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Theoretical and experimental estimates of the Peierls stress

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ABSTRACT

The Peierls stress is the stress required to move a dislocation through a perfect crystal lattice. Theoretical estimates show an exponential dependence on the ratio of the spacing between gliding planes and the unit slip distance. Nabarro corrected an error of a factor of 2 in this exponent in Peierls's original estimate. A revised estimate by Huntington introduced a further factor of 2. Three experimental estimates are available, from the Bordoni peaks (which agrees with the Huntington theory), from the flow stress at low temperatures (which agrees with the P–N (Peierls–Nabarro) theory) and from the rate of Harper–Dorn creep (which agrees with the P–N theory). Since the Huntington theory is clearly better founded than that of P–N, the agreement of two experimental results with P–N is unexpected. The discrepancy is resolved by using a recent result by Schoeck.

§ 1. INTRODUCTION

In an elastically isotropic crystal of shear modulus μ, the shear stress required to move the material on one side of the glide plane rigidly over that on the other side was estimated by Frenkel (1929) to be $\mu/2\pi$. Later estimates (for example Seeger (1958)) suggested $\mu/30$, far higher than the flow stress of a soft single crystal. A dislocation should move through an otherwise perfect crystal at the Peierls stress σ_P. Section 2 describes how, after the pioneering calculation by Peierls (1940), two distinct families of estimates have developed, which we may call the Peierls–Nabarro (P–N) formula and the Huntington (H) formula. It is argued that H, which gives a much higher stress than P–N, represents the correct analysis of the model on which P–N was based. Section 3 describes experimental estimates of the Peierls stress, which fall into three groups. The first is based on an analysis of the Bordoni internal friction peaks, and agrees with H. The second is based on the assumption that the yield stress of a single crystal at low temperatures should be equal or close to σ_P, and agrees with P–N. The third is based on an analysis of Harper–Dorn creep, and also agrees with P–N. It is disturbing that two sets of measurements should agree with a theoretical formula whose derivation has been shown to be false.

Section 4 shows that the theoretical formulae and the experimental observations can be brought into an orderly pattern. Benoit, Bujard and Gremaud (1987) showed that internal stresses could suppress the Peierls stress to zero in the case in which dissociated dislocations were gliding on a closed-packed plane. Schoeck (1994), by

applying second-order perturbation theory, showed that this reduction would be to a small, but finite, value. We point out that this small value is essentially that given by P–N, so that the P–N formula is sometimes valid for reasons which were not considered in its original derivation. It is argued that the conditions of each type of experiment determine whether the P–N or the H formula is appropriate.

§ 2. THEORETICAL ESTIMATES

Peierls's original estimate was based on a simple cubic lattice with elastic isotropy and Poisson's ratio ν.

The result was

$$\sigma \approx 20\mu \exp\left[-4\pi/(1-\nu)\right]. \tag{1}$$

This value is so small that a detailed discussion of its accuracy would be pointless.

Nabarro (1947) corrected an algebraic error in Peierls's calculation, and at the same time neglected some terms in the pre-exponential factor. His result was

$$\sigma_{PN} \approx 3\mu \exp\left[-2\pi/(1-\nu)\right]. \tag{2}$$

Cottrell (1953) extended the calculation to the case of a rectangular lattice in which the distance h between glide planes differs from the unit slip distance b. The result is

$$\sigma_{PN} = \frac{2\mu}{1-\nu} \exp\left(1 - 4\pi\zeta/b\right), \tag{3}$$

where ζ is given by

$$\zeta = h/2(1-\nu), \tag{4}$$

and it is this result which is generally called the P–N formula.

In a strict sense, these calculations are not self-consistent. They are based on the assumption that the width 2ζ of the dislocation core (full width to half height) is many interatomic spacings. One of the most favourable cases is that of the motion of a dislocation in a close-packed cubic plane, where it is assumed that the dislocation is dissociated into two partials which travel independently. If the lattice spacing is a, we have $b = a/\sqrt{6}$, $h = a/\sqrt{3}$, $h/b = \sqrt{2}$, and $2\zeta/b = \sqrt{2}/(1-\nu) \approx 2\cdot1$. The result (3) can be expected to provide a rough guide.

In comparison with experiments, eqn. (3) is often used for values of h/b much less than $\sqrt{2}$. The justification is that if one extrapolates (3) back to the lowest experimental values of h/b, about 0·3, and takes $\nu = \frac{1}{3}$, one obtains $\sigma_P \approx 0\cdot18\ \mu$. Since both the calculated values of $\sigma_{P/\mu}$ and the experimental values of the ratio of the flow stress to μ cover four orders of magnitude, one can claim that (3) should be an acceptable approximation for $h/b \approx \sqrt{2}$, gives a reasonable order of magnitude when extrapolated back to $h/b - 0\cdot3$, and therefore may be at least a reasonable guide for intermediate values of h/b.

The disturbing feature of the derivation of (3) is that the energy varies with wavelength $\frac{1}{2}b$ as the core of the dislocation moves, the two symmetrical configurations of the core having equal values. If the energy is expressed as a Fourier series in the position of the core, with period b, the leading term is absent. This leading term, if present, would be of order

$$\sigma_P = \frac{\mu}{1 - \nu} \exp(-2\pi\zeta/b), \tag{5}$$

much greater than that given by eqn. (3).

Huntington (1955) (H) showed that the vanishing of the leading term in the Fourier series was an accidental consequence of the details of Peierls's model, and confirmed this by showing that this term re-appeared and led to a Peierls stress of the order given by (5) if Peierls's model in which atoms on one side of the glide plane faced those on the other side (F) was replaced by one in which these atomic sites alternated (A) as they would in a close packing of circles.

Huntington made a greater advance in moving to a modified model (M) in which the displacement of each atom is a prescribed function of its actual displaced position, whereas in the P–N model it is a prescribed function of its original undisplaced position. For the alternating arrangement of atoms, both the P–N and the H calculations lead to the result (5). For the facing arrangement, P–N leads to (3), while H leads to

$$\sigma_H = \frac{(0\cdot15 + 0\cdot03\ b/\zeta)\mu}{1 - \nu} \exp(-2\pi\zeta/b), \tag{6}$$

which is of the same order of magnitude as (5). Wang's recent attempt (Wang 1996a) to recover a result of this form is vitiated by the change of sign between his eqns (11) and (17).

Not only does Huntington's approach seem more plausible, but it also avoids the great sensitivity to the assumed model of the undislocated crystal. Yet the Huntington modification is rarely quoted, probably because its mathematical details are complicated.

As has been mentioned, all of these calculations are of very limited accuracy because they assume $\zeta/b \gg 1$ and then determine a value of ζ/b of order unity.

The method of Peierls can be extended to the case of potentials across the glide plane which are not sinusoidal, but for which the dislocation is still divided into components all having the same direction of Burgers vector (Foreman, Jaswon and Wood 1951). The method would have to be substantially extended to treat dislocations moving on close-packed planes, which dissociate into two partial dislocations whose Burgers vectors have different directions. In the following discussion we shall use the rough model in which each partial feels the influence of the other only through the tension of the stacking fault which joins them. The only atomistic calculations for a close-packed structure seem to be those of Basinski, Duesbery and Taylor (1971) for a hypothetical h.c.p. sodium structure and of Bacon and Martin (1981) for two model potentials. Basinski *et al.* found a value of $\sigma_P/\mu \approx 0\cdot0004$ for a screw dislocation. This is considerably closer to the Huntington value for an isolated partial than to the P–N value. Bacon and Martin found critical shear strains for a screw dislocation in basal slip of $0\cdot015$ for one potential and $0\cdot016$ for the other, while for an edge dislocation in basal slip the critical strain was $0\cdot011$ for one potential and could not be calculated in view of the low stacking-fault energy for the other potential. These estimates lie, on a logarithmic scale, about as far above the Huntington estimate for an isolated partial as the estimate of Basinski *et al.* lie below it. Since dislocations across close-packed planes have components of the Burgers vector which are not parallel to the resultant Burgers vector, a substantial extension of Peierls's method will be required to treat them consistently.

For non-screw dislocations in the bcc lattice, the Peierls stress has been computed for $\frac{1}{2}[\bar{1}11]$ dislocations lying in various directions on a (110) plane, using various pair potentials. Except for potentials yielding a very narrow core, values of σ_P/μ of the order of 0·0015 were found (Vitek and Yamaguchi 1973, Duesbery 1989). For these dislocations, $h/b = (\frac{2}{3})^{1/2} \approx 0\cdot816$, a value lying very close to the P–N line. However, as suggested by Kuhlmann-Wilsdorf (1960) and emphasized by Duesbery (1989), the effective value of b to be inserted into a formula of the P–N or Huntington type is not the Burgers vector but the distance between successive crystal planes normal to the line of the dislocation. For [001] and [110] dislocation lines this halves the value of b, giving a point which falls almost exactly on the H line. The question arises of why the computed value for a [113] dislocation line, for which the effective value of b would be reduced by a factor of 11, is not extremely small. The answer is probably that, although the mean direction of the dislocation line is [113], its detailed configurations in positions of equal energy a distance of $(\frac{2}{3})^{1/2}a/11$ apart are very different, and there is a substantial energy barrier between neighbouring configurations of low energy.

When dislocations dissociate off the glide plane, as occurs for screws in bcc and $L1_2$ structures, the glide processes are still not completely understood, and it is most unlikely that any direct extension of the Peierls model would give useful insight into their behaviour.

Atomistic calculations such as those of Sanders (1962), Ishioka (1974) or Zhou, Carlsson and Thomson (1994) sometimes show a very sensitive dependence of σ_P/μ on the details of the potential, with occasional very low values, the reasons for which are understood (Kratochvil and Indenbom 1963, Nabarro 1989a), but are more usually values of the order 10^{-2}–10^{-3}, or 'nearly 10^4 times Nabarro', corresponding roughly to (5) or (6). The calculations of Ohsawa, Koizumi, Kirchner and Suzuki (1994) cover a wide range of h/b using three different atomic pair potentials V_1, V_2 and V_3, and show a close general agreement with Huntington's result (fig. 1).

§ 3. Experimental estimates

Using and developing the analysis of Seeger (1956), it is possible to derive from the activation energy of the Bordoni internal friction peaks the energy of a kink where a dislocation crosses from one Peierls valley to the next, and from this to derive the Peierls stress. The analysis of Bujard, Gremaud and Benoit (1987) considers the advance of the dislocation by the Burgers vector of a single partial dislocation, and leads to the values $\sigma_P/\mu = 1\cdot2 \times 10^{-3}$ for copper and 8×10^{-3} for aluminium, in order of magnitude agreement with the predictions of Huntington's formulae (5) and (6).

Ohsawa et al. (1994) assembled experimental results on the flow stress, and found (fig. 2) that they were quite well represented by the P–N formula (3) with ν in (4) taken as 0·3. The value $h/b = \sqrt{2}$ for the close-packed metals again corresponds to the motion of single partial dislocations. Since the P–N and H estimates differ by a factor of over 300 for this value of h/b, the H formula is clearly not applicable here.

One might expect some microplasticity arising from the motion of dislocation segments not trapped in Peierls valleys, but this would not lead to strains of the conventional order of 0·2%. It has been suggested that dynamical effects could lead to these segments overshooting their Peierls valleys and initiating macroscopic deformation, but Suzuki and Koizumi (1993) showed that such overshooting would occur only for applied stresses in excess of $0\cdot7\,\sigma_P$.

Fig. 1
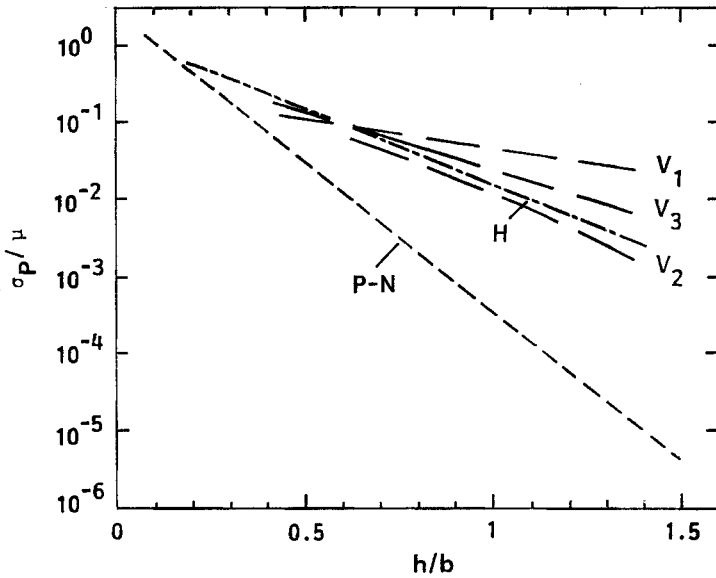
Ratio of the Peierls stress to the shear modulus as a function of h/b ($h =$ spacing between glide blanes, $b =$ Burgers vector) calculated for three pair potentials V_1, V_2 and V_3, and by the Peierls–Nabarro and Huntington formulae (Ohsawa *et al.* 1994).

Fig. 2
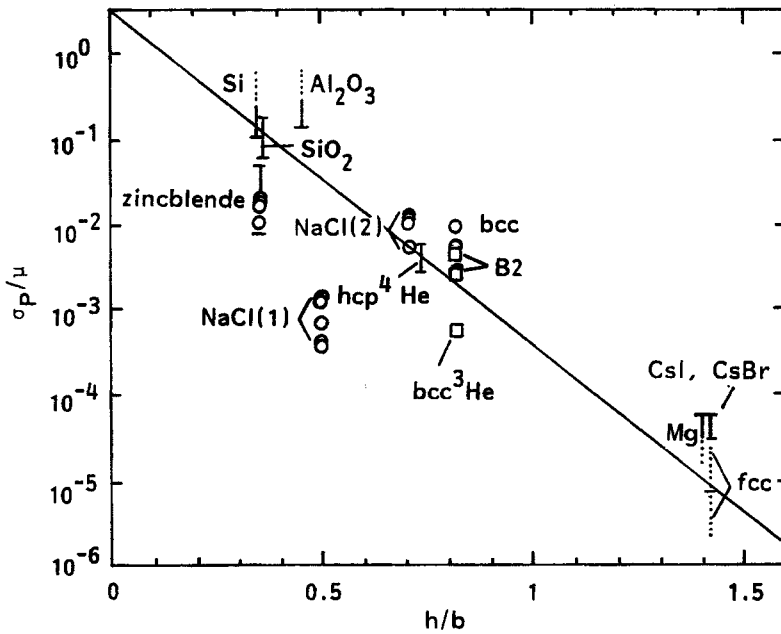
Experimental flow stresses normalized to the shear modulus as functions of h/b (Ohsawa *et al.* 1994).

The Peierls stress may also be derived from an analysis of Harper–Dorn creep. This is creep at a rate linear in the stress and independent of grain size. It is characterized by a dislocation density which is independent of the applied stress. It was recognized early that the observed creep rates could be accounted for by the climb of edge dislocations at the observed density under the influence of the applied stress. By analysing the observations on aluminium, Nabarro (1989b) was led to propose that the characteristic dislocation density was that at which the stress exerted on each dislocation by its nearest neighbour was equal to the Peierls stress. Wang (1993, 1996b) refined the model, and established its validity by identifying Harper–Dorn creep in many materials. The agreement between the observed dislocation density and the calculated Peierls stress is shown in fig. 3 to cover three orders of magnitude. Wang's calculated Peierls stress is half of that given by (3) and (4), that is to say essentially the P–N value.

There is thus one class of experiments which supports the H formula, while two classes support the ill-founded P–N formula.

§ 4. Resolution of the contradictions

Analytic formulae such as (3), (5) and (6) can be expected to have approximate validity only for the extreme values of $h/b \lesssim; 0 \cdot 5$ and $h/b \approx 1 \cdot 414$ encountered in practice. For the low values of h/b, theory and experiment both show that disloca-

Fig. 3

$$b \rho^{\frac{1}{2}} = 1.3 \times \frac{\sigma_P}{\mu}$$
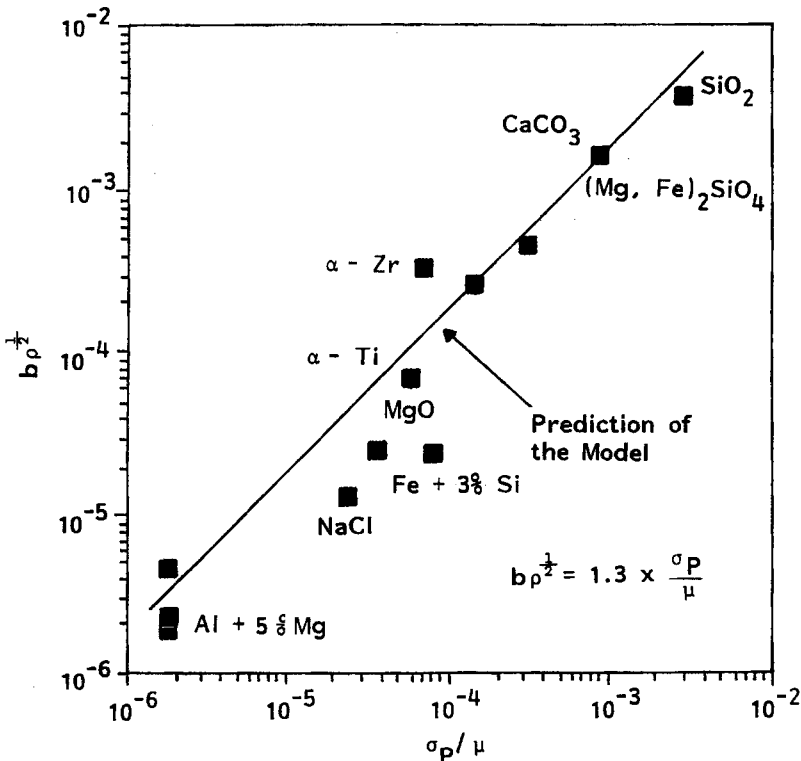
Dislocation densities during Harper–Dorn creep as functions of the normalized Peierls stress using the P–N formula (Wang 1996b).

tions will move only under stresses of the order of $\mu/20$. For $h/b \approx 1.414$, the analytical results are based on approximations which are reasonably acceptable. For intermediate values of h/b we are concerned with a simple interpolation. We therefore concentrate attention on the close-packed metals in which $h/b \approx \sqrt{2}$ for a partial dislocation.

The first step in resolving the discrepancies was taken by Benoit *et al.* (1987). Suppose the structure of a dissociated dislocation is rigid, so that the separation of the cores of the partial dislocations is fixed. If this separation is an integral multiple of the unit distance of advance, the two partials climb Peierls hills together, and the effective Peierls stress is, apart form small geometrical factors, equal to that for an isolated partial dislocation, and should be given by (5) or (6). If, on the other hand, their separation is a half-integral multiple of the unit distance of advance, the effective Peierls stress is zero. The structure is not entirely rigid, and the argument assumes that the Peierls stress can alter the separation of the partials by a distance much less than b. Benoit *et al.* then assume that the larger stresses created by point defects may alter the separation by distances of order $\frac{1}{2}b$. They assume that in general the equilibrium separation is neither an integral nor a half-integral multiple of the unit distance of advance. Then, in the absence of point defects, the Peierls stress will be of order (5) or (6), though smaller. The presence of point defects can shift the spacing to a half-integral multiple and reduce the stress almost to zero.

The next advance came in the work of Schoeck (1994), who effectively introduced a second-order perturbation treatment. Suppose that the equilibrium separation of the partials is a half-integral multiple of the unit distance of advance. Then, when one partial dislocation is on the top of a Peierls hill and the other is in a valley, the Peierls potential does not influence this separation. When the dislocation advances by $\frac{1}{4}b$, one partial dislocations is on the steepest part of the forward slope of the Peierls potential, and one on the steepest part of the backward slope. The coupling between the partial dislocations is not rigid, and the partial dislocations each sink towards the nearest Peierls valley. In a linear approximation, the reduction in energy is the same whether the perturbation causes the separation between the partial dislocations to increase or to decrease. The energy of the configuration is therefore modulated as the dislocation moves, the period of the modulation being $\frac{1}{2}b$ and the amplitude proportional to the square of the Peierls stress for a single partial.

Schoeck's result is that the amplitude of the energy modulation ΔE is related to the Peierls energy E_P (crest to trough) per unit length of partial dislocation by

$$\frac{\Delta E}{E_P} = 88 \frac{\sigma_P}{\mu}, \tag{7}$$

where σ_P is the Peierls stress for a single partial.

Neglecting small geometrical factors, we have

$$E_P = \sigma_P b_P 2/\pi, \tag{8}$$

and

$$\Delta E = \sum_P b_P^2/2\pi, \tag{9}$$

where $\sum_P$ is the observed Peierls stress arising from the second-order perturbation. The additional factor of 2 appears because the period of the second-order perturbation is $\frac{1}{2}b_P$. These equations lead to

$$\sum_{\mathrm{P}} = 176\sigma_{\mathrm{P}}^2/\mu. \tag{10}$$

The appropriate value of σ_{P} is given by (5), with b replaced by b_{P}, and thus the effective Peierls stress is given by

$$\sum_{\mathrm{P}} = \frac{176\mu}{(1-\nu)^2} \exp\,(-4\pi\zeta/b_{\mathrm{P}}). \tag{11}$$

This shows the same exponential dependence as that of the P–N formula (3) with b replaced by b_{P}, although the estimated pre-exponential is large.

The discrepancies between the different experimental estimates of the Peierls stress can now be understood. The Bordoni peak represents a localized and quasi-reversible process which can occur on any segment of the dislocation network. It is dominated by the segments which are not perturbed by local stresses, and the relevant Peierls stress is of the order calculated by Huntington for a single partial dislocation. If the equilibrium spacing of the partial dislocations is an integral number of partial Burgers vectors, the stress is equal to this Huntington value; otherwise, it is smaller, but of the same order.

Small long-range internal stresses will broaden the peak, but not shift it significantly.

The flow stress, on the other hand, is controlled by the least strongly pinned segments. Once these become mobile, plastic deformation spreads by the mitigation of kinks. The flow stress is thus of the order given by (11), which is of the P–N form.

Finally, the process of dislocation annihilation which determines the equilibrium dislocation density, and so the rate of Harper–Dorn creep, is again one which can be initiated in the regions where internal stresses have caused the separation of partial dislocations to be a half-integral multiple of the partial Burgers vector. The dislocation can then spread by kink migration. The effective Peierls stress is again given by (11), with the same exponent as in the P–N formula.

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