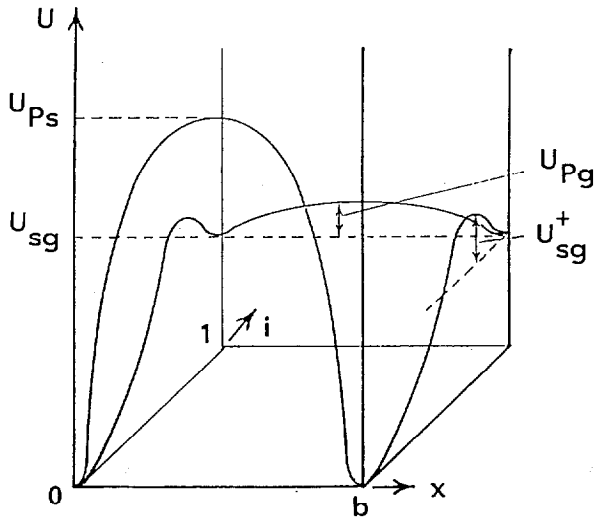

Fig. 10. Traces of the potential energy curve of a dislocation which moves by the locking-unlocking mechanism. The core of the dislocation moves in the x direction and its energy is periodic with period b. The core has two configurations of mechanical stability, represented by the reaction coordinate i. When $i=0$, the core has its lowest energy at $x=0$, but the Peierls energy at $x=\frac{1}{2}$ has the high value U_{Ps}. When $i=1$, the core energy at $x=0$ is U_{sg}, and this increases by only a small amount U_{Pg} as x increases to $\frac{1}{2}$. The high-energy glissile state with $i=1$ can revert to the low-energy sessile state with $i=0$ only by overcoming an activation energy for locking $U^{\dagger}_{gs}$.

that the unlocked or locked configuration spreads rapidly along the length of a dislocation segment, the segments will remain locked for a finite time, run forward rapidly, and again become locked. For segments of a given length, the probability that a locked segment will remain locked decreases exponentially with time. For an unlocked segment, the probability of a jerky forward jump lasting a time t decreases exponentially with t. If the stress is constant the velocity is constant, and the probability that a single jerky advance will cover a distance greater than l decreases exponentially with l. Both of these predictions are verified experimentally.

8. Conclusions

The Peierls model has great heuristic value.

The Peierls–Nabarro formulation has been superseded by the Huntington formulation.

The result of the calculation is so sensitive to the details of the model that its value is only heuristic.

For dislocations lying between close-packed planes, the argument of Benoit et al. shows that the stress required to move a dislocation segment may be reduced almost to zero.

The arguments show that this reduced value contains an exponential dependence on the width of a partial

dislocation which has twice the exponent of that for the flow stress of an isolated partial, converting the Huntington expression to the Peierls–Nabarro expression.

Some experimental techniques probe the average stress required to move a dislocation segment, while others probe the stress required to move the most weakly anchored segments.

Bearing these considerations in mind, the experimental theoretical estimates are reasonably compatible.

The locking-unlocking model is an extension of the Peierls model, in which the dislocation core has distinct low-energy sessile and high-energy glissile mechanically stable configurations.

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