The Role of Dislocations in the Flow Stress Grain Size Relationships

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Calculations involving pileups of dislocations, both analytical and numerical, using either discrete dislocations or continuous distribution of dislocations of infinitesimal Burgers vectors, are reviewed in the light of their effects on the relation between yield or flow stress and grain size. The limitations of the pileup models are discussed and some nonpileup theories of yielding are critically reviewed also. More critical experiments are still needed to reveal the fundamental mechanicm of yielding.

FOLLOWING the work of Hall[1] and Petch,[2] many experimental and theoretical studies have been conducted to understand the linear relationship between the flow stress and the reciprocal square root of grain size, see Fig. 1. The original mechanism proposed by Hall[1] involves a pileup of dislocations against the grain boundary as shown in Fig. 2. The flow stress is the external stress which, with the help of the pileup, creates a critical stress concentration at a certain distance ahead of the pileup. His model was modified later by Cottrell[3] who suggested that the critical stress concentration is that which can unpin a dislocation source near the grain boundary. A similar mechanism was proposed by Petch[2] except that the stress concentration is *at* the grain boundary. Yielding is to take place when such stress concentration reaches the strength of the grain boundary.

Since all these early mechanisms involve pileups of dislocations, many theoretical studies have been conducted to examine the properties of various kinds of pileups. These include single-layer single-ended pileups in homogeneous, heterogeneous, and anisotropic media, single-layer double-ended pileups, circular pileups, and multiple-layer pileups. No attempt will be made to review all these studies. Some relevant ones will be selected and their effects on the Hall-Petch relation examined.

More recently observations have been reported which indicate the need to search for mechanisms which do not involve pileups. These observations include the lack of direct evidence of pileups in pure metals, dislocation generation in the preyield microstrain region, an increase of Hall-Petch slope in alloys where pileups are observed, and the effect or segregation of impurities to grain boundaries. Some of these nonpileup mechanisms will be reviewed and critically assessed.

1) THEORY OF DISLOCATION PILEUPS

There are two approaches to the studies of dislocation pileups, the discrete approach and the continuum approach. In the first approach, discrete dislocations of normal Burgers vectors are arranged to assume equilibrium positions. It is a problem of solving simultaneous nonlinear algebraic equations. In the second approach, a continuous distribution of dislocations of infinitesimal Burgers vectors is used to replace the discrete dislocations. It is a problem of solving an integral equation involving such a distribution function. Analytical as well as numerical methods are available for both approaches.

1.1) Single-Layer Pileups. This is the case in which all dislocations are in the same slip plane.

1.1.1) *Single-Ended Pileups.* a) *The original Eshelby-Frank-Nabarro problem.* Eshelby, Frank, and Nabarro[4] gave exact solutions to a single-layer single-ended pileup of discrete edge, screw, or mixed dislocations in isotropic or anisotropic media. Their solution is briefly described below. Consider a pileup of dislocations, all of the same Burgers vector, as shown in Fig. 2. The slip plane is the xz plane and all dislocations are parallel to the z axis. At equilibrium, the force exerted on each free dislocation is zero.

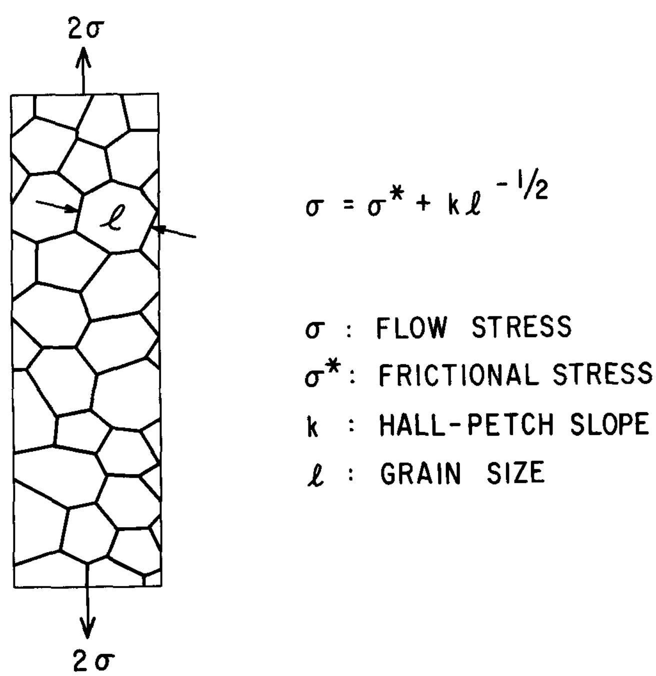

Fig. 1—The Hall-Petch relation.

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$$\frac{A}{x_i} + \sum_{\substack{j=1 \\ j \neq i}}^{n-1} \frac{A}{x_i - x_j} - \sigma = 0, \quad i = 1, 2, \ldots, n-1 \qquad [1]$$

where $A = \mu\mathbf{b}/2\pi$ and $\sigma = \sigma_{yz}$ for screw dislocations, and $A = \mu\mathbf{b}/2\pi(1-\nu)$ and $\sigma = \sigma_{xy}$ for edge dislocations in an isotropic medium of shear modulus μ and Poisson's ratio ν. For mixed dislocations in an isotropic medium,

$$A = \mu\mathbf{b}[\sin^2\phi + (1-\nu)\cos^2\phi]/2\pi(1-\nu) \qquad [2]$$

and

$$\sigma = \sigma_{xy}\sin\phi + \sigma_{yz}\cos\phi \qquad [3]$$

where ϕ is the angle between the dislocation line and the Burgers vector. For an anisotropic medium,

$$A = (\mathbf{b}/2\pi)(K_e\sin^2\phi + K_s\cos^2\phi) \qquad [4]$$

where K_e and K_s are for pure edge and pure screw pileups, respectively. These can be expressed explicitly in terms of elastic constants if the mixed dislocation has simple orientations, see for example, Chou and Mitchell.[5]

For simplicity, let the unit of distance be $A/2\sigma$ so that Eq. [1] becomes

$$\frac{1}{x_i} + \sum_{\substack{j=1 \\ j \neq i}}^{n-1} \frac{1}{x_i - x_j} - \tfrac{1}{2} = 0, \quad i = 1, 2, \ldots, n-1 \qquad [5]$$

Now consider the following polynomial whose zeros are the solutions of Eq. [5]:

$$f(x) = (x - x_1)(x - x_2)\ldots(x - x_{n-1}) \qquad [6]$$

Then

$$\frac{f'(x)}{f(x)} - \frac{1}{x - x_i} = \sum_{\substack{j=1 \\ j \neq i}}^{n-1} \frac{1}{x - x_j} \qquad [7]$$

When $x \to x_i$, the left side of Eq. [7] approaches $f''(x_i)/2f'(x_i)$ and the right hand side approaches $\frac{1}{2} - (1/x_i)$ according to Eq. [5]. Hence the problem can be solved if $q(n, x)$ in the following second order differential equation

$$f''(x) + \left(\frac{2}{x} - 1\right)f'(x) + q(n, x)f(x) = 0 \qquad [8]$$

can be so chosen that the differential equation has a polynomial solution of the $(n-1)$ degree with all real and distinct roots, and that $q(n, x)$ has no pole at any of the roots. It turns out that the following equation

$$xf''(x) + (2 - x)f'(x) + (n-1)f(x) = 0 \qquad [9]$$

is satisfied by the first derivative of the nth Laguerre polynomial $L'_n(x)$:

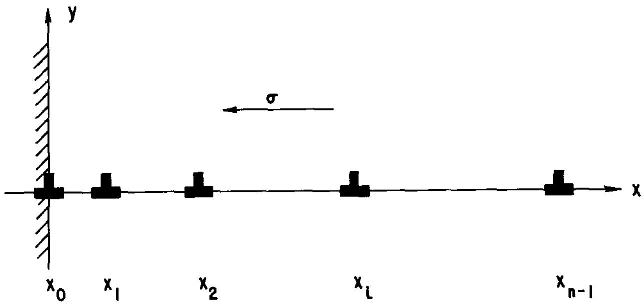

Fig. 2—A pileup of dislocations against a grain boundary.

$$L'_n(x) = -\sum_{k=0}^{n-1} \frac{n!(-x)^k}{k!(k+1)!(n-k-1)!} \qquad [10]$$

the roots of which are then solutions for Eq. [5].

With the substitution of $v(x) = xf(x)\exp(-x/2)$, Eq. [9] is transformed into

$$v''(x) + \left(\frac{n}{x} - \frac{1}{4}\right)v(x) = 0 \qquad [11]$$

which, for $x \ll 4n$, has the solution:

$$v(x) = \sqrt{x} \cdot J_1(2\sqrt{nx}) \qquad [12]$$

and hence near the tip of the pileup the position of the ith dislocation is given by

$$x_i \simeq j_i^2/4n \qquad [13]$$

in units of $A/2\sigma$ with j_i being the ith zero of the Bessel function J_1. In particular, $x_1 = 1.84A/n\sigma$. Furthermore, since v'' and v must differ in sign, an upper limit for x is $4n$. Hence for large n, the length of the pileup approaches:

$$l = 4n(A/2\sigma) = 2nA/\sigma \qquad [14]$$

Although the lower limit of l is given by Eshelby *et al.*,[4] this result is the simplest and is pertinent to the subject of this review.

The stress concentration σ_{tip} exerted on the pinned dislocation can be obtained from the external forces exerted on all the free dislocations which sum up to $(n-1)\sigma\mathbf{b}$. Since the system is at equilibrium, $(\sigma_{\text{tip}} - \sigma)\mathbf{b} = (n-1)\sigma\mathbf{b}$, and hence,

$$\sigma_{\text{tip}} = n\sigma \qquad [15]$$

Following Petch,[2] these results can be used to derive the flow-stress grain size relationship by assuming a yield condition of $\sigma_{\text{tip}} = \sigma_c$, a critical stress required at the grain boundary in order to propagate the plastic deformation, and by assuming that the length of the pileup, l, is the same as the grain size. By substituting $n = \sigma_c/\sigma$ into Eq. [14] and solving for σ and by including a possible frictional stress, σ^*, inside the grain, the Hall-Petch relation is obtained:

$$\sigma = \sigma^* + \sqrt{2A\sigma_c}\, l^{-1/2} \qquad [16]$$

The Hall-Petch slope, k, is then identified as $\sqrt{2A\sigma_c}$. For $\sigma_c = \mu/30$ and $A = \mu\mathbf{b}(2-\nu)/4\pi(1-\nu)$ for mixed dislocations, this slope is $0.115\mu\sqrt{\mathbf{b}}$ for $\nu = \frac{1}{3}$. Direct numerical determination by Li and Liu[6] using only a few mixed dislocations gives a slope of $0.1\mu\sqrt{\mathbf{b}}$ indicating the extent of applicability for small n. Experimentally, using Hall's data[1] for mild steel, $k = 1$ kg/mm$^{3/2}$ (the shear stress is taken as one half of tensile stress), and taking $\mu = 7.9 \times 10^3$ kg/mm^2 and $\mathbf{b} = 2.48$Å, σ_c is found to be $\mu/6.3$, a reasonable value.

Numerical computations of the equilibrium positions or the roots of the Laguerre polynomials are given by Head,[7] by Chou *et al.*,[8] and by Mitchell *et al.*[9] Stress contours are plotted by Mitchell,[10] and by Basinski and Mitchell.[11]

b) *The effect of the pinned dislocation having a different Burgers vector*. Chou[12] modified the foregoing problem by considering the case in which the pinned dislocation is of a different Burgers vector. This is motivated by the fact that the pinned dislocation is at the grain boundary and therefore could have a Burgers vector, $m\mathbf{b}$, different from the lattice dislocations forming the pileup. The problem can be solved by following the procedure given by Eshelby *et al.*,[4] by starting with an extra factor m (a positive real number) at the first term of Eq. [1], and similarly of Eq. [5]. The factor $(2/x) - 1$ in Eq. [8] becomes $(2m/x) - 1$ and the factor $(2 - x)$ in Eq. [9] becomes $2m - x$. Then instead of Eq. [10] the solution is the generalized Laguerre polynomial:

$$L_{n-1}^{(2m-1)} = \sum_{k=0}^{n-1} \binom{n + 2m - 2}{n - k - 1} \frac{(-x)^k}{k!} \qquad [17]$$

A substitution of $v(x) = x^m f(x) \exp(-x/2)$ gives the following differential equation instead of Eq. [11]:

$$v''(x) + \left[\frac{n + m - 1}{x} - \frac{m(m-1)}{x^2} - \frac{1}{4}\right] v(x) = 0 \qquad [18]$$

which, for small x (so that $\frac{1}{4}$ can be neglected in the bracketed quantity) has the solution (Jahnke and Emde,[13] p. 146):

$$v(x) = \sqrt{x} \cdot J_{2m-1}(2\sqrt{(n + m - 1)x}) \qquad [19]$$

and, hence, near the tip of the pileup the position of the ith dislocation is given by

$$x_i = (j_{2m-1,i})^2/4(n + m - 1) \qquad [20]$$

in units of $A/2\sigma$ with $j_{2m-1,i}$ being the ith zero of the Bessel function J_{2m-1}. In particular, for

$m = \frac{1}{2}$, $\quad x_1 = 0.723A/(n - \frac{1}{2})\sigma$

$m = 1$, $\quad x_1 = 1.84A/n\sigma$

$m = 2$, $\quad x_1 = 5.1A/(n + 1)\sigma$

and for

$$m = 3, \qquad x_1 = 9.6A/(n + 2)\sigma \qquad [21]$$

Here again, since $v''(x)$ and $v(x)$ must differ in sign, the bracketed quantity in Eq. [18] must be positive and hence for large n, the length of the pileup approaches

$$l = 2(n + m - 1)A/\sigma \qquad [22]$$

The stress concentration σ_{tip} exerted on the pinned dislocation can be obtained as before, namely, $(\sigma_{\mathrm{tip}} - \sigma)m\mathbf{b} = (n - 1)\sigma\mathbf{b}$, and hence

$$\sigma_{\mathrm{tip}} = (n + m - 1)\sigma/m \qquad [23]$$

By using a yield condition of $\sigma_{\mathrm{tip}} = \sigma_c$ at the grain boundary, Eq. [23] can be combined with Eq. [22] and, after introducing the lattice friction stress σ^*, the Hall-Petch relation becomes

$$\sigma = \sigma^* + (2Am\sigma_c)^{1/2} l^{-1/2} \qquad [24]$$

from which the Hall-Petch slope, k, is identified as $\sqrt{2Am\sigma_c}$. A comparison with Eq. [16] shows that the slope is modified by a factor of $\sqrt{m}$. By using Hall's data[1] again for mild steel, $m\sigma_c$ is found to be $\mu/6$. This gives $m = 5$ if σ_c is $\mu/30$. Based on the ledge structure of grain boundaries to be discussed later, it is conceivable that grain boundary ledges can have large Burgers vectors.

c) *Continuous distribution of dislocations.* Instead of discrete dislocations each having the same Burgers vector $\mathbf{b}$, the pileup problem can be viewed as a continuous distribution of dislocations of infinitesimal Burgers vectors. A distribution function $f(x)$ is sought such that $\mathbf{b}f(x)dx$ is the total Burgers vector of dislocations between x and $x + dx$ and hence it produces a stress field $Af(x)dx/(t - x)$ at a distance t. Such distribution function has to satisfy the following integral equation:

$$A \int_0^l \frac{f(x)dx}{t - x} = \sigma \quad \text{for any } 0 < t < l \qquad [25]$$

The number of dislocations in the pileup is then given by:

$$\int_0^l f(x)dx = n \qquad [26]$$

The solution is given by Leibfried[14] and by Head and Louat:[15]

$$f(x) = \frac{\sigma}{\pi A}\sqrt{\frac{l - x}{x}} \qquad [27]$$

from which the total number of dislocations is given by $n = \sigma l/2A$ in agreement with Eq. [14]. The stress concentration can be calculated from the total applied force on the system by assuming that this force is exerted on the pinned dislocation of Burgers vector $\mathbf{b}$:

$$\sigma_{\mathrm{tip}} = \int_0^l f(x)\sigma dx = \frac{\sigma^2 l}{2A} = n\sigma \qquad [28]$$

in agreement with Eq. [15]. By using the same yield criterion, namely a critical stress concentration σ_c at the grain boundary, the same Hall-Petch relation, Eq. [16], is obtained.

The strain energy of the pileup can be obtained by making a cut in the slip plane from $x = 0$ to $x = R$ (R is the size of specimen), replacing the external stress with equal and opposite forces on the two cut surfaces to maintain the elastic state of the system, and reversibly reducing these forces to zero so as to remove the pileup. Per unit area of the slip plane, these forces are σ within the pileup, and are σ_ξ at a distance ξ outside the pileup:

$$\sigma_\xi = A \int_0^l \frac{f(x)}{\xi - x} dx = \sigma\left(1 - \sqrt{\frac{\xi - l}{\xi}}\right) \qquad [29]$$

The displacement u inside the pileup is

$$u = \mathbf{b} \int_0^x f(x)dx \qquad [30]$$

and outside the pileup at $\xi \geq l$ is

$$u_\xi = \mathbf{b} \int_0^l f(x)dx = n\mathbf{b} = \mathbf{b}\sigma l/2A \qquad [31]$$

The energy is then (per unit length in the z direction):

$$E = \int_0^\sigma \int_0^l \sigma\left(\frac{\partial u}{\partial \sigma}\right)_x dx d\sigma + \int_0^\sigma \int_l^R \sigma_\xi \left(\frac{\partial u_\xi}{\partial \sigma}\right)_x dx d\sigma$$

$$= \frac{\mathbf{b}\sigma^2 l^2}{8A}\left(\ln\frac{4R}{l} + \frac{1}{2}\right) = n^2 \frac{A\mathbf{b}}{2}\left(\ln\frac{4R}{l} + \frac{1}{2}\right) \qquad [32]$$

which is given also by Stroh.[16]

This result can be used to derive Eq. [28] as follows: The change of energy for constant σ from a pileup of length l to that of length $l + \Delta l$ can be obtained from Eq. [32]. This change can be obtained also by direct reversible extension of the pileup. This would involve the work of σ and σ_ξ upon a change of displacement in u and u_ξ caused by the extension of l, as well as the work of σ_{tip} (negative) which amounts to $\mathbf{b}\sigma_{\mathrm{tip}}\Delta l$. The procedure is an application of Moutier's theorem[17] and will be used later in the case of double ended pileups for which the stress concentration cannot be obtained from the total force exerted on the system.

Another continuum approach is advanced by Webster and Johnson[18] for screw pileups. Since the field of a screw dislocation is mathematically equivalent to the velocity field of a vortex in fluid flow, it is possible to apply the complex potential method used in hydrodynamics to screw pileups. The results are of course the same, but one important advantage is that, for certain boundary conditions, the conformal mapping technique can be exercised.

d) *The effect of nonuniform stress field.* So far the stress field other than that produced by the dislocations themselves is uniform along the slip plane. The effect of a nonuniform stress field on the continuous distribution of dislocations has been examined by Chou and Louat.[19] The problem is the same as the previous one except that Eq. [25] is now

$$A \int_0^l \frac{f(x)dx}{t-x} = \sigma(t) \qquad [33]$$

where $\sigma(t)$ is a given function and Eq. [33] has to be satisfied for any t between 0 and l. For this case in which $f(x)$ is unbounded at $x = 0$ and bounded at $x = l$, the solution is, according to Mushelishvili[20]

$$f(x) = \frac{1}{\pi^2 A}\sqrt{\frac{l-x}{x}} \int_0^l \sqrt{\frac{t}{l-t}}\,\frac{\sigma(t)}{t-x}\,dt \qquad [34]$$

A simple example is $\sigma(t) = \sigma_0[1 + (\lambda t/l)]$ where λ is a constant. Then for $\lambda > -\frac{2}{3}$:

$$f(x) = \frac{\sigma_0}{\pi A}\sqrt{\frac{l-x}{x}}\left(1 + \frac{\lambda}{2} + \frac{\lambda x}{l}\right) \qquad [35]$$

$$n = \int_0^l f(x)dx = \frac{\sigma_0 l}{2A}\left(1 + \frac{3\lambda}{4}\right) \qquad [36]$$

The stress concentration is again obtained from the total external forces exerted on the system:

$$\sigma_{\text{tip}} = \int_0^l f(x)\sigma(x)dx = \frac{\sigma_0^2 l(\lambda+2)^2}{8A} \qquad [37]$$

By using the yield criterion mentioned earlier and by taking σ_0 as the applied stress and $\sigma_0\lambda x/l$ as the internal stress, the Hall-Petch relation becomes:

$$\sigma_0 = \sigma^* + \frac{\sqrt{8A\sigma_c}}{\lambda+2}\, l^{-1/2} \qquad [38]$$

which reduces to Eq. [16] for $\lambda = 0$. The Hall-Petch slope, k, is now $\sqrt{8A\sigma_c}/(\lambda + 2)$ and is seen to be affected by the internal stress through the magnitude and sign of λ. However, Eq. [38] shows that the Hall-Petch relation is exact only if λ is independent of l. If instead of λ, $\sigma_0\lambda$ is independent of l, the Hall-Petch relation becomes inexact. This signals caution in applying the Hall-Petch relation to work hardened states in which cells or subgrains are formed so that nonuniform internal stresses exist within a grain.

Although in the foregoing example the internal stress is of one sign within the pileup region, it is to be remembered that a pileup of negative dislocations under the influence of the same internal stress distribution except for the sign should exist somewhere in another grain in the same specimen. Thus, the average internal stress is zero as required by elastic equilibrium without the external stress.

The effects of nonuniform stress distribution upon the dislocation distribution and upon the stress concentration are discussed also by Yokobori and Ichikawa,[21] by Chaudhari and Scattergood,[22] and by Smith.[23,24]

e) *Pileups of extended dislocations.* The effect of stacking fault energy, or the extent each dislocation dissociates into partial dislocations, on the properties of pileups has been studied by Li.[25] The equilibrium positions of all the partial dislocations are determined numerically. As expected, the equilibrium width of the stacking fault varies along the length of the pileup—being smaller near the tip than farther away from the tip. However, the stress concentration at the tip and the number of dislocations for a given pileup length are both independent of the stacking fault energy. Hence for a given critical stress concentration for yielding, the Hall-Petch slope is also independent of stacking fault energy. This result is somewhat expected in view of the fact that the results of discrete dislocations and those of continuous distribution of dislocations of infinitesimal Burgers vectors are the same, indicating that any prescribed interaction between dislocations of infinitesimal Burgers vectors is immaterial.

f) *Dynamic effects involving dislocation pileups.* In view of the large effect of stress on the dislocation mobility, Rosenfield and Hahn[26] pointed out that the time for the formation of a pileup depends greatly on the parameter $\beta = \mu(\partial \ln v/\partial\sigma)$ where v is dislocation velocity and μ is the shear modulus. By assuming that β is independent of stress, the time for the tip stress to reach $\frac{1}{2}$ of the equilibrium value is computed numerically and is given approximately by

$$t_{1/2}/t_0 = \exp(0.75 \times 10^{-4}\beta) \qquad [39]$$

where t_0 is the time required for the case of $\beta = 0$. These dynamic effects undoubtedly contribute to the yield stress at different strain rates and to the delay time phenomena.

g) *The effect of a second phase.* Dislocation pileups against a second phase were studied by Chou[27] for a single-layer, single-ended pileup of screw dislocations. The second phase in front of the pileup is assumed rigid. The results, based on a continuous distribution of dislocations, are

$$f(x) = \frac{2\sigma}{\pi^2 A'}\cosh^{-1}\left|\frac{l}{x}\right|, \quad \bar{K} = 1 \qquad [40]$$

and

$$n = \frac{\sigma l}{\pi A'} \qquad [41]$$

where

$$\bar{K} = \frac{\mu_2 - \mu_1}{\mu_2 + \mu_1}, \quad A' = \frac{\mu_1 \mathbf{b}}{2\pi} \qquad [42]$$

and μ_1 and μ_2 are the shear moduli of the first and second phase, respectively. For a more general case, Chou[27] proposed a linear relation as implied by the numerical results of Head:[28]

$$l = \frac{A'}{\sigma}[2 + (\pi - 2)\bar{K}]n, \quad 0 \le \bar{K} \le 1 \qquad [43]$$

Eq. [43] was proved fairly accurate with a maximum error of 1 pct by Smith[29] and by Barnett.[30] Using Eq. [40] Barnett was able to find the following general solution

$$f(x) = \frac{\sigma}{\pi A'} \frac{1}{\sin(\lambda\pi/2)} \sinh\left(\lambda \cosh^{-1} \frac{l}{x}\right),$$

$$\lambda = \frac{2}{\pi} \sin^{-1} \sqrt{\frac{1 - \bar{K}}{2}} \qquad [44]$$

$$n = \frac{\sigma l}{A'} \frac{\lambda}{\sin \lambda\pi} \qquad [45]$$

and the stress component σ_{yz} near the tip in the second phase at $y = 0$,

$$\sigma''_{yz} = -\frac{\sigma \cos \frac{\lambda\pi}{2}}{2 \sin^2 \frac{\lambda\pi}{2}} \left\{\left(2\left|\frac{l}{x}\right|\right)^{\lambda} - 2 \cos \frac{\lambda\pi}{2}\right\}, \quad \left|\frac{l}{x}\right| \gg 1 \qquad [46]$$

The validity of Eq. [43] was checked also by Barnett and Tetelman[31] in the case where the second phase is a circular inclusion. By using a critical force criterion, the Hall-Petch relation can be derived as shown by Chou.[32]

More recently, Kuang and Mura[33] analyzed the case of single-layer, single-ended pileups of edge dislocations, using the Wiener-Hopf technique.[34] The analysis is rather complex but the results show that Eq. [43] is also valid in the case of edge dislocations.

Numerical calculations for pileups in two-phase media were performed by Head,[28] Armstrong and Head,[35] and Chou.[36]

1.1.2) *Double-Ended Pileups.* a) *Continuous distribution of dislocations.* Instead of piling up against one boundary, a more realistic situation is for a source inside the grain to emit dislocations of both signs so that they pile up at diametrically opposite grain boundaries as shown in Fig. 3. Analytical methods for calculating the equilibrium positions of discrete dislocations are not yet available. Leibfried[14] and Head and Louat[15] give solutions for the continuous distribution of dislocations of infinitesimal Burgers vectors. The distribution function is

$$f(x) = \frac{\sigma}{\pi A} \frac{x}{\sqrt{a^2 - x^2}} \qquad [47]$$

and the number of dislocations of either sign is

$$n = \int_0^a f(x)dx = \sigma a/\pi A \qquad [48]$$

The strain energy of the pileup can be obtained by making a cut in the slip plane between the two ends of the pileup, replacing the external stress by equal and opposite forces (σ per unit area) on the two cut surfaces, and reversibly reducing these forces to zero so as to remove the pileup. The displacement at x is

$$u = \mathbf{b} \int_x^a f(x)dx = \frac{\sigma \mathbf{b}}{\pi A} \sqrt{a^2 - x^2} \qquad [49]$$

The energy is then (per unit length in the z direction):

$$E = \int_0^{\sigma} \int_{-a}^{a} \sigma\left(\frac{\partial u}{\partial \sigma}\right)_x dx d\sigma = \frac{\mathbf{b} a^2 \sigma^2}{4A} \qquad [50]$$

which is given also by Hirth and Lothe.[37]

The stress concentration at the tip can be calculated by application of Moutier's theorem. The energy difference between pileups of length $2a$ and $2(a + \Delta a)$ is $\Delta E = \mathbf{b} a \sigma^2 \Delta a/2A$. This difference can be obtained also by direct reversible extension of the pileup. In this reversible extension, both σ and σ_{tip} contribute to the work. The part with σ is, from Eq. [49]:

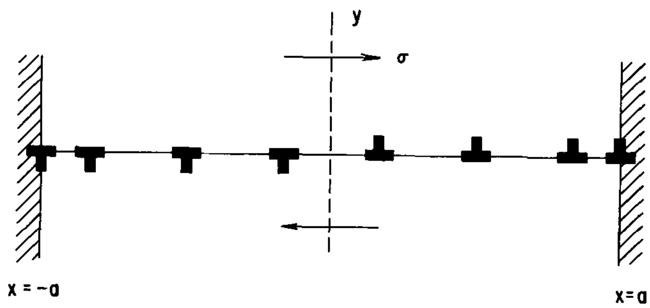

Fig. 3—Single-layer, double-ended pileups.

$$\frac{\sigma^2 \mathbf{b}}{\pi A} \left[\int_{-(a+\Delta a)}^{a+\Delta a} \sqrt{(a + \Delta a)^2 - x^2}\, dx - \int_{-a}^{a} \sqrt{a^2 - x^2}\, dx \right] = \frac{\mathbf{b} a \sigma^2 \Delta a}{A}$$

The part with σ_{tip} is $-2\mathbf{b}\sigma_{tip} \Delta a$. Hence

$$\sigma_{tip} = \frac{\sigma^2 a}{4A} = \frac{\pi}{4} n\sigma \qquad [51]$$

This result is given also by Hirth and Lothe[37] except that their application of Moutier's theorem is incomplete.

Eq. [51] leads to the following Hall-Petch relation based on the yield condition that σ_{tip} reaches a critical value σ_c and taking $l = 2a$:

$$\sigma = \sigma^* + 2\sqrt{2A\sigma_c}\, l^{-1/2} \qquad [52]$$

A comparison of this result with Eq. [16] shows that the Hall-Petch slope is exactly twice as much in the case of the double-ended pileups as in the case of the single-ended pileup. By using Hall's data[1] again for mild steel, $k = 1$ kg/mm$^{3/2}$, σ_c is found to be $\mu/25$ based on the double-ended pileups of screw dislocations.

The effect of a second phase on double-ended screw pileups was recently studied by T. W. Chou[116] and by Smith.[117] For a pileup between $x = 0$ and $x = l$ against a boundary at $x = 0$,

$$f(x) = \frac{\sigma}{\pi A'} \frac{1}{\sin(\lambda\pi/2)} \left\{\sinh\left(\lambda \cosh^{-1} \frac{l}{x}\right) - \frac{\lambda l}{\sqrt{l^2 - x^2}} \cosh\left(\lambda \cosh^{-1} \frac{l}{x}\right)\right\} \qquad [53]$$

where A' is given by Eq. [42] and λ by Eq. [44]. It is of interest to note that the result given by Eq. [53] is a superposition of two separate distribution functions. The first term is the distribution of a single-ended pileup of positive screw dislocations under the applied stress σ, see Eq. [44]; whereas the second term represents the distribution of a double-ended pileup of negative screw dislocations under zero stress. Such superposition is in fact generally applicable. The stress distribution near the tip of the pileup was found[116] to be the same as in a single-ended pileup, Eq. [46], as expected.

Eq. [53] takes simpler forms for the limiting cases of $\mu_1/\mu_2 \to 0$ or $\lambda \to 0$ and $\mu_1/\mu_2 \to \infty$ or $\lambda \to 1$. In each case the number of positive or negative screw dislocations can be found by integration. For the case of $\mu_1/\mu_2 \to 0$, the number is $0.8438\ (\sigma l/2\pi A')$ and for the case of $\mu_1/\mu_2 \to \infty$, the number is 2 $(\sigma l/2\pi A')$ where $(\sigma l/2\pi A')$ is the number for the homogeneous case, namely, $\mu_1 = \mu_2$.

b) *Numerical solutions for discrete dislocations.* Armstrong *et al.*[38] studied the equilibrium positions by numerical methods and found that, for any n, σ, and a, there are two configurations, one is stable and the other unstable. These two configurations will approach each other upon reducing σ until a critical σ is reached such that the two configurations become identical. A further reduction of σ will lose a pair of dislocations and two possible new configurations will result with one pair less of dislocations. Since the yield stress is taken to be the minimum applied stress required to create a given stress concentration at the boundary, it is also the stress that can maintain the largest number of dislocations. This is the situation discussed previously in the continuous distribution.

By using a different yield criterion based on a critical separation (10**b**) between the first two dislocations in a pileup, Armstrong *et al.*[38] compared numerical results for discrete dislocations with analytical results for a continuous distribution and found that the Hall-Petch relation can be extended to very small grain sizes with only a few dislocations in the pileup at the time of yielding. The Hall-Petch slope for the double-ended pileups is about twice that for the single-ended pileups.

By using a critical stress concentration of $\mu/30$, Li and Liu[6] calculated numerically for the double-ended pileups of mixed dislocations a Hall-Petch slope of $0.22\,\mu\sqrt{\mathbf{b}}$. For the same stress concentration, Eq. [52] predicts a slope of $0.23\,\mu\sqrt{\mathbf{b}}$. The agreement also indicates the applicability of continuous distribution even for only a few dislocations.

1.1.3) *Circular Pileups.* a) *Continuous distribution of dislocation loops.* The application of the Hall-Petch relation to very small grain sizes requires consideration of more realistic pileups such as circular or polygonal loops instead of infinite straight dislocations. An equilibrium continuous distribution of circular dislocations within a circular boundary of radius a can be obtained from the displacement of a shear circular crack in an isotropic medium:

$$f(r) = \frac{8\sigma(1-\nu)}{\pi\mu\mathbf{b}(2-\nu)}\frac{r}{\sqrt{a^2-r^2}} \qquad [54]$$

where $f(r)dr$ is proportional to the density of loops between r and $r+dr$. The total number of loops is then:

$$n = \int_0^a f(r)dr = \frac{8\sigma a(1-\nu)}{\pi\mu\mathbf{b}(2-\nu)} \qquad [55]$$

The displacement at r is

$$u = \mathbf{b}\int_r^a f(r)dr = \frac{8\sigma(1-\nu)\sqrt{a^2-r^2}}{\pi\mu(2-\nu)} \qquad [56]$$

These results can be used to calculate the energy of the pileups as illustrated before:

$$E = \int_0^\sigma\int_0^{2\pi}\int_0^a \sigma\left(\frac{\partial u}{\partial\sigma}\right) r\,dr\,d\theta\,d\sigma = \frac{8a^3\sigma^2(1-\nu)}{3\mu(2-\nu)} \qquad [57]$$

which can be used to calculate an average stress concentration by the application of Moutier's theorem:

$$\bar{\sigma}_{\text{tip}} = \frac{4a\sigma^2(1-\nu)}{\mu\mathbf{b}(2-\nu)\pi} = \tfrac{1}{2}n\sigma \qquad [58]$$

Eq. [52] leads to the following Hall-Petch relation

$$\sigma = \sigma^* + \left(\frac{\mu\mathbf{b}(2-\nu)\pi\sigma_c}{2(1-\nu)}\right)^{1/2} l^{-1/2} \qquad [59]$$

where $l = 2a$ and the yield condition is $\bar{\sigma}_{\text{tip}} = \sigma_c$. A comparison of Eq. [59] with Eq. [16] shows that the Hall-Petch slope in the case of circular pileups is π times that of single-ended pileups of mixed straight dislocations [$A = \mu\mathbf{b}(2-\nu)/4\pi(1-\nu)$ in isotropic medium].

b) *Numerical results on discrete circular loops.* Li and Liu[6] examined circular dislocation pileups by numerical means so as to compare with the results for a continuous distribution. Equilibrium configurations are obtained by requiring that all the loops are circular and that the average force exerted on each free loop is zero. The outermost loop is of radius a and is blocked everywhere by grain boundaries. Under an applied shear stress σ, n loops are introduced and their equilibrium radii determined. For each set of values of a, σ, and n, two equilibrium configurations are possible, one stable and the other unstable, similar to the case of double ended pileups. Upon reduction of σ, these two configurations approach each other and become identical when a critical σ is reached. Further reduction of σ loses one loop and two possible configurations appear again with one less loop. Since the yield stress is taken to be the minimum stress required to create a given stress concentration at the boundary, the largest number of loops is used for each set of a and σ. This is the case studied in the continuous distribution.

An added complication in the case of discrete loops is the line tension of dislocations which is neglected in the continuous distribution. This introduces a parameter r_0, the core radius of dislocations, which is of the order of **b**. For $a = 1000r_0$, the minimum stress necessary to maintain n loops in units of $\mu\mathbf{b}/2a\pi(1-\nu)$, is compared with Eq. [55] as follows ($\nu = \frac{1}{3}$):

n	2	3	4	5	6	7	8
σ	8.8	13.1	17.3	21.4	25.6	29.9	33.9
Eq. [55]	8.2	12.3	16.5	20.6	24.7	28.8	32.9

It is seen that the numerical results agree with those required for continuous distribution, especially at large n.

The Hall-Petch slope for discrete loops is found to be $0.37\mu\mathbf{b}/\sqrt{r_0}$ for a critical stress concentration at the boundary, $\mu\mathbf{b}/30r_0$. For the same critical stress concentration, Eq. [59] predicts a slope of $0.36\mu\mathbf{b}/\sqrt{r_0}$. The slight difference could be caused by the line tension neglected in the continuous distribution.

1.2) Double-Layer Pileups. This is the case in which dislocations are arranged in two identical layers, one above the other. Because of their mutual interaction, the results are different from those of a single layer.

1.2.1) *Single-Ended Pileups.* Two identical layers of a continuous distribution of edge dislocations at $y = 0$ and $y = h$ are piled up between $x = 0$ and $x = l$ against a grain boundary at $x = 0$. The dislocation lines are all parallel to the z axis. The distribution function $f(x)$ along each layer should satisfy the following:

$$A\int_0^l \frac{f(x)}{t-x}\left\{1 + \frac{(t-x)^2[(t-x)^2-h^2]}{[(t-x)^2+h^2]^2}\right\}dx = \sigma \qquad [60]$$

An analytical solution for $f(x)$ is not yet available. By approximating part of the integrand with a finite Fourier series of $m + 2$ terms (m being arbitrary, and the larger the more accurate) Yokobori and Ichikawa[40] solved numerically the system of $m + 2$ simultaneous equations. The results on the number of dislocations, n_2, in each layer as compared with that of a single layer, n_1, are

h/l	0	0.15	0.30	0.50	1.0	2.0	∞
n_2/n_1	0.5	0.674	0.805	0.948	1.0656	1.0437	1.000

The limiting ratio of 0.5 at $h = 0$ is expected because then it becomes a single pileup of dislocations of double Burgers vectors. When h/l increases it is seen that n_2/n_1 first increases, reaches a maximum, and then decreases. This is reasonable since for small h/l, most dislocations repel each other across the two layers and for large h/l they attract each other instead. Based on the critical stress concentration at the boundary, the ratio of Hall-Petch slopes is simply $k_2/k_1 = (n_1/n_2)^{1/2}$.

1.2.2) *Double-Ended Pileups.* Two identical layers (separation h) of double-ended pileups of a continuous distribution of screw dislocations within a length $2a$ were considered by Smith[41] for the case of $a < h$. The integral equation was approximated by expanding the distribution function into a power series of a/h. The number of dislocations in each half layer is found to be

$$n = \frac{2\sigma a}{\mu \mathbf{b}}\left(1 - \frac{a^2}{2h^2} + \frac{7a^4}{8h^4} + \cdots\right) \qquad [61]$$

For edge dislocations, the result is

$$n = \frac{2\sigma a(1-\nu)}{\mu \mathbf{b}}\left(1 + \frac{a^2}{2h^2} - \frac{13a^4}{8h^4} + \cdots\right) \qquad [62]$$

It is seen that, relative to the single-layer pileups, less screw dislocations but more edge dislocations can be contained in the double-layer pileups. Accordingly, the Hall-Petch slope is larger for screw dislocations and smaller for edge dislocations in the case of double-layer pileups. However, for $h \ll a$, $n = \sigma a/\mu\mathbf{b}$ for screw dislocations and $\sigma a(1-\nu)/\mu\mathbf{b}$ for edge dislocations since they both approach single-layer, double-ended pileups of dislocations of twice the Burgers vector.

1.3) Triple-Layer Pileups. Three layers ($y = 0$, h, and $2h$) of single-ended pileups of a continuous distribution of edge dislocations ($0 \le x \le l$) against a grain boundary at $x = 0$ were investigated by Yokobori and Ichikawa[40] by approximating the integral equation with eleven terms of a finite Fourier series. The number of dislocations in the outer layer, n_3, and that in the middle layer, n_3', are calculated numerically and are compared with that for a single layer pileup, n_1, as follows:

h/l	0	0.15	0.30	0.50	1.00	2.00	∞
n_3/n_1	0.333	0.635	0.818	1.0106	1.1170	1.0597	1.000
n_3'/n_1	0.333	0.392	0.606	0.8902	1.1372	1.0890	1.000

It is seen that for large h/l, the stress concentration is larger at the tip of the middle layer than at the tips of outer layers. However, the situation is the opposite for small h/l. The Hall-Petch slope, k_3, for the triple-layer pileups, is given by $k_3/k_1 = \sqrt{n_1/n_3}$ or $\sqrt{n_1/n_3'}$ whichever is smaller. Similarly, when compared with double-layer pileups, $k_3/k_2 = \sqrt{n_2/n_3}$ or $\sqrt{n_2/n_3'}$ whichever is smaller.

1.4) Infinite-Layer Pileups. 1.4.1) *Single-Ended Pileups.* a) *Continuous distribution of screw dislocation walls.* An infinite number of layers of screw dislocations, with a uniform spacing h between layers, are here considered to pile up between $x = 0$ and $x = l$ against a grain boundary at $x = 0$. The slip planes are parallel to $y = 0$ and all the dislocation lines are parallel to the z axis. The distribution function along each layer is given by Louat[42] and later also by Webster and Johnson:[18]

$$f(x) = \frac{2\sigma}{\mu\mathbf{b}}\left(\operatorname{sech}\frac{\pi l}{2h}\right)\left\{\frac{\sinh[\pi(l-x)/h]}{\sinh(\pi x/h)}\right\}^{1/2} \qquad [63]$$

The number of dislocations in each layer is

$$n = \int_0^l f(x)dx = \frac{2\sigma h}{\mu\mathbf{b}}\tanh\frac{\pi l}{2h} \qquad [64]$$

Since l is usually larger than h, the hyperbolic tangent function in Eq. [64] is very close to unity. The simplified Eq. [64] can be obtained directly from the stress field of screw dislocation walls[43] which is $\mu\mathbf{b}/2h$ per wall at any distance larger than h from the wall. This gives $\sigma = (n-1)\mu\mathbf{b}/2h$ which agrees with Eq. [64].

From equilibrium considerations the stress concentration at the tip is $n\sigma$. Hence by the critical stress criterion for yielding, the Hall-Petch relation is

$$\sigma = \sigma^* + \sqrt{\mu\mathbf{b}\sigma_c l/2h}\, l^{-1/2} \qquad [65]$$

It is seen that, for the Hall-Petch relation to be valid, l/h must remain constant for all l. If, however, h is constant instead of h/l, Eq. [65] predicts a stress which is independent of l. This casts some doubt on the multilayer pileup model for yielding.

To compare with the Hall-Petch slope k_1 for a single-layer pileup of screw dislocations, $\sqrt{\mu\mathbf{b}\sigma_c/\pi}$, Eq. [64] gives k_∞ as

$$k_\infty/k_1 = \sqrt{(\pi l/2h)\coth(\pi l/2h)} \qquad [66]$$

which is shown in Fig. 4 together with that for the pileup of edge dislocation walls.

b) *Numerical results on the pileups of discrete screw dislocation walls.* Since the number of dislocations, n, is proportional to stress but is nearly independent of l, it is interesting to see how the dislocations arrange themselves in the slip planes. This is obtained numerically[44] and is shown in Fig. 5 for twenty walls of screw dislocations. The dotted line is for the case of a single layer. It is seen that upon increasing l or decreasing h, more and more dislocations are concentrated at the tip of the pileup. The stress to maintain the pileups is shown in Fig. 6. For $n \to \infty$, the stress approaches that required for continuous distribution as expected. For any realistic value of $\pi l/h$ such as 10 or more, the stress required is almost exactly $(n-1)\mu\mathbf{b}/2h$ for any $n \ge 2$.

c) *Pileups of edge dislocation walls.* An analytical solution for the continuous distribution of pileups of infinite edge dislocation walls is not yet available. Yokobori and Ichikawa[40] approached the problem numerically based on a method proposed by Hanaoka.[45] The following integral equation

$$\int_0^l \frac{f(x)}{t-x}\left[\frac{\pi(t-x)}{h}\operatorname{csch}\frac{\pi(t-x)}{h}\right]^2 dx = \sigma/A \qquad [67]$$

where $A = \mu\mathbf{b}/2\pi(1-\nu)$, is approximated by expanding part of the integrand into a finite Fourier series of $m+2$ terms (m being arbitrary, the larger the more accurate) so that the integral equation becomes a set of simultaneous equations of $m+2$ unknowns which is then solved numerically. The results on the number of dislocations, n_∞ (as compared to that of single pileup, n_1), are as follows ($m = 19$):

h/l	∞	2.0	1.5	1.0	0.65	0.6
n_∞/n_1	1.0000	1.1839	1.3040	1.5810	2.0674	2.4963
h/l	0.4	0.3	0.2	0.15	0.12	0.10
n_∞/n_1	2.966	3.753	5.30	6.7	7 to 8	6 to 10

The Hall-Petch slope, k_∞, when compared with that for a single layer pileup of edge dislocations, k_1, is

$$k_\infty/k_1 = \sqrt{n_1/n_\infty} \qquad [68]$$

which is shown in Fig. 4.

Numerical results on the pileup of discrete edge dislocation walls[44] are shown in Figs. 7 and 8. Fig. 7 shows the equilibrium positions for a pileup of 20 walls of edge dislocations as a function of the relative size of l/h. It is seen that the distribution becomes more uniform upon increasing l/h. This arises from the decreasing repulsion between walls. Fig. 8 shows the stress required to maintain n walls of edge dis-

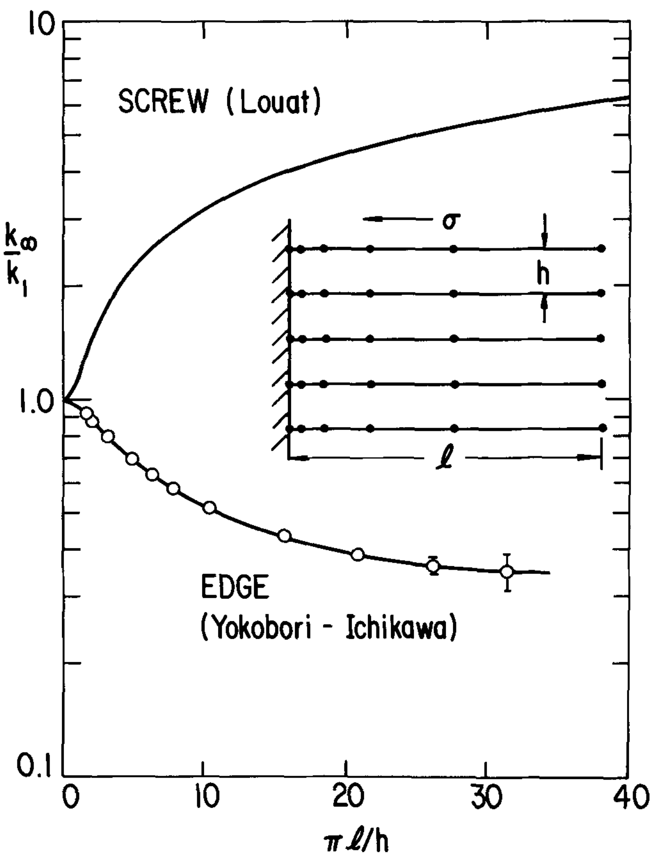

Fig. 4—Effect of multiple-layer pileups on the Hall-Petch slope.

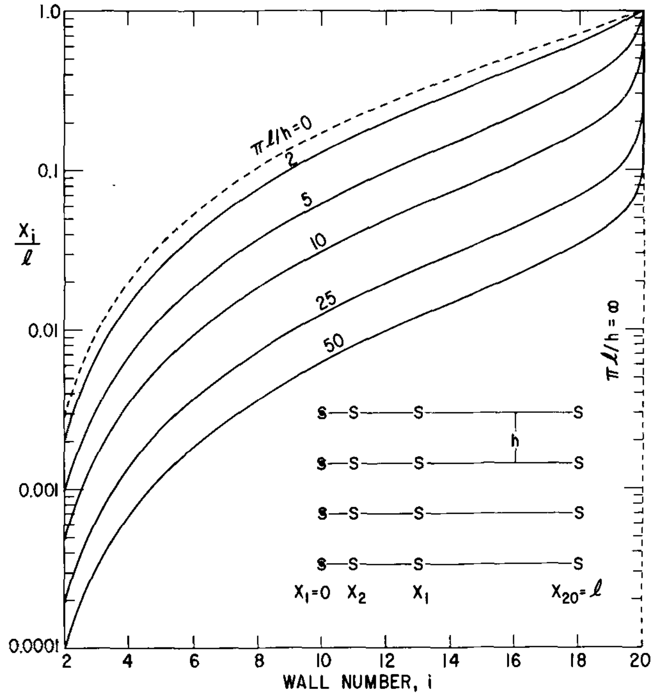

Fig. 5—Equilibrium positions in a pileup of twenty walls of screw dislocations.

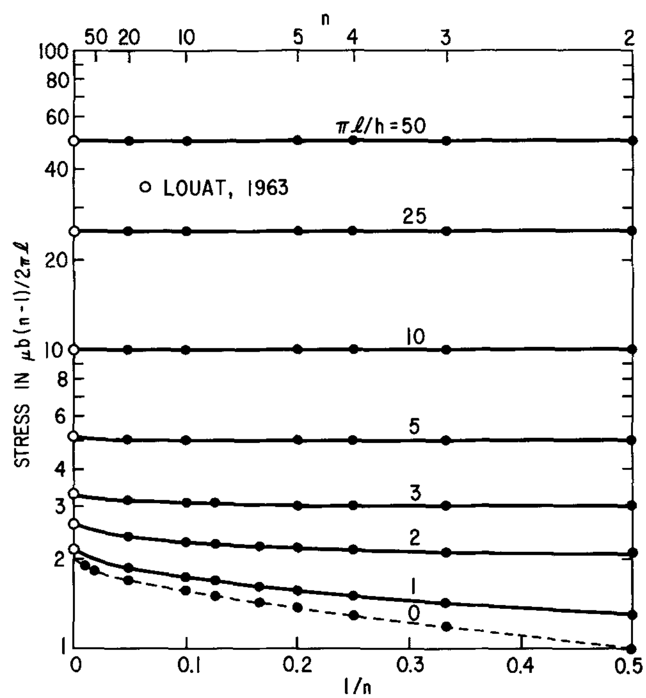

Fig. 6—Stress to maintain a pileup of n walls of screw dislocations.

locations. When $n \to \infty$, the results agree with those of Yokobori and Ichikawa[40] for the continuous distribution of dislocations.

1.4.2) *Double-Ended Pileups.* a) *Continuous distribution of screw dislocation walls.* Infinite layers of identical double-ended pileups of screw dislocations between $x = -a$ and $+a$ and of a uniform spacing h between layers were investigated by Louat.[42] He obtained the following distribution function:

$$f(x) = \frac{2\sigma}{\mu \mathbf{b}} \frac{\sinh(\pi x/h)}{[\sinh^2(\pi a/h) - \sinh^2(\pi x/h)]^{1/2}} \quad [69]$$

which is given also by Smith.[46] The number of dislocations in each half layer is given by Smith:[46]

$$n = \int_0^a f(x)dx = \frac{2\sigma h}{\mu \mathbf{b} \pi} \tan^{-1} \sinh \frac{\pi a}{h} \quad [70]$$

It is seen that n decreases with decreasing h and hence the Hall-Petch slope increases with increasing a/h.

The distribution of screw dislocation walls in anisotropic media is given by Chou.[47] Chou and Barnett[48] studied pileups of screw dislocation walls against a second phase.

b) *Continuous distribution of edge dislocation walls.* Infinite layers of identical double-ended pileups of edge dislocations between $x = -a$ and $+a$ and of a uniform spacing h between layers were examined by Smith[46] for the case of $a < h$. The integral equation is approximated by expanding the distribution function into a power series of a/h, with the following result

$$f(x) = \frac{2\sigma(1-\nu)}{\mu \mathbf{b}} \frac{x}{\sqrt{a^2 - x^2}} \left(1 + \frac{\pi^2 a^2}{6h^2} + \cdots\right) \quad [71]$$

$$n = \int_0^a f(x)dx = \frac{2(1-\nu)\sigma a}{\mu \mathbf{b}} \left(1 + \frac{\pi^2 a^2}{6h^2} + \cdots\right) \quad [72]$$

It is seen that n increases with decreasing h, contrary to the results of screw dislocation walls. The Hall-Petch slope decreases with increasing a/h in this case.

2) NONPILEUP THEORIES OF YIELDING

Several considerations lead one to question the general applicability of the pileup model for yielding.

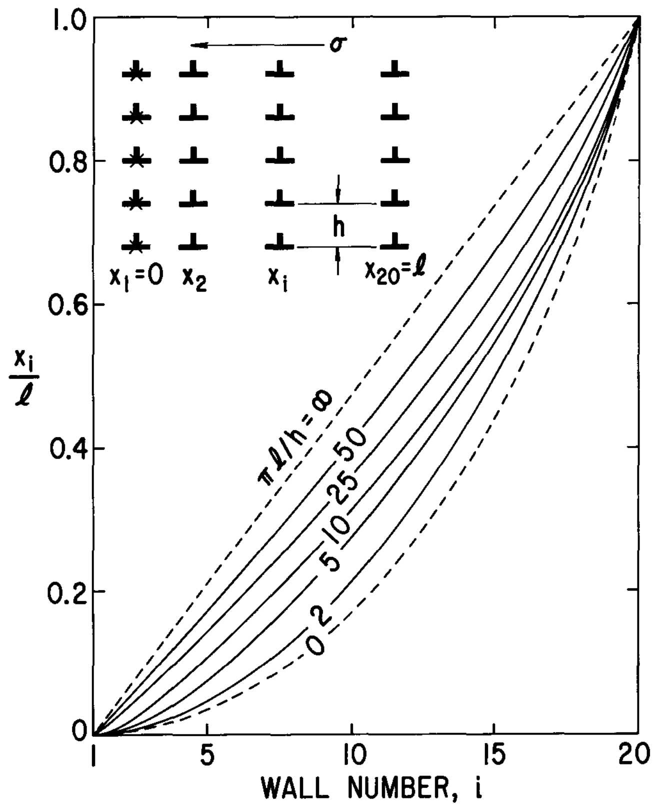

Fig. 7—Equilibrium position in a pileup of twenty walls of edge dislocations.

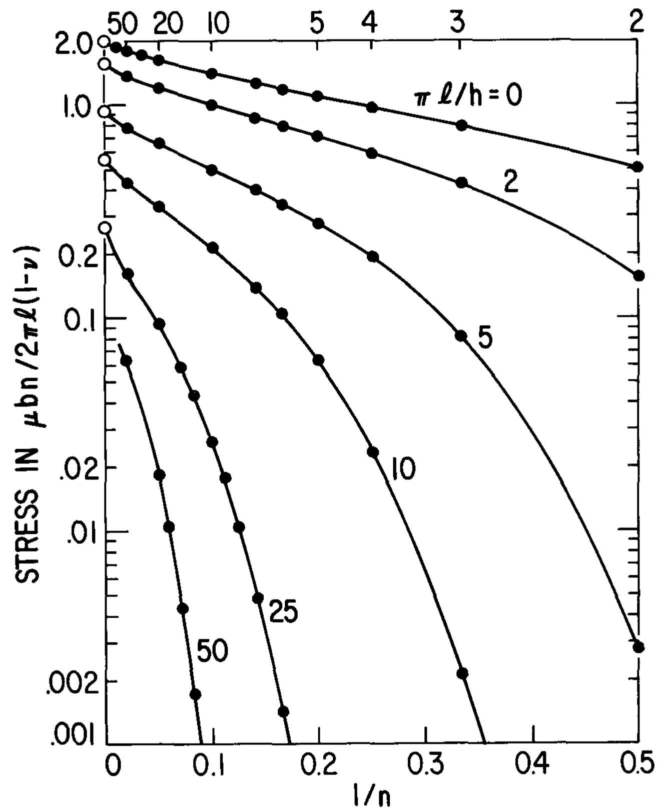

Fig. 8—Stress to maintain a pileup of n walls of edge dislocations.

The first is the lack of direct observation of pileups in pure metals although pileups are seen in alloys of low stacking fault energy or of long range order. Yet the Hall-Petch relation is found valid in both pure metals and alloys. In fact, Ku, McEvily, and Johnston[49] examined the Hall-Petch slopes in copper and its alloys as a function of stacking fault energy and found that the Hall-Petch slopes have one value when pileups are not observed and increase to a higher value when the pileups are observed. Such increase is not easily understood in terms of solute pinning of dislocations or of grain boundaries. Secondly, Worthington and Smith[50] found that in Fe-3 pct Si, dislocations are emitted from grain boundaries at stresses much below the yield stress without the help of pileups and that these stresses do not seem to depend on grain size. According to the pileup model for yielding, the function of the pileup is to create a stress concentration at the grain boundary so as to activate dislocation sources. If these dislocation sources can be activated without a pileup and at stresses below the yield stress, the function or the usefulness of the pileup is then lost. Motivated by these considerations, theories without the use of pileups have been proposed and some of them are reviewed here.

2.1) Work Hardening Theories. In this class of theories pileups are disregarded and a linear relation between yield or flow stress and the square root of dislocation density is taken as an established experimental fact:

$$\sigma = \sigma^* + \alpha\mu\mathbf{b}\sqrt{\rho} \quad [73]$$

where σ is one half of the tensile yield or flow stress,

ρ is average dislocation density, and α is about 0.4 according to Keh[51] for iron. The value of α would be different if a different Taylor factor (see Wilson and Chapman[52] and Worthington and Smith[53]) is used and/or a forest density is preferred instead of the average density for dislocations. The essence of the work hardening model is that the average distance of slip of dislocations, $\bar{x}$, is proportional to the grain size, l:

$$\bar{x} = \beta l \qquad [74]$$

Since the plastic strain is given by

$$\epsilon = \rho \mathbf{b} \bar{x} \qquad [75]$$

the total dislocation density could be calculated by assuming that all the dislocations remain in the system:

$$\rho = \epsilon/\mathbf{b}\bar{x} = \epsilon/\mathbf{b}\beta l \qquad [76]$$

Substituting Eq. [76] into Eq. [73] gives

$$\sigma = \sigma^* + \alpha\mu\mathbf{b}\sqrt{\epsilon/\mathbf{b}\beta}\, l^{-1/2} \qquad [77]$$

which is a Hall-Petch relation with the following slope

$$k = \alpha\mu\mathbf{b}\sqrt{\epsilon}/\sqrt{\mathbf{b}\beta} \qquad [78]$$

The model or its equivalent seems to have been proposed by many people including Louat as quoted by Marcinkowski and Fisher,[54] Meakin and Petch,[55] and Conrad.[56] Although no quantitative treatment was attempted, Johnson[57] seemed to be the first to suggest that $kd^{-1/2}$ could be due to work hardening.

2.1.1) *Supporting Evidences and Limitations.* Since Eq. [77] demands a parabolic stress-strain curve, the work hardening model of yielding is applicable only to those systems possessing such stress-strain behavior. Such behavior is found in niobium (columbium) by Conrad, Feuerstein, and Rice.[58,59] They showed that the flow stress is linear with the square root of strain as required by Eq. [77] with a constant intercept, except for the case in which the grain size is larger than the specimen thickness. They showed further that the dislocation density is linear with strain as required by Eq. [76] with a small intercept which they believe to be the density after recrystallization and before deformation. These observations do imply the validity of Eq. [74] which is the fundamental hypothesis of this model.

On the other hand, in Fe-Co alloys, Marcinkowski and Fisher[54] did not observe a linear relation between the Hall-Petch slope and the square root of strain as required by Eq. [78]. Neither did they observe a strain-independent σ^* as suggested by Eq. [77]. Contrary to Eq. [78] the Hall-Petch slope was found to decrease with strain by Carreker and Hibbard[60] for copper, by Carreker[61] for silver, by Carreker and Hibbard[62] for aluminum, and by Ohba[63] for iron. In almost all the cases, the intercept σ^* was found to increase with strain, contrary to Eq. [77]. Also inconsistent with Eq. [76], Dingley and McLean[64] found for iron that the net rate of increase of dislocation density is greater at the beginning of straining than later on. All the foregoing observations are not in support of the work hardening model of yielding. A demonstration of the validity of Eq. [73] is only relevant to the theory of work hardening and not to that of yielding.

2.1.2) *Other Considerations.* Instead of Eq. [74], nonlinear relations between the average distance of slip and the grain size have been proposed by Conrad[65,66] and by Conrad and Christ.[67] Such relations, when combined with Eqs. [73] and [75] would invalidate the Hall-Petch relationship. The data collected by Conrad[65] for iron and steel in an attempt to show a linear relation between stress and $\sqrt{\epsilon}\, l^{-1/4}$ actually showed curvature in almost all cases.

The effect of plastic strain on the Hall-Petch slope was discussed also by Li[68] using a kinetic equation for dislocation density as proposed by Johnston and Gilman[69] to include dynamic recovery. It was found that without recovery, the Hall-Petch slope increases with strain but the intercept σ^* remains unchanged. However, with recovery, the Hall-Petch slope may decrease with strain and the intercept may increase depending on the relative rates of work hardening and recovery.

2.2) Grain Boundary Source Theories. In this class of theories, grain boundaries are assumed to act as sources of dislocations. Their capacity to emit dislocations may change with the structure and composition of the grain boundary but is independent of grain size. Let m be the total length of dislocations emitted per unit area of grain boundary at the time of yielding. Then the density of dislocations at the time of yielding is, for a spherical grain:

$$\rho = \tfrac{1}{2}(\pi l^2 m)/\tfrac{1}{6}\pi l^3 = 3m/l \qquad [79]$$

where the factor $\frac{1}{2}$ arises from the fact that each boundary is shared by two grains. Substituting Eq. [79] into Eq. [73] gives

$$\sigma = \sigma^* + \alpha\mu\mathbf{b}\sqrt{3m}\, l^{-1/2} \qquad [80]$$

which is a Hall-Petch relation with the following slope:

$$k = \alpha\mu\mathbf{b}\sqrt{3m} \qquad [81]$$

The original version was proposed by Li[68] with a slightly different k. A similar version was proposed by Crussard.[70,71]

2.2.1) *Evidences of Grain Boundary Sources.* Eq. [81] does not contain plastic strain and hence this theory is not considered as a work hardening theory although Eq. [73] is still accepted as an established experimental fact. The theory does depend, however, on the assumption that grain boundaries can act as dislocation sources. Hornbogen[72] has shown a clear example of dislocation loops emitted from grain boundaries in an Fe-3.17 at. pct P alloy although whether such emission is caused by a pileup is not known. More recently Carrington and McLean[73] observed slip lines originating at grain boundaries in Fe-3 pct Si at stresses between σ^* and the lower yield stress. They concluded the following: 1) The observed percentage of yielded grains as a function of stress did not agree with a relation calculated by Suits and Chalmers[74] based on uniform distribution of sources inside the grains. 2) About 95 pct of all the slip lines which did not completely cross a grain are in contact with a grain boundary at one end. 3) Typically there are slip lines only on one side of the grain boundary in the early stages of yielding. Similar results were observed by Worthington and Smith.[50] All these seem to confirm the suggestion that grain boundaries can act as dislocation sources without the stress concentration created by a pileup.

2.2.2) *Observation of Grain Boundary Ledges.* The next question is how a grain boundary can act as a dislocation source. The original suggestion was made by Mott[75] and later independently by Li[76] based on a picture of a grain boundary structure taken by Keh.[51] The dislocation-like images in the grain boundary were suggested[76] as ledges which were supposedly to act as dislocation donors. The fact that a ledge can actually become a dislocation is first indicated by a picture taken by Swann[76] showing a dislocation partly in the grain and partly in the grain boundary as a ledge. Further electron microscopic observations of ledges in grain boundaries were made by many people including Fisher *et al.*[77] in iron, Weissmann[76] in tungsten, Lin and McLean[78] in nickel, Ishida and Brown[79] and Ishida *et al.*[80] in Fe-0.75 pct Mn alloy, and Wilson[81] and Hook[82] in steels. Fig. 9 shows a picture taken by Goodrich[83] indicating, probably for the first time, the coexistence of positive and negative ledges in a grain boundary. The possibility of dislocation-ledge interconversion was shown also by Ishida and Brown.[79] Direct observation of ledges in the field ion microscope was reported by Ryan and Suiter.[84,85] Some considerations of the interaction of dislocations with high angle boundaries are given recently by Brandon.[86] Hook and Hirth[87] called attention to the effect of both elastic and plastic compatibility stresses at the grain boundaries. While undoubtedly these stresses could contribute to the operation of grain boundary sources, the plastic part which depends on grain size is a result of plastic strain and hence depends on the availability of grain boundary sources. In other words, grain boundary sources still may be the controlling factor.

2.2.3) *Effects of Quenching and Annealing*. The foregoing observations indicate that the ability of a grain boundary to emit dislocations could be related to the density of ledges in the grain boundary. The next question is what factors may affect the ledge density. An earlier thought[68] was that both the annealing temperature and the solute concentration could affect the density of ledges in the grain boundary. It was based on the hypothesis that segregation of solute atoms onto the grain boundary may help to stabilize the ledge structure and thereby increase the ledge density in

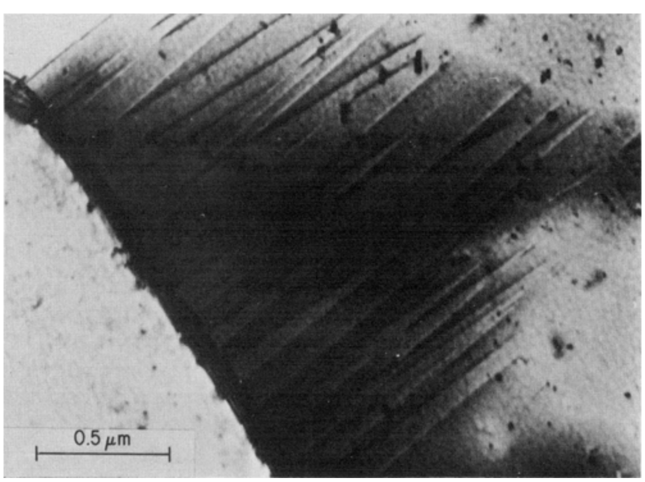

Fig. 9—Positive and negative ledges in a grain boundary. (Aluminum-killed steel, annealed and temper rolled, courtesy of Robert S. Goodrich, Materials Science Division, Vanderbilt University.)

the boundary. Several experiments have shed light on this question: Cottrell and Fisher[88] found that quenched iron (10 ppm C and N) had a smaller Hall-Petch slope than furnace cooled. Aging at 140°C after quenching increased the Hall-Petch slope. Dingley and McLean[64] examined the Hall-Petch slope of iron (70 ppm C and N) as a function of test temperature and found a maximum around 450°K. Wilson[81] studied the effect of aging at 90°C after quenching on the Hall-Petch slope and concluded from the time required to reach the slowly cooled value that the effect was caused by the diffusion of carbon onto the grain boundaries. If Wilson's interpretation was correct, aging would reduce the carbon concentration in the lattice. Based on the work hardening theory of yielding, aging should increase β in Eq. [74] and thereby decrease k in Eq. [78] contrary to Wilson's finding. However, the effect of aging could be understood if diffusion of carbon onto the grain boundary increased the ledge density in the boundary.

Evidences for the segregation of solute atoms onto grain boundaries have been reviewed by Westbrook.[89] Many studies showed that solute atoms can diffuse onto grain boundaries during aging. Floreen and Westbrook[90] reported that microhardness of grain boundaries increases with the time of aging at 200°C in a quenched Ni-6 ppm S alloy until a saturation value is reached. Similar behavior is observed by Seybolt and Westbrook[91] in Ni-Ga containing oxygen, and by Braunovic *et al.*[92] in an Fe-0.002 at. pct W alloy.

Recent results of Ohba,[63] on the effects of quenching on the Hall-Petch slope for iron, seem to differ from those of Cottrell and Fisher,[88] of Dingley and McLean,[64] and of Wilson.[81] The trouble may be traced to the fact that Ohba prepared specimens of different grain sizes by recrystallizing at and quenching from different temperatures. Hook[82] corrected Ohba's data by using the known effects of quenching and showed that the corrected results agree with those of previous workers.

In his studies of quenching and aging on the lower yield and Lüders strain in steels, Hook[82] found that quenched samples contain many dislocations (10^9 per sq cm) but furnace-cooled ones contain none. While undoubtedly these dislocations may affect the inhomogeneity of yielding and Lüders strain, the available amount of information seems insufficient to formulate a theory for the grain size effect based on the number and arrangement of these dislocations. Hook[82] reported further that the ledge density in the grain boundary seemed to decrease upon annealing. It is to be noted that when the ledge density is too high, the individual contrast of ledges is smeared, as shown by Ishida *et al.*[80]

2.2.4) *Effects of Neutron Irradiation*. Another factor which may affect the ledge density is neutron irradiation. Chow and McRickard[93] found in Fe-C alloys that irradiation reduced the Hall-Petch slope and increased σ^*. The latter effect was expected because irradiation introduced vacancies and interstitials into the lattice. Interaction between carbon and vacancies[94] could reduce the activity of carbon and thereby cause desorption of carbon from the grain boundary. Such desorption then could reduce the ledge density and hence the Hall-Petch slope. For higher carbon concentration, the change of Hall-Petch slope was smaller for the same neutron dose, or larger neutron doses were needed to produce the same change in the Hall-Petch slope as found by Chow and McRickard,[93] all to be expected from the foregoing considerations. The results of Hull and Mogford[95] on high carbon alloys also can be explained on this basis.

2.2.5) *Effects of Pressurization.* Pressurization may be yet another factor which affects ledge density in the grain boundary. Yajima and Ishii[96] found that the Hall-Petch slope decreases after pressurization. They found also that pressurization creates new dislocations around oxide particles. These new dislocations could interact with carbon in the lattice, reduce the carbon activity, cause carbon desorption from the grain boundary, reduce the ledge density there, and thereby reduce the Hall-Petch slope. These considerations are supported by the fact that the effect of pressurization is prominent only if enough oxides (600 ppm O) are there to create sufficient dislocations. A smaller amount (200 ppm O) of oxides produces a small effect and a still smaller amount (68 ppm O) produces no effect. On the other hand, Yajima and Ishii[96] suggested that the new dislocations are the main reason for the reduced Hall-Petch slope. By assuming that the density of mobile dislocations is a constant fraction of the total dislocation density, they obtained a relation between the Hall-Petch slope, the Lüders strain, and the initial dislocation density. The $kd^{-1/2}$ term is attributed to the effective stress which determines the average velocity of dislocations based on a relation suggested by Gilman.[97] While the new dislocations introduced by pressurization may affect yielding in many ways, it is difficult to believe that they play a direct role in the lower yield stress-grain size relationship.

2.2.6) *Effects of Temperature and Strain Rate.* According to Eq. [81], the Hall-Petch slope should not change with test temperature unless the temperature is such that it changes the ledge density in the grain boundary or it alters α by changing the dislocation arrangement. For iron, Petch[98] found that k is virtually independent of temperature between 18° and −79°C; Conrad and Schoeck[99] reported a similar finding between 110° and 300°K. However, at 77°K, Hull and Mogford[95] found a higher k, probably because of a larger α due to a different dislocation arrangement, as shown by Keh.[51] At higher temperatures, Dingley and McLean[64] found that k decreases in the temperature range 300° to 600°K except for a hump between 400° and 500°K; Brindley and Barnby[100] found a similar behavior. For niobium, the value of k is small at all temperatures and within experimental error, it is insensitive to temperature between 76° and 293°K as found by Johnson,[101] and Churchman,[102] and Adams *et al.*[103] In chromium, Marcinkowski and Lipsitt[104] found that k is independent of temperature between −150° and 97°C. In magnesium, Hanser *et al.*[105] found that k decreases from 78° to 473°K and Wilson and Chapman[52] found that it decreases from 78° to 290°K. Similar results are found by Hauser *et al.*[105] in Mg-2 pct Al alloys. In all cases σ^* decreases with increasing temperature except when strain aging occurs.

Also according to Eq. [81], the Hall-Petch slope should not change with strain rate unless it alters α by changing the dislocation arrangement. Heslop and Petch[106] found that k in iron at −79°C is independent of strain rate between 2×10^{-3} and 10^{-6} per sec. Campbell and Harding[107] found in both iron and steel, that k is independent of the mean strain rate at 10^{-3}, 960, and 2600 per sec by impact testing at room temperature. In all cases σ^* increases with strain rate as expected.

2.2.7) *Other Considerations.* Some results on Fe-Ti alloys by Castagna *et al.*[108] indicate that the Hall-Petch slope is greatly reduced (~20 pct of the usual value) by as little as 0.04 pct Ti addition. This is consistent with the grain boundary source model by considering that the addition of titanium reduces interstitial segregation onto the grain boundaries.

Gouzou[109] proposed a theory of yielding also based on grain boundary sources. Unfortunately his theory involved an assumption that the yield stress required to emit dislocations from the grain boundary was to supply the interaction energy between solute atoms and grain boundary dislocations by moving the dislocation a distance which is proportional to the grain size. The validity of this assumption is not obvious. As mentioned earlier, Worthington and Smith[50] observed dislocation emission from grain boundaries at stresses much below the lower yield stress independent of grain size. Obviously the stress necessary for emitting dislocations from grain boundaries is not the stress required for yielding.

Cottrell and Fisher[88] also used the concept of grain boundary sources but required stress concentration at the end of a pileup as did Dingley and McLean.[64] These should be classified as pileup theories of yielding.

2.3) Dislocation Dynamics Theories. Both the work hardening theory and the grain boundary source theory suggest that at low temperatures $kd^{-1/2}$ is the athermal part of the flow stress due to dislocations. The other part σ^* consists of the thermal part σ^{**} and the athermal part σ_s of other origin such as precipitates. Let $\bar{v}$ be the average velocity of all the mobile dislocations and let the stress dependence of $\bar{v}$ be given by[69]

$$\bar{v} = B(\sigma^{**})^{m^*} \tag{82}$$

where B and m^* may depend on temperature. Then

$$\sigma = \sigma_s + kd^{-1/2} + (\bar{v}/B)^{1/m^*} \tag{83}$$

The quantity σ^{**} is also known as the effective stress which is approximately equal to the difference between the applied stress and the internal stress.[110] The athermal part $\sigma_s + kd^{-1/2}$ should depend on temperature only as the shear modulus, provided that the structure is independent of temperature.

2.3.1) *The Problem of Strain Rate in Inhomogeneous Deformation.* A question often being asked is "what is the strain rate in inhomogeneous deformation?" The answer is really very simple: it depends on the definition of the density of mobile dislocation. The essence of dislocation theory is that no deformation is homogeneous on the microscale. Whether all the mobile dislocations are uniformly distributed on a macroscopic scale, or concentrated at the Lüders front will not affect the elongation rate of the specimen provided that they have the same average velocity. Hence, if the strain rate is the elongation rate divided by the gage length, the dislocation density is the total length of dislocations divided by the volume of the specimen independent of the distribution of these dislocations. On the other hand, if one insists that the density of mobile dislocations should be defined as the local one at the Lüders front, the strain rate is then defined likewise. However, one then has to know the strain profile at the Lüders front.

Thus, the strain rate amplification suggested by Gokyu and Kihara[111] is not really needed. However, if the number of mobile dislocations associated with each Lüders front is independent of the number of Lüders fronts, the average velocity $\bar{v}$ of these dislocations is inversely proportional to the number of Lüders fronts for the same elongation rate of the specimen as suggested correctly by Gokyu and Kihara and earlier by Butler.[112] Gokyu and Kihara suggested further that the strain rate amplification is inversely proportional to the grain size. What they really suggested was that $\bar{v}$ is inversely proportional to the grain size, or that σ^{**} decreases with increasing grain size. Qualitatively it follows that the activation area,[110] $kT(\partial \ln \dot{\epsilon}/\partial\sigma^{**})$, increases, or the strain rate sensitivity decreases with increasing grain size, as indeed observed by Gokyu and Kihara.[111]

2.3.2) *The Problem of Stress in Inhomogeneous Deformation.* Another problem in inhomogeneous deformation is that a specimen has at least two cross sectional areas. Which area should be used in calculating the lower yield stress? Based on the pileup theory or the grain boundary source theory, the stress should be that immediately behind the Lüders front. The area to use is then the area of the undeformed region. On the other hand, based on the work hardening theory, the stress is that of the strained region; the same strain should be used for all grain sizes.

To apply dislocation dynamics, the applied stress varies from the strained region to the unstrained region according to the strain profile:

$$\sigma = \sigma_0 \exp \epsilon \qquad [84]$$

where σ_0 is the stress at zero strain. Let the velocity of a Lüders front be v_L, the local strain rate at any point is

$$\dot{\epsilon} = v_L \frac{d\epsilon}{dx} = \rho_m \mathbf{b} B(\sigma - \sigma_i)^{m^*} \qquad [85]$$

where x is in the direction of propagation, ρ_m is the local density of mobile dislocations, and σ_i is internal stresses of all origins. The elastic strain rate is neglected. Hahn[113] seems to be the first to apply dislocation dynamics to inhomogeneous deformation. He integrated Eq. [85] to obtain a strain profile by making the following assumptions: 1) ρ_m is a constant fraction of the total dislocation density ρ which is linear with a single power of strain. 2) The internal stress is proportional to strain. With proper choice of parameters, the calculated profiles indeed resemble the experimental ones.

The average dislocation velocity in Eq. [83] can be obtained from Eq. [85]:

$$\bar{v} = \frac{\int(\dot{\epsilon}/\rho_m \mathbf{b})\rho_m A dx}{\int \rho_m A dx} = \frac{A_0 v_L}{bL}(1 - e^{-\epsilon_L}) \simeq \frac{A_0 \dot{x}}{\mathbf{b}L} \qquad [86]$$

where A is local cross sectional area, A_0 is A at $\epsilon = 0$, ϵ_L is Lüders strain, L is the total length of mobile dislocations, and $\dot{x}$ is the cross head speed, which is equal to $v_L \epsilon_L$. Eq. [86] suggests that the velocity of Lüders front or the cross head speed can be used to approximate the average velocity of mobile dislocations if L can be assumed to be nearly constant. It suggests also that if one knows $\bar{v}$ by other means, L can be calculated.

Eq. [86] suggests that the stress σ at which $\dot{x} = 0$ is given by

$$\int(\sigma - \sigma_i)^{m^*} \rho_m A dx = 0 \qquad [87]$$

where the sign of $(\sigma - \sigma_i)^{m^*}$ is that of $\sigma - \sigma_i$, no matter what m^* is. This stress is an average internal stress, as can be seen for $m^* = 1$:

$$\bar{\sigma}_i = \frac{\int \sigma_i \rho_m A dx}{\int \rho_m A dx} \qquad [88]$$

and can be determined experimentally such as in a stress relaxation test. On the other hand, Eq. [83] shows that the internal stress is equal to $\sigma_s + kd^{-1/2}$. These problems are being studied by Prewo.[114]

2.3.3) *The Stress Dependence of Lüders Band Velocity.* Prewo[114] found that the average internal stress during the propagation of a Lüders band in polycrystalline iron obtained by a stress relaxation technique[115] is independent of the velocity of the Lüders band, the Lüders strain, or the applied stress but depends on material variables such as grain size and carbon content. However, the Lüders band velocity is a simple power function of effective stress with an exponent of 3.5 at 300°K, 5.5 at 243°K, 7.5 at 213°K, and 10 at 183°K, independent of carbon content or heat treatment. During stress relaxation, the Lüders band is found to propagate further at a rate and to the extent predictable from dislocation dynamics.

3) SUMMARY AND CONCLUSIONS

It is seen from this review that calculations on pileups of dislocations are quite extensive. However, the following are still lacking: 1) analytical solutions for discrete dislocations in double-ended, circular, elliptical, or multilayer pileups, 2) analytical solutions for continuous distribution of dislocations of infinitesimal Burgers vectors in double-layer and triple-layer pileups, and in infinite-layer pileups of circular or edge dislocations, and 3) numerical results for discrete dislocations in double layer or triple-layer pileups. The significance of these calculations has diminished considerably because of the lack of direct observation of these pileups in many systems. Even for alloys in which dislocations do tend to stay on their slip planes, grain boundaries seem to act as dislocation sources without the help of pileups. These and other observations give rise to serious doubt of the validity of the pileup model of yielding as a fundamental mechanism.

It is indeed disappointing that simple arrangements of dislocation pileups are not sufficient to understand yielding. Nonpileup models are still vague in their details. Among them the work hardening model demands a dislocation density-strain relationship which is valid only for certain systems. It has no provision for the understanding of Lüders strain nor the effect of grain boundary structure. The grain boundary source model avoids these difficulties by introducing the concept of source density in the grain boundary. Although there are numerous observations of grain boundary ledges, dislocation emission from these ledges, and indirect evidence of how the ledge density can be changed by heat treatment, pressurization, and neutron irradiation, direct quantitative determination of source density in the grain boundary is still lacking. After dislocations are emitted from grain boundaries, they immediately interact with each other and move according to the stress dependence of dislocation velocity. It seems unavoidable that the Lüders front velocity and the strain profile must be understood from the dynamics of dislocations. Experiments along these lines are needed to shed light on the mechanistic details of yielding.

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