60 Years of Hall-Petch: Past to Present Nano-Scale Connections

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Pioneering research results reported in the early 1950’s by E. O. Hall and N. J. Petch on iron and steel materials have led to an expanded description of the grain size dependence of the yield stress at ambient temperature and of the yield and cleavage fracture stresses at low temperatures, both with investigators employing the same relationship

\[ \sigma = \sigma_0 + k \ell^{-1/2}. \]  

In eq. (1), \( \ell \) is the average polycrystal grain diameter and \( \sigma_0 \) was specified as the friction resistance for dislocation movement within the polycrystalline grains while \( k \) was described as a measure of the local stress needed at a grain boundary for transmission of plastic flow (\( k_y \)) or, at the lower temperature, for cleavage fracturing (\( k_C \)). Different values of friction stress, \( \sigma_{0y} \) or \( \sigma_{0C} \), applied for yielding or cleavage. The dislocation pile-up model of Eshelby, Frank and Nabarro has been employed at the tip of a blocked slip band was employed also both by Hall and Petch to explain eq. (1).

During subsequent years, Hall pointed out that the hardness of metals followed an analogous grain size dependence to that observed for the yield stress, with constants \( H_0 \) and \( k_{H0} \) and summarized in a book his researches on the yield point behavior and on related subsequent serrated plastic flow behavior observed in stress-strain curves. Petch, with a number of students and colleagues, took up several related topics, first, of the dependencies on steel compositions and heat treatments of the \( \sigma_0 \) and \( k \) parameters obtained from eq. (1) and, then with Cottrell, showed extension of the grain size dependent relationship to other material properties such as the ductile-brittle transition in steel and, much later with Armstrong, to the fracture toughness properties of a number of steel materials.

The present report carries on this theme of development of Hall-Petch results with a description in roughly chronological order of the following topics:

- The Cottrell-Petch theory for the ductile-brittle transition properties of steel and related bcc metals and alloys and extension to fracture mechanics.
- Application of the H-P analysis to describing the full stress-strain behavior of mild steel and to the yield behavior of other engineering materials.
- An H-P dependence for other material properties, such as hardness, fatigue and low-temperature creep.
- Relation of the H-P microstructural stress intensity, \( k_n \), to the Griffith theory and to fracture mechanics.
- An H-P based interpretation of hot spots and shear banding produced by dislocation pile-up avalanches.
- Thermal-activation in \( k_t \) for needed prism or pyramidal slip at hcp grain boundaries and for cross-slip at fcc grain boundaries.
- An H-P explanation of the strength and strain rate sensitivity of nanocrystals, including an H-P reversal at limiting smallest nanometer-scale grain sizes.
- Reduction in \( k_t \) for disordered grain boundaries.

2. The Cottrell-Petch Theory for the Ductile to Brittle Transition

A first successful application of the H-P equations for yielding and cleavage fracture was to description of the transition in brittleness exhibited at low temperatures and/or high loading rates by steel and related body-centered cubic (bcc) metals. Cottrell obtained an implicit description of the ductile-brittle transition temperature (dbtt) occurring in terms of the grain size, \( \ell \) and H-P yield stress parameters, \( \sigma_{0y} \) and \( k_y \), in the relationship

\[ k_y (\sigma_{0y} \ell^{1/2} + k_y) = CG\gamma \]  

On the right side of eq. (1), \( G \) is the shear modulus, \( \gamma \) is the cleavage crack surface energy and \( C \) is a numerical constant. Thus by increasing \( k_y \), \( \sigma_{0y} \), or \( \ell \), the condition would be met more quickly for cleavage cracking and failure to occur. Hull and Mogford reported an increase in the dbtt produced...
by an increase in $\sigma_{0y}$ from neutron irradiation damage, thus raising the magnitude of the left-side of eq. (2) and promoting brittleness.

Petch obtained an explicit temperature dependence of the dbtt. The temperature dependent component of the friction stress, was employed with a stress coefficient, $B$ and exponential temperature coefficient, $\beta$. Petch also had presented evidence earlier that the true ductile fracture stress followed an analogous grain size dependence with constants, $\sigma_{0d}$ and $k_*$. On such basis, an equation was obtained for $T_C$ as:

$$T_C = (1/\beta)\ln B - \ln((CG\gamma/k_* - k_*) - \ln \epsilon^{-1/2}) \quad (3)$$

In eq. (3), $B$ is the limiting value of the temperature dependent component of the friction stress at temperature, $T = 0$ and $\beta$ is the exponential temperature coefficient that is smaller at greater strain rate.

Figure 1 provides an illustration produced at the U.S. Oak Ridge National Laboratory of the dbtt behavior as obtained on the basis of computed tensile test results applicable to grain size and neutron irradiation hardening. In the figure, a comparison is made between the temperature dependences of the yield and cleavage fracture stresses of two annealed mild steel materials, “A” having a conventional grain size of $\sim 100 \mu$m and “B” having a grain size of $\sim 5 \mu$m. In addition, the yield stress is shown to be raised after neutron irradiation hardening of steel “A”, now labeled “A*”, but for which its cleavage stress is unchanged. As indicated in the figure, steel A has a lower dbtt because of the H-P inequality: $k_C > k_p$. And steel “A*” has an appreciably raised dbtt due to addition of the athermal component $\Delta\sigma_{0y}$ to $\sigma_{0y}$, in the manner described by Hull and Mogford, thus raising the ambient temperature yield strength up to that of steel “B”. The danger indicated in the figure, which was deemed important at the time, was that steels “B” and “A*” could have the same ambient yield strengths and temperature dependencies of them while exhibiting appreciably different values of the dbtt.

A historical note is that Orowan had drawn attention to the condition of the yield stress being raised to the level of the cleavage fracture stress as a criterion for the onset of brittleness in steel; and, this consideration, taken together with a plastic constraint factor for the notch in a Charpy impact test, provided for a quantitative description of the dbtt in the same vein as described by Cottrell and Petch. Wessel reported at ICF1 (see Section 6), in Sendai, on the correlation of changes in $T_C$ associated with changes in $\sigma_{0y}$ and $k_*$ for a structural pressure vessel steel.

3. H-P for the Complete Stress–Strain Behavior of Mild Steel

After establishment of an H-P dependence for the yield stress of iron and steel materials and with successful employment of the H-P parameters in understanding the occurrence of a ductile to brittle transition in steel, particularly as influenced by neutron irradiation hardening, it seemed only natural to inquire about the grain size dependence during the post-yield deformation behavior. Figure 2 shows a compilation of results obtained for two early investigations made on mild steel. Armstrong, Codd, Douthwaite and Petch provided a rational explanation of the $\sigma_{0y}$ and $k_*$ coefficients shown for the yield and flow stress dependencies in Fig. 2. The analysis led to an extended application of the H-P dependence in the relationship

$$\sigma_\epsilon = m[\tau_{0y} + k_{Sc} \epsilon^{-1/2}] \quad (4)$$

In eq. (4), $m$ was designated as a Taylor type orientation factor for the needed distribution of slip systems within the polycrystal grain volumes, $\tau_{0y}$ was the average resolved shear stress on the slip systems, so giving $m\tau_{0y} = \sigma_{0y}$ and in like manner, $k_{Sc}$ was proposed to apply for the average shear stress concentration at the tip of a slip band, so giving $mk_{Sc}$ in place of $k_*$, A value of $k_{Sc} = \sim 24 \text{MPa} \cdot \text{mm}^{1/2}$ applies for the lower yield point (l.y.p.) results shown in Fig. 2. The
values of $\sigma_{0e}$ at increasing strains were attributed to the influence of dislocation density on determining plastic deformation within the polycrystal grain volumes as was described in the grain size independent plasticity theory of Taylor\textsuperscript{23} while $k_c$ was attributed to the continued need for local stress concentrations to effect transmission of plastic flow across grain boundaries. Additional H-P type measurements were presented in Ref. 10) for copper, $\alpha$-brass, aluminum, aluminum–magnesium alloy, decarburized iron and zinc materials. And a tabulation of $\sigma_{0e}$ and $k_c$ values was given for a greater number of body-centered cubic (bcc), hexagonal close-packed (hcp) and face-centered cubic (fcc) metals and alloys.

In later investigation of the grain size and brittleness aspects of deformations in polycrystal magnesium and beryllium materials, the value of $k_{Se}$ was expressed in terms of the concentrated shear stress on the lead dislocation of a pile-up as\textsuperscript{24}:

$$k_{Se} = [m^*Gb\tau_{C}/2a]^{1/2}$$

(5)

In eq. (5), $m^*$ was identified as a Sachs type orientation factor for the most favorable slip system, $b$ is the dislocation Burgers vector, $\tau_{C}$ is the concentrated shear stress and $a = -0.8$ is an average of screw and edge type factors for a circular dislocation loop. The reported temperature dependencies of $\sigma_{0e}$ and $k_c$ for polycrystal magnesium were shown to follow reported single crystal resolved shear stresses for basal slip ($\sigma_{0b}$) and prism slip ($\tau_{C}$), respectively, thus extending Taylor’s consideration of single crystal and polycrystal strength levels in $\sigma_{0e}$ to single crystal connection and in $\tau_{C}$ to $k_c^2$. Such evaluations of $k_c$ in terms of the concentrated stress on the lead dislocation in a pile-up led to its designation as a microstructural stress intensity, $K$, as will be discussed in a subsequent section.

4. H-P for hcp and fcc Metals and Alloys

There are major differences and some similarities in the H-P dependencies to be described for hcp and fcc metals and their alloys. For the hcp crystal structure, both a relatively high value of $m = \sim 6.5$ is proposed to apply because of the limited orientation dependence of the primary basal slip system until deformation twinning intervenes and, also, a much higher value of $\tau_{C}$ is required for activation of the secondary prismatic or pyramidal slip systems needed to effect accommodation of plastic strains at grain boundaries. Chun and Davies have recently compared the basal, prism and pyramidal slip stresses for magnesium AZ31 alloy material in terms of favoring a material texture involving prism slip for warm rolling of plate material.\textsuperscript{26} In the fcc case, as will be described, a lowest value of $m = 3.1$ applies for the multiple available slip systems and there is need for cross-slip to occur at grain boundaries for transmission of plastic flow. For both crystal structure types, however, there is thermal activation in $k_c$.

4.1 H-P for the hcp case

Figure 3 shows a compilation of H-P results reported for polycrystal magnesium\textsuperscript{27,28} and AZ31 alloy material.\textsuperscript{29–31} The dashed rectangular box of magnesium results contains measurements over a conventional range of grain size for which it had been established that a random crystallographic texture had been achieved. H-P $k_c$ values of $\sim 8.8$ and $\sim 10.8$ MPa·mm$^{1/2}$ had been determined for these measurements in comparison with a computed value of $mk_{Se} = \sim 10.6$ MPa·mm$^{1/2}$ from eqs. (4) and (5) taking a value of $\tau_{C}$ given by prism slip.\textsuperscript{32} Hauser, Landon and Dorn\textsuperscript{33} had reported metallographic observations of such prism slip activity at grain boundary regions in the strained material.

An important increase in $\sigma_{0e}$ and reduction in $k_c$ to $\sim 4.2$ MPa·mm$^{1/2}$ are shown in Fig. 3 for the broader tabulation of measurements for AZ31 materials. The smallest grain size material was obtained by Lee and Chang for material subjected to various conditions of equal channel angular extrusion, ECAP.\textsuperscript{31} Both of the H-P parameters are largely associated with the development of a recrystallized texture of oriented grains favoring prism slip within the material. The consequence is an increase in prism and/or pyramidal slip in $\sigma_{0e}$ and reduction in $m$ in $k_c$ plus involvement in it of basal slip. A lowered value of $m = m^* = \sim 3.7$ would account for the influence of texture alone in reducing $k_c$ for the AZ31 material results. Caceres and Lukace\textsuperscript{34} had proposed that $m = 4.5$ for the magnesium in which case $m = m^* = \sim 2.6$ is obtained and should be taken to indicate that basal slip was playing an important role in the grain boundary straining.

Yuan, Panigrahi, Su and Mishra\textsuperscript{35} have produced for AZ31 material prepared by the ECAP-related equal channel angular pressing (ECAP) method and other processing techniques a tabulation of texture-influenced H-P parameters in line with the results shown in Fig. 3. The H-P results involved grain sizes smaller than $\sim 10$ micrometers and a range in microstructural stress intensities of $5.1 \leq k_c \leq 11.0$ MPa·mm$^{1/2}$. In this connection, it should be mentioned that Wilson and Chapman had established in a pioneering report a range in $k_c$ for textured magnesium materials developed at larger grain sizes and leading to a lowest value of $k_c = \sim 1.6$ MPa·mm$^{1/2}$ for flat bar extruded product.\textsuperscript{36} Related results had been reported by Chapman and Wilson of a strong increase in material ductility as the grain size was
refined even carrying on to demonstration of superplastic flow at the finer grain sizes of a few micrometers.\textsuperscript{37} The results were later incorporated into a compilation of H-P type results for the true fracture strain of conventional and ultrafine grain size magnesium results\textsuperscript{38} beginning from an even earlier pioneering report made by Herenguel and Lacombe.\textsuperscript{39} Koike has reported on ductility, including grain boundary sliding and deformation twinning observations in magnesium alloy materials.\textsuperscript{40} Watanabe, Mukai and Higashi have reported on the threshold stress for superplastic flow of a fine grained magnesium alloy material tested at 473 K and higher temperatures.\textsuperscript{51} Latest results on magnesium are observations of deformation twinning dependence on grain size in Luleders bands produced within inhomogeneous grain size material, by Tsai and Chang,\textsuperscript{42} and of strengthening produced by nano-spaced stacking faults in ultra-strong alloyed magnesium material as part of a cooperative research effort by Jian, Cheng, Xu, Yuan, Tsai, Wang, Koch, Zhu and Mathaudhu.\textsuperscript{43}

4.2 H-P for the fcc case

Great interest in the mechanical properties of newly available aluminum single crystal and polycrystalline material was generated in the first part of the twentieth century. The interest pre-dated the 60 years of H-P based researches. For example, an historical consideration of grain size effects in aluminum, or lack thereof, was an important topic at a 1928 Faraday Society Discussion meeting that featured important participations from Taylor and from Polanyi, both researchers later being co-discoverers of era.

Detailed observations of H-P dependencies for the complete stress–strain behaviors of relatively pure aluminum materials have been reported by Hansen\textsuperscript{49} and by Al-Haidary, Petch and de Los Rios.\textsuperscript{50} Figure 4 shows a log/log compilation of other H-P results reported for aluminum at conventional and nanopolycrystal grain sizes and includes comparison with copper and nickel material results. On a log/log basis, the H-P relation leads at large grain size to a relatively constant value of $\sigma_0$ and, at limiting small grain size, goes over to a linear dependence of slope $-1/2$.

In Fig. 4, the open square\textsuperscript{51}, circle\textsuperscript{52} and triangle\textsuperscript{53} points apply for conventional grain size materials at different proof stress values, thus demonstrating a significant influence of the strain hardening behavior of fcc metals in comparison with the $k_\epsilon \epsilon^{-1/2}$ term. For example, a value of $k_\epsilon = 2.15 \text{MPa} \cdot \text{mm}^{-1/2}$ applies for the nickel material result of Keller and Hug\textsuperscript{53} at the given $\epsilon = 0.14$ whereas a value of $k_\epsilon = 5.17 \text{MPa} \cdot \text{mm}^{-1/2}$ applied at $\epsilon = 0.01$; in the latter case, nearly the same value as that of $k_\epsilon = 5.0 \text{MPa} \cdot \text{mm}^{-1/2}$ corresponding to the open circle copper result of Hansen and Ralph\textsuperscript{52} at $\epsilon = 0.05$. In contrast to the nickel result, $k_\epsilon$ was constant during straining. Other Narutani and Takamura\textsuperscript{54} nickel results to be described with regard to H-P influence on the strain rate sensitivity, showed a constant value of $k_\epsilon$ throughout the stress–strain curve and of value near to that mentioned for $\epsilon = 0.01$. The relatively pure aluminum results of Hansen\textsuperscript{49} and of Al-Haidary \textit{et al.}\textsuperscript{50} showed a relatively constant value of $k_\epsilon = 2.3 \text{MPa} \cdot \text{mm}^{-1/2}$ with straining; and, this strain independence of $k_\epsilon$ seems more often than not to be generally observed.\textsuperscript{10}

The open square aluminum points of Careeker and Hibbard\textsuperscript{51} in Fig. 4 are for relatively less pure material and correspond to a value of $k_\epsilon = 2.3 \text{MPa} \cdot \text{mm}^{-1/2}$. The filled square, smaller grain size results shown from the investigation by Tsuji, Ito, Saito and Minamino\textsuperscript{55} present an interesting case of $k_\epsilon$ increasing first from a value of $\sim 3.5$ to $\sim 4.8 \text{MPa} \cdot \text{mm}^{-1/2}$ for a relatively impure material. These results relate to a follow-up report on the $\epsilon = 0.002$ proof stress of conventional and ultrafine grain size material produced by accumulative roll-bonding (ARB) and annealing, or by cold rolling (CR) and annealing by Kamikawa, Huang, Tsuji and Hansen,\textsuperscript{56} as shown by the open triangle and circle points in Fig. 5. Kamikawa \textit{et al.} tracked the complete stress–strain behaviors for the specimens labeled A to F in the figure. The A to D specimens showed significant H-P type strengthening from the outset of straining and reduced values of uniform elongation associated with rather rapid onset of plastic instability whereas the E and F specimens underwent substantial strain hardening until reaching the plastic instability condition. The filled circle points are plotted in the figure for the true stress at maximum load, $\sigma_{UL} = \sigma_{UTS} [1 + \epsilon_U]$. Thus, $\sigma_{UL}$ is shown to follow a same grain size dependence with $k_\epsilon = 1.3 \text{MPa} \cdot \text{mm}^{-1/2}$ as for the initial yielding behavior of the conventional grain size.

![Fig. 4 H-P compilation for conventional and ultrafine grain size Al, Cu and Ni materials.](image-url)
material. And the finer grain size A to D “ARB + Annealed” materials are indicated to have produced variously increased values of $\sigma_0$, prior to an additional smaller extent of strain hardening before reaching $\sigma_U$.

The preceding aluminum results and those shown in Fig. 4 for the filled circle points for copper compiled in Ref. 57) and the filled triangle point measurements for nickel give indication of approaching an order of magnitude increase in strength level even for fcc metals at nano-scale grain sizes. The reported value of $k_c = \sim 6.2$ MPa·mm$^{1/2}$ for the nano-scale nickel results were obtained as one-third of hardness, $k_{Hc}$ measurements and can be compared with $k_c = \sim 5.0$ MPa·mm$^{1/2}$ for copper. The vertical shift upwards of the nickel points is attributed in part to a relatively larger value of the nickel $\sigma_0 = \sim 300$ MPa, also obtained as one-third of the intercept hardness, $H_0$.

There are important examples of stronger H-P dependencies established for fcc alloy materials, most notably for $\alpha$-brass and aluminum–magnesium alloys, in another report pre-dating Hall-Petch, demonstrated a strong grain size dependence of the flow stress of $\alpha$-brass material and including evidence for yield point behavior. A value of $k_f = \sim 12.6$ MPa·mm$^{1/2}$ applies for the reported yield stress results. Meakin and Petch followed up with demonstration of H-P dependencies for $\sigma_f$ including an increase in $k_f$ with increased straining. Nakanishi and Suzuki produced two important articles on H-P, firstly, on experimental demonstration of H-P dependencies for copper–aluminum and copper–nickel alloys, and, secondly, on a theoretical description of the results. The theoretical model was based on pinning of grain boundaries by solute atoms and the need for dislocation pile-ups to push their leading dislocations into the boundary so as to effect transmission of plastic flow. Armstrong and Douthwaite have reported on compiled H-P results for a number of aluminum–magnesium, aluminum–lithium, the copper–aluminum alloys of Nakanishi and Suzuki and a number of $\alpha$-brass materials. Zhang, Tao and Lu have reported H-P results for ultrafine copper–aluminum materials involving both slip and twinning deformations as affected by stacking fault energy.

5. H-P for the Hardness, Fatigue and Low Temperature Creep Behavior

As mentioned in the Introduction, Hall had pointed out that the hardness might be expected to follow a Hall-Petch dependence (4). Figure 6 shows supporting results for nickel electroplate material extending into the nano-scale regime of grain size. The newly added filled square points for measurements of Torrents et al. are those that have been transformed to flow stress measurements in Fig. 4 by taking $\sigma_f = H/3$. Other H-P type hardness measurements, particularly at ultrafine grain sizes have been compiled recently for chromium, $\alpha$-titanium and tungsten materials by Armstrong and Elkan.

The fatigue behavior of materials involves H-P related grain size effects but their determination and analysis of them are more complicated. Figure 7 provides a schematic view of surface intrusions/extrusions under a cyclically applied shear stress and the corresponding internal dislocation arrangements. An individual slip band stress concentration in one direction is weakened by an oppositely directed pile-up. A dislocation dipole structure is produced as first described in pioneering numerical calculations reported by Head. The closer stress dependence on distance of such dipoles has been associated with a greater number of dislocations being squeezed into a persistent slip band whose intrusion/extrusion behavior leads to cracking.

Hall-Petch measurements for low cycle fatigue stresses have been compiled for $\alpha$-iron, low carbon steel and $\alpha$-brass materials involving consideration at large grain sizes of a specimen size effect and at small grain sizes of a reduced grain size dependence at stresses below the yield stress of the material. Additional confirming H-P dependencies have been shown for the fatigue stress of $\alpha$-brass material at several stress levels.

Figure 8 shows recent results reported by Lukas, Kunz, Navratilova and Bokuvka for the high cycle fatigue behavior of copper material at an ultrafine grain size of 300 nm and a conventional grain size of 60–70 micrometers. The 300 nm material exhibited a 0.1 yield stress of 349 MPa, consistent with results shown in Fig. 4 and ultimate tensile stress of 387 MPa. H-P $k_f$ values of $\sim 1.3$ MPa·mm$^{1/2}$ apply for the
results at $\sim 10^6$ cycles and $\sim 0.9 \text{MPa mm}^{1/2}$ at $\sim 10^9$ cycles. Fatigue cracking in the ultrafine grain size material was observed just underneath the observation of highly localized surface extrusions/intrusions. A mechanism was proposed of dislocation interactions producing atomic vacancies which then migrate along grain boundaries to form cracks.

For Hall-Petch type consideration of strain rate and creep, it seems instructive to start with Nabarro who presented an interesting limit analysis for the influence of grain size on the several mechanisms of creep deformation proceeding downward from strain rates above conventional power law (P-L) creep, to the slowest mechanisms of creep relating in one or another to deformations enhanced by mechanisms of mass transport by diffusion. A summary of the model considerations for copper is plotted in Fig. 9 taken from Armstrong, Conrad and Nabarro. The presence of any friction stress has been neglected in the analysis.

In Fig. 9, N-H is for the Nabarro-Herring creep model, $\sigma_p$ is the Peierls stress and H-D is the Harper-Dorn model for creep. For a constant stress test at effective low temperature in the absence of mass diffusion, Armstrong had earlier pointed to the plastic strain rate for thermally-activated dislocation motion being exponentially lowered by the presence of the $k_c \ell^{-1/2}$ term. Otherwise at effective high temperature, the combination of mass transport by diffusion and the occurrence of grain boundary weakening mechanisms enter into a reversed prediction of material strengthening at larger grain sizes. The issue is to be discussed in Sections 9–11, particularly with regard to important results reported for copper at nano-scale grain sizes.

6. Relation of H-P $k_c$ to Fracture Mechanics $K_{IC}$

At the other end of the scale from low or negative $k_c$ values for effective high temperature deformation, the largest values of microstructural stress intensity occur for $k_c = k_c$ that applies for essentially brittle cleavage fracturing. Such brittle consideration leads naturally to comparison of the H-P relation for cleavage cracking and the Griffith equation for fracture stress, $\sigma_F$, as expressed in terms of the plane strain stress intensity defined on a fracture mechanics (FM) basis for a pre-crack half-length, $c$, as

$$\sigma_F = K_{IC}(\pi c)^{-1/2}. \quad (6)$$

In eq. (6), $K_{IC}$ is the plane strain fracture mechanics stress intensity parameter. Equations (1) and (6), with $\ell$ and $c$ taken as analogous quantities, are only different because of the presence of $\sigma_0$ and a numerical constant. Alternatively, the two equations are different in terms of their application, respectively, to microscopic crack-free as compared with macroscopic pre-crack test conditions. Yokobori drew attention in the founding of the International Conference on Fracture, beginning at ICF1, to the need for reconciling microscopic and macroscopic concepts in fracture.

A connecting link between the H-P and FM views of brittle cracking was provided by the Bilby, Cottrell and Swinden continuum dislocation based description of essentially brittle
crack propagation occurring with an associated plastic zone at the crack tip.\(^7^9\) The analysis led to the condition for unstable growth of a crack with a plastic zone of length \(s\) at the crack tip of
\[
\frac{s}{c} = \left[ \sec \left( \pi \sigma_f/2 \sigma_y \right) \right] - 1. \tag{7}
\]
For connection to the Griffith equation, eq. (7) was re-arranged in the well-approximated relationship\(^8^0\)
\[
\sigma_f = A \sigma_f [s/(c + s)]^{1/2}. \tag{8}
\]
In eq. (8), \(A\) is a constant equal to \((\pi/2)\) for \((s/c) < 1.0\) and is equal to \(1.0\) for \((s/c) \to 1.0\). Also, \(\sigma_y\) in eq. (7) has been replaced by \(\sigma_f\) for the fracture stress of crack-free material.\(^8^1\) Equation (8) had been shown to fit experimental results reported for several steel materials and for the brittle fracture stresses of two polymethylmethacrylate (PMMA) materials\(^8^2\) and later proved useful in the interpretation of both conventional FM and indentation FM results reported for WC-Co composite materials.\(^8^1\)

The form of eq. (8), with \(A = \pi/2\), leads to the following relationship of \(K_{fc}\) and the H-P expression for \(\sigma_f\)\(^7^7\)
\[
K_{fc} = \left( 8/3 \pi \right)^{1/2} [\sigma_{fc} + k_c \epsilon^{-1/2}]^{1/2} \tag{9}
\]
Figure 10 shows agreement with a compilation of results for \(\alpha\)-iron and mild steel materials.\(^8^2\)\textendash\(^8^6\) The lowest \(K\) = \(\sim 600\) MPa-mm\(^{1/2}\) obtained by extrapolation in Fig. 10 compares with an average \(k_c = \sim 100\) MPa-mm\(^{1/2}\) for cleavage of similar \(\alpha\)-iron and steel materials;\(^8^7\) compare with \(k_c = \sim 1.3\) MPa-mm\(^{1/2}\) for the yielding of pure aluminum.

Petch and Armstrong have reported on the influence of an increase in \(\sigma_y\) reducing the value of \(K_{fc}\) and the reverse effect for a reduction in grain size, both of these influences being in the same direction, respectively, of raising or lowering the dbht.\(^8^9\) The effect of grain size reduction on increasing \(K\) may be understood in the following manner that relates to the condition of \(k_c > k_c\). During initial loading, plastic yielding is initiated at the root of the notch, at higher H-P stress as the grain size is smaller, but greater strain hardening is needed to reach a higher H-P determined cleavage stress, hence the measured value of \(K\) is greater; see also the physical interpretation for ductile and brittle fracturing of ferritic steel given by Qiu, Wang, Hanamura and Torizuka.\(^8^8\)

7. Dislocation Pile-up Avalanche Mechanism for Hot Spots and Shear Banding

The importance of a substantial value of the H-P \(k_c\) in affecting cleavage was proposed relatively more recently to provide a fundamental explanation for the occurrence of shear banding behavior based on sudden release of a dislocation pile-up.\(^8^9\)\textendash\(^9^0\) Head had provided an analytic description of pile-up release from a blocking obstacle\(^9^1\) and Gerstle and Dvorak had provided numerical calculations for a pile-up pushing through a viscous boundary resistance.\(^9^2\) Armstrong, Coffey and Elban proposed the following relationship for the temperature rise, \(\Delta T\), accompanying sudden release of a pile-up\(^6^9\)
\[
\Delta T = (k_s \varepsilon^{1/2} v / 16 \pi K^*) \ln (2K^* / \varepsilon^* c b) \tag{10}
\]
In eq. (10), \(k_s\) is the shear stress intensity at pile-up release, \(v\) is dislocation velocity, \(K^*\) is thermal conductivity and \(c^*\) is the specific heat at constant volume. At the highest limiting dislocation velocity, \(v\), corresponding to the elastic shear wave speed, the principal dependence is in the ratio of \(k_s / K^*\). Furthermore, Armstrong and Elban\(^1^3\) took an upper limiting value of \(k_s\) to be given by the shear stress required to bring the leading dislocations in the pile-up to a closest separation of \(b\), after Armstrong and Head,\(^9^3\) and proposed that the ordinate slope to points of \((k_s, K^*)\) could be taken as a measure of the susceptibility to shear banding. Figure 11 provides evidence for validity of the model consideration. The titanium alloy, Ti6Al4V, is known to be susceptible to shear banding\(^8^4\) and copper and aluminum are known to be much less so. More realistic values of \(\Delta T\) are obtained at lower thermal-stress-dependent values of \(v\), say, of two orders of magnitude or so lower than the material elastic shear wave speed. The pile-up avalanche model consideration was also applied to understanding the localized generation of hot spots leading to the initiation of explosion in energetic materials.\(^9^5\)

8. Thermal Activation in the H-P \(k_c\)

Mention of thermal dependence for the dislocation velocity in eq. (10) relates also to the implicit consideration that \(\tau_C\) in
9. Nanopolycrystal Strength of Copper

Despite the relatively low $k_c$ values of the fcc metals, say $k_c = \approx 5 \text{ MPa}\cdot\text{mm}^{1/2}$ for copper as compared with $\approx 24 \text{ MPa}\cdot\text{mm}^{1/2}$ for mild steel, there is substantial strengthening to be gained for fcc nano-scale grain size material. Figure 13 shows an example of the case for copper based on the production of nano-twinned material in which the twin thickness has been proposed to contribute to effective grain boundary strengthening.\textsuperscript{52,101–103} Armstrong \textit{et al.} had earlier pointed out that only slip systems with $b$ values contained in the twin interface plane could be transmitted through the boundary.\textsuperscript{10} In Fig. 13, Armstrong and Smith\textsuperscript{102} had extended to nano-scale grain sizes the experimental H-P dependence established by Hansen and Ralph\textsuperscript{52} and drew attention to the condition at ultratine grain size of achieving the limiting case of a single dislocation loop expanding against the grain boundary resistance. Such condition is contained in Fig. 13 by employing the results from Li and Liu for a single dislocation loop expanding against the grain boundary obstacle\textsuperscript{103} for which such stress is joined at $n = 1.0$ to the extended H-P dependence shown at larger grain size. Thus there is prediction of a transition to a raised reciprocal grain diameter dependence that, because of the grain boundary resistance, is raised to a somewhat higher stress than the extrapolated H-P dependence. In Fig. 13, the open circle points are those reported by L. Lu, Chen, Huang and K. Lu for the stress dependence on (growth) twin thicknesses taken as the effective grain size for pulsed electro-deposited copper materials.\textsuperscript{101} A similar H-P strengthening dependence was shown to have been obtained in their larger nano-scale regime in agreement with other compiled results for copper shown earlier in Fig. 4. In a companion article, K. Lu, L. Lu and Suresh pointed to achievement of an increased ductility for the nano-twinned material.\textsuperscript{104} Credit for the result was given to the importance of coherency of the twin boundaries with the adjacent matrix, the boundary stability and small boundary spacing.\textsuperscript{105} The combined features are in line with an H-P expectation for boundary resistance to cracking,\textsuperscript{10} for example, at a limiting small number of dislocations in a pile-up, including the condition of $n = 1.0$, the local concentrated stress is sharply reduced and the applied stress must necessarily reach on its own the theoretical value required for cleavage initiation or plastic instability. In this regard, Armstrong and Antolovich have presented preliminary predictions for cleavage being unfavorable in $\alpha$-iron at nano-scale grain sizes.\textsuperscript{87}

At the smallest nano-twin thicknesses shown in Fig. 13, Lu \textit{et al.} measured a reverse strength dependence on the nano-twin thickness.\textsuperscript{101} Such reversal of the H-P relation is normally-attributed to grain boundary weakening\textsuperscript{79} and is
suggested to follow an effective high temperature-type stress dependence of the form\(^{15}\)

\[
\frac{d\varepsilon}{dt} = (AD_Gb/k_B T)(b/c)\eta^p\sigma^q
\]  

(11)

In eq. (11), \(D_G\) is either lattice \((i = L)\) or grain boundary \((i = G)\) diffusion coefficient; \(k_B\) is the Boltzmann constant; and, \(A, p\) and \(q\) are experimental constants. The latter two constants relate to the Nabarro-Herring (N-H) mechanism of creep described in Nabarro’s Fig. 8 with values of \(p = 2.0\) and \(q = 1.0.\) More is to be described on this issue in the next Section in which the thermal activation-strain rate analysis (TASRA) for dislocation slip in polycrystalline material is examined in greater detail, particularly, for a grain size dependence of the reciprocal activation volume, \(v^*\), defined as.\(^{106}\)

\[
v^* = mk_BT[\partial(\ln(d\varepsilon/dt)/\partial\sigma)_{T}] \quad (12)
\]

In eq. (12), \((d\varepsilon/dt)\) is the plastic strain rate obtained as \((1/m)\) times the shear strain rate.

10. H-P Dependencies for the Reciprocal Activation Volume, \(v^{* -1}\)

Narutani and Takamura\(^{54}\) reported careful measurements of \(v^*\) for conventional polycrystalline nickel material and employed the measurements to determine dislocation densities that could be compared with independent measurements separately determined by a calibrated electrical resistivity technique. The \(v^*\) results are shown in Fig. 14 on a reciprocal H-P type \(v^{* -1}\) basis adapted from an analysis developed by Rodriguez.\(^{107}\) An H-P type dependence for \(v^{* -1}\) had been predicted by Prasad and Armstrong.\(^{108}\) The H-P type dependence is obtained by differentiation of eq. (4) while taking into account that \(k_S\) in eq. (5) would potentially also exhibit a thermal dependence in \(\tau_c.\)

On the basis of the \(v^*\) separations in intercept and slope values in Fig. 14, Rodriguez was able to account for (larger) \(v_0^*\) values corresponding to the dislocation intersection mechanism operative within the grain volumes of the nickel material and (smaller) \(v_C^*\) values corresponding to cross-slip at grain boundaries.\(^{107}\) The same \(v^*\) values at \(\varepsilon = 0.05\) are shown in the combined compilation of nickel and copper results in Fig. 15. In this case, the total results are plotted over a large range in grain size, \(\ell\) and for the open circle points, twin thicknesses, \(\lambda,\) so as to include both H-P strengthening and weakening effects.\(^{109-112}\) The lower and upper solid H-P type curves in the figure apply for the temperatures of 300 and 195 K. The highest values of \(v^{* -1}\) determined at the smallest nano-scale \(\lambda\) values in Fig. 15 were obtained from eq. (12) taking \(p = q = 1.0.\) The corresponding small values of \(v^*\) are proposed to be characteristic of boundary deformations, as was previously demonstrated for even smaller \(v^*\) values determined for results reported by Conrad and Narayan of grain boundary weakening in nanocrystalline zinc material.\(^{32,113}\)

11. Disorder at Nanopolycrystal Grain Boundaries

A last topic in the present report involves returning to the subject of the width of grain boundaries in polycrystals, which issue was resolved in the latter half of the twentieth century in favor of a sharp atomic scale transition between adjacent grains.\(^{114}\) The nature of grain boundaries in at least some nanocrystalline materials may be a different situation.\(^{116}\) Armstrong has proposed that such boundaries may consist of a wider region of disordered material in agreement with a number of studies leading to atomic model constructions. Figure 16 possibly shows a compilation of results that can be interpreted to provide indirect evidence for the proposal. The solid curve is the H-P dependence established at conventional grain sizes for the yield stress of the mild steel material previously shown here in Fig. 2.\(^{10}\) The nano-scale open square points were obtained by Embury and Fisher\(^{115}\) for patented pearlitic (piano) wire and the open circle points were obtained by Jang and Koch\(^{116}\) for heavily ball-milled \(\alpha\)-iron material. Both material results fit dashed shifts of the H-P lines that are partly accounted for by reduced values of \(k_s.\) The results for Jang and Atzmon were obtained by transformation of highest reported hardness measurements.\(^{117}\) A lowered \(k_s\) is expected for disordered grain boundaries. For comparison, the open triangle points in Fig. 16 have been plotted from recent results reported by Purnek, Saray, Karaman and Maier\(^{118}\) for interstitial-free steel material processed to ultrafine grain
size by the ECAE method and annealing. The dashed H-P relation for the open triangle points was obtained with \( \sigma_0 = 43 \text{ MPa} \) and \( k = 11 \text{ MPa mm}^{-1/2} \), down from \( 24 \text{ MPa mm}^{-1/2} \) for the conventional mild steel result. In this case, \( k \) is lowered by the removal of carbon.\(^{10}\) Zhang, Godfrey, Huang, Hansen and Liu\(^{19}\) have reported more recent results for cold-drawn pearlitic steel wire in which lowered values of \( k \) between 6.3 and 12.7 \text{ MPa mm}^{-1/2} \) were determined along with increasing values of \( \sigma_0 \) for greater dislocation densities at increasing stages of drawing. In another study of an ultra-low carbon thermo-mechanically controlled processing of conventional grain sizes within a microalloyed steel material, Shukla, Das, Ravi Kumar, Ghosh, Kundu and Chatterjee\(^{20}\) obtained a value of \( k = 18.1 \text{ MPa mm}^{-1/2} \).

12. Summary

The reciprocal square root of grain size dependence observed for mild steel materials in pioneering measurements reported by Hall and Petch and interpreted by them on a dislocation pile-up model basis has been reviewed in terms of a wider application to a diverse number of materials and their more inclusive mechanical properties. In this regard, connection has been made between the H-P analysis and the ductile to brittle transition behavior of steel and related materials, the broader stress–strain behavior of bcc, hcp and fcc materials, the hardness property, fatigue, fracture mechanics, shear banding and strain rate sensitivities. Particular attention has been given to H-P application to nanocrystalline material properties, including both grain size and nano-twin strengthening behaviors and, at the smallest nano-scale dimensions, effective grain size weakening. The dislocation pile-up model is shown to relate through the friction stress, \( \sigma_0 \), to the Taylor theory for a dislocation density explanation of material strength and through the H-P \( k \) to a fracture mechanics explanation of the macroscopic stress intensity \( K \) for pre-cracked material. The accumulated references presented for the various H-P results give strong indication of continuing progress being made on the topic.

REFERENCES
