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Editorial

The Dislocation Mechanics of Crystal/Polycrystal Plasticity

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Abstract: A brief history and update are given in four examples demonstrating that polycrystals are generally stronger than their individual component crystal grains because of obstructed dislocation pile-ups at grain boundaries. The example cases constitute diverse applications of a Hall–Petch dependence involving one or another aspects of the full polycrystal stress–strain behavior: (1) a Hall–Petch based description for a compilation of delayed yielding measurements compiled for steel; (2) computations for an H-P grain size dependent, tensile, plastic instability behavior of copper; (3) an H-P relationship for the true maximum stress for the limit of uniform straining of aluminum; and (4) the onset of a ductile-to-brittle transition in steel cleavage fracturing measurements that are connected to the material fracture toughness properties.

Keywords: dislocations; crystals; polycrystals; Hall–Petch relation; delayed yielding; constitutive relations; strain hardening; plastic instability; cleavage fracturing; fracture toughness

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1. Introduction

Polycrystal grain boundaries block dislocation slip (or deformation twin) bands from exiting the crystal grain volumes, thus leading to a Hall–Petch (H-P) inverse square root of average grain diameter, $\ell^{-1/2}$, dependence of the full polycrystal stress (σ_ε)-strain (ε) behavior in the relationship:

$$\sigma_\varepsilon = \sigma_{0\varepsilon} + k_\varepsilon \ell^{-1/2} \quad (1)$$

In Equation (1), $\sigma_{0\varepsilon}$ measures the strain dependence of the yield strength of the individual crystals or grains; and, k_ε measures the stress intensity required for transmission of plastic flow across the grain boundaries. At the crystal lattice level, dislocation pile-ups in normal slip band structures are required to overcome the grain boundary resistances. The subsequent multi-slip system condition for yielding and strain hardening is in $\sigma_{0\varepsilon}$ and occurs both because of an increase in dislocation density and, very importantly, because of the consequent dislocation interactions/reactions that occur during plastic straining [1].

Early evidence for the later development of a thus-described H-P relationship was expressed by Polanyi [2] in a 1927 Faraday Society meeting. The scientific gathering was devoted to understanding the new mechanical properties being determined for multi-crystal deformations being made on the 20th century metal: aluminum. Polanyi pointed to the observation that tensile straining of an aluminum multi-crystal produced on the tensile specimen surface a record of in-place grain boundary ridges that were indicative of the boundary resistance to the overall plastic deformation. Taylor [3] gave, in opposition, emphasis to internally measured lattice distortions being essentially no different for individual single crystals or multi-crystals, as measured by X-ray diffraction; and so, he discounted any direct grain boundary effect on the polycrystal strength. Aluminum polycrystal measurements reported much later by Hansen [4] gave evidence that the H-P grain size effect was easily missed by Taylor and co-workers because the material has a lowest k_ε in Equation (1), except for lead [4] and for a very good dislocation mechanics-based reason of easy cross-slip needed at the aluminum grain boundaries. Thus, modern strength-dependent H-P measurements have corrected the situation for aluminum and related face-centered cubic metals, as will be described in the present report, which begins with H-P measurements for iron and steel materials, for which the importance of a grain size effect could not be missed.

2. An H-P Dependence for the Delayed Yielding of Iron and Steel

Hall [5] and Petch [6] initially accounted for the application of Equation (1) to grain size dependent yield (and cleavage) strength measurements made on steel materials. The results were explained in terms of dislocation pile-ups needing to overcome a grain boundary resistance. Here, we note that quite independent of that earlier work, Suh and Lee [7] investigated the grain size dependence of delayed yielding in iron and steel materials in terms of the modeled time period required for dislocation pile-ups to travel to the material grain boundaries. The model consideration can be assessed on an H-P basis that was extended to include the thermally activated rate dependence for dislocation movement. Such strain rate ($d\varepsilon/dt$) and temperature (T) dependence for bcc iron and steel materials is expressed in the relationship [8]:

$$\sigma_\varepsilon = \sigma_{0G\varepsilon} + B\mathbf{exp}(-\beta T) + A\varepsilon^n + k_\varepsilon \ell^{-1/2} \tag{2}$$

In Equation (1), $\sigma_{G\varepsilon}$ is an athermal stress component dependent on the dislocation density and solute concentration, B is the thermal stress at T = 0, $\beta = \beta_0 - \beta_1 \mathbf{ln}(d\varepsilon/dt)$, and A and n are constants measuring the material strain hardening. Thus, the first three terms in Equation (2) are an expanded interpretation of $\sigma_{0\varepsilon}$ in Equation (1). It should be noted that the ($d\varepsilon/dt$) and T dependencies are in the yield stress for bcc metals while the strain hardening is essentially athermal. The constants in Equation (1) have been evaluated previously for dynamic material computations made for the deformation of ARMCO iron material [8].

Figure 1 provides the compilation of measurements collected by Suh and Lee as fitted by a band of curves centered on the shorter delay time results. In the figure, an extended constitutive equation-based H-P type dependence has been added to provide H-P connection with the otherwise same model based description given by Suh and Lee. The thermal stress term in Equation (2) was utilized on the basis of an inverse dependence of ($d\varepsilon/dt$) on the material delay time, t_d. The constants k_ε = 22 MPa.mm$^{1/2}$; $\sigma_{0G\varepsilon} = 0$; β_0 = 0.00698 K^{-1}; β_1 = 0.000415 K^{-1} and an average grain diameter of ℓ = 0.094 mm were employed in the calculation. Thus, reassuringly, the Equation (2) material constants taken from Table 1 of reference [8] have led to a reasonable H-P description of the delay time measurements for a closely related Suh and Lee model description of grain size dependent delay time measurements.

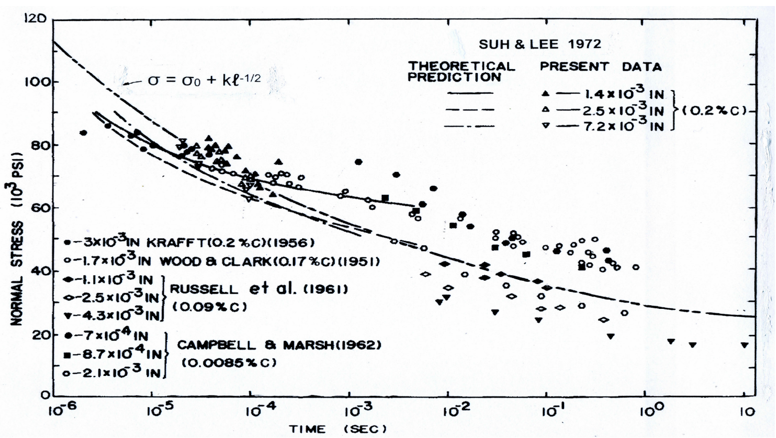

Figure 1. A compilation of delay time measurements for the yielding of carbon steel materials, also with several theoretical model predictions reported by Suh and Lee [9], and also including an extended curve for Hall–Petch dependence; 10^3 psi = 6.9 MPa and 1.0 in = 2.54 cm.

3. Grain-Size-Dependent Plastic Instability Computations for Copper

A different constitutive equation has been validated for copper and related face centered cubic (fcc) metals in the form [9]:

$$\sigma_\varepsilon = \sigma_{0G\varepsilon} + B_0[\varepsilon_r(1 - \mathbf{exp}\{\varepsilon/\varepsilon_r\})]^{1/2}(\mathbf{exp}[-\alpha T) + k_\varepsilon \ell^{-1/2} \quad (3)$$

In Equation (3), the $\sigma_{0G\varepsilon}$, B_0 and $k_\varepsilon \ell^{-1/2}$ terms and factor have the same meaning as for Equation (2) while ε_r is a recovery strain and $\alpha = \alpha_0 - \alpha_1 \mathbf{ln}(d\varepsilon/dt)$, as for β in Equation (2). Thus, in contrast to the bcc case, fcc strain hardening is thermally dependent and the maximum true stress determined by uniform straining is counter intuitively greater at an increasing strain rate. At small strain, a Taylor-type parabolic stress–strain dependence is obtained.

Hansen and Ralph [10] have reported very complete H-P dependencies for the tensile stress–strain behavior of copper over the range of true strain values of ε = 0.03, 0.05, 0.10, 0.15, 0.20 and 0.30. A constant value of k_ε = 5.0 MPa.mm$^{1/2}$, independent of strain, was obtained. In the present investigation, Equation (3) was fitted to the cumulative $\sigma_\varepsilon - \varepsilon$ measurements with estimated values of $B = B_0$ = 500 MPa, $\sigma_{0G\varepsilon} = 0$ and ε_r = 1.2. Figure 2 shows the resultant computations of the so-determined $\sigma_\varepsilon - \varepsilon$, curves at the two grain sizes of ℓ = 40 and 4.0 μm and with evaluation of the strain hardening, $(d\sigma_\varepsilon/d\varepsilon)$, in this case, equal to $(d\sigma_{0\varepsilon}/d\varepsilon)$. At ℓ = 40 μm, the important influence of ε_r on stress reduction is shown between the dashed and solid $\sigma_\varepsilon - \varepsilon$ curves. The computed maximum uniform strain values are consistent with the largest ε = 0.30 values determined by Hansen and Ralph for their H-P dependencies. The reduction in uniform strain values, ε_u, at smaller grain size are also consistent with a previous tabulation reported for tensile deformation measurements [11].

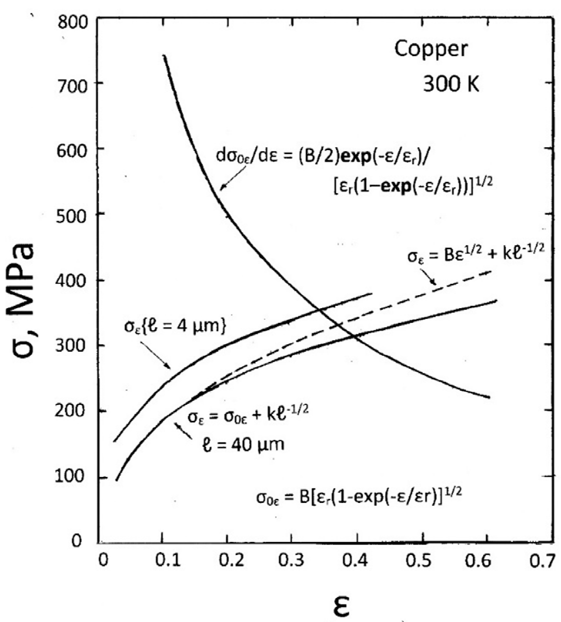

Figure 2. H-P based plastic instability computations demonstrating a decrease in the tensile uniform strain at reduced grain size for copper material.

4. An H-P Dependence for the True Stress at Maximum Load of Aluminum

Kamikawa, Huang, Tsuji and Hansen [12] extended the obtainment of H-P measure ments for aluminum to nanostructured material produced by accumulative roll-bonding (ARB). An increase in k_ε was interpreted to occur at ultrafine grain sizes for the materials exhibiting discontinuous yielding behaviors. Alternatively, a same H-P dependence to that for initial yielding was shown to apply for the true stress at the maximum uniform strain, σ_u [1]. More recently, Kamikawa, Hirooka and Furuhara [13] have reported related H-P measurements both for aluminum and for aluminum-magnesium alloy materials. Quantitative electron back-scattered diffraction (EBSD) measurements were made to establish a mean value, d_r, of low-angle and high-angle grain boundary spacings. Figure 3 is an illustration of the H-P dependence for the tabulated σ_u measurements. Again, a same H-P k_ε is obtained for both the yield stress and σ_u value at maximum uniform strain.

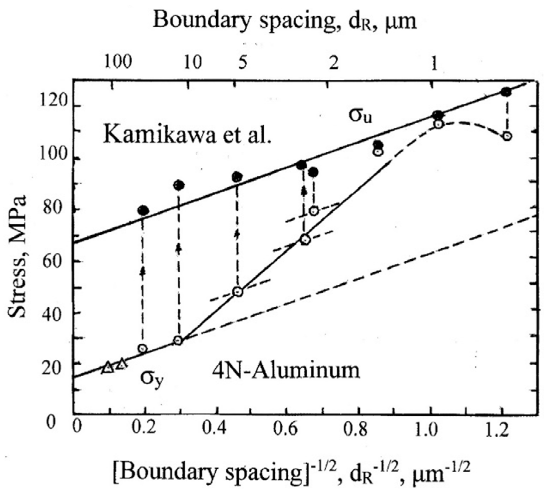

Figure 3. The yield stress, σ_y, and true stress at maximum uniform strain, σ_u, for aluminum material as obtained from measurements reported by Kamikawa, Hirooka and Furuhara [13].

The $k_u = k_y$ result in Figure 3 provides a possible alternative explanation to k being increased at smaller grain sizes. In the figure, the dashed vertical lines apply for the strain hardening between σ_y and σ_u whereas the dashed segments of slope k_y at the several points of increasing stress might be taken to represent increasing values of $\sigma_{0\varepsilon}$ at those corresponding points. Such issue separating a possible "residual strain" effect contained in $\sigma_{0\varepsilon}$ from an annealed grain size effect is imagined to be a problem in assessing the strength levels measured for materials produced by severe plastic deformation.

5. The Ductile-Brittle Transition Steel and Its Fracture Toughness

A notable extension of the original H-P analysis was to explain the onset of catastrophic brittleness in steel, particularly as specified in terms of achieving a cleavage stress, σ_C, and a ductile-to-brittle transition temperature, dbtt, Tc, that was shown to be raised by neutron irradiation damage [14]. Charpy v-notch impact testing has been employed to evaluate the effect of temperature and strain rate on the dbtt. Figure 4 is an example of very complete measurements made by Sandström and Bergström [15] on mild steel. A value of k_C = 107 MPa.mm$^{1/2}$ had been determined for the cleavage stress in bend tests. Measurements for a thermally activated description of $\sigma_{0\varepsilon}$, essentially the same as given in Equation (2), was expressed for the T and $(d\varepsilon/dt)$ dependencies. Otherwise, the dbtt was determined from the condition that $\sigma_\varepsilon = \alpha\sigma_y\{T,(d\varepsilon/dt)\}$, for which a notch stress-concentration factor, α, was also determined to take into account that the yield stress was greater under the combined state of stress present at the root of the notch [15]. In Figure 4, a somewhat raised dbtt was attributed to the presence in the smaller grain size material of relatively larger carbide particles [14].

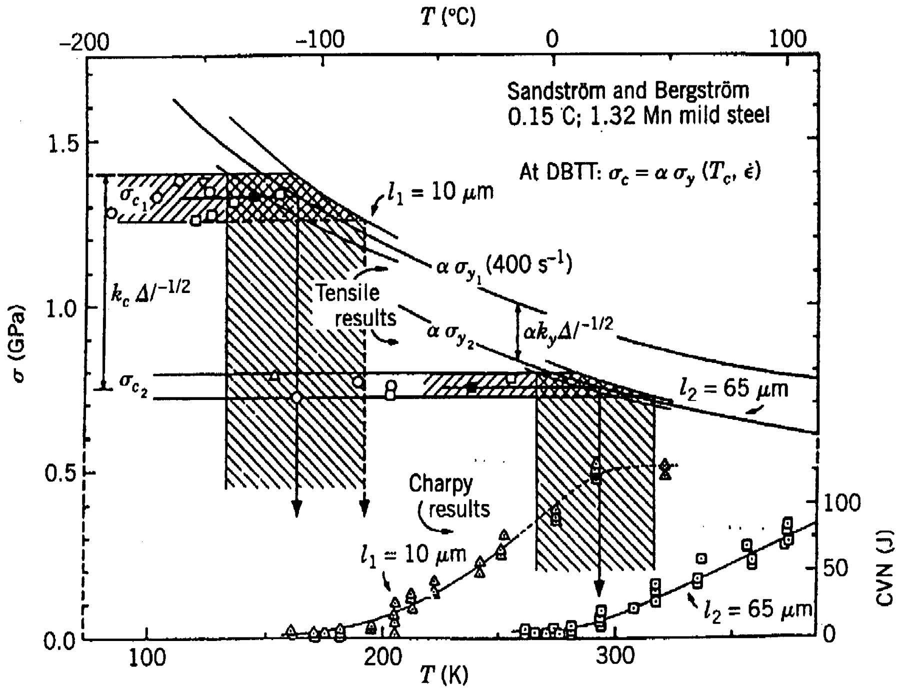

Figure 4. A compilation of tensile test and Charpy impact test results obtained by Sandström and Bergström in determining a ductile-to-brittle transition in behavior at two grain sizes [14,15].

Petch and Armstrong [16] followed-up on such dbtt results by investigating the same type considerations for the fracture toughness aspects of plastic deformation at the root of a notch leading to cleavage fracturing. Emphasis was given to the bcc-type strain hardening via A and n in Equation (2) being athermal. At sufficient stress application, plastic deformation was taken to be initiated at the notch and to lead via strain hardening to achievement of the higher cleavage stress. A positive influence of grain size resulted in this case also because of the greater dependence on k_C over k_y. A fracture mechanics stress intensity, K_C, was obtained on a dislocation mechanics model basis, involving a constant reference, K_C', and the strain hardening factors given in Equation (2) as

$$K_C = K_C'\mathbf{exp}(-\sigma_y/nA) \tag{4}$$

Equation (4) was shown to be in agreement with K_C decreasing with an increasing value of σ_y, except for the influence of an increasing grain size. In this case, although the yield stress is greater at smaller grain size, the cleavage stress is raised more so and the re quired strain hardening required to reach the cleavage stress is larger. A relatively recent report by N.H. Heo, Y.-U. Heo, Kwon et al. [17] has included a consideration of inter granular fracturing to that of the Hall–Petch model for yielding and cleavage in determining the overall fracture strength behaviors of bcc steel materials.

6. Summary

Four Hall–Petch based sub-topics have been described: (1) delayed yielding in in iron and steel materials; (2) grain size dependent uniform strain values for the tensile plastic instability properties of copper; (3) an H-P dependence for the tensile maximum uniform strain of aluminum at ultrafine grain sizes; and (4) H-P connection of the ductile-brittle transition and fracture toughness properties of steel. In each case, a crystal-to-polycrystal connection has been made in terms either of the importance of one or another of the H-P parameters, $\sigma_{0\varepsilon}$ and k_ε.

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