

## NEW CONCEPTS OF A MODIFIED HALL - PETCH TYPE RELATIONSHIP

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### Abstract

A modified form of the Hall - Petch equation, where the average grain diameter is replaced by the surface to volume ratio of internal boundaries ( $S_v$ ), is considered. Working with this model, a flow stress –  $S_v$  relationship dominated by geometrically necessary dislocations (GNDs) is derived for the low strain region.

At higher strains, a more complicated relationship between the flow stress and  $S_v$  is anticipated. The role of statically stored dislocations (SSDs) in the high strain region is emphasized. The Stacking fault energy (SFE), through the density of the SSDs may control the character of the Hall - Petch slope  $K_y$  with increasing strain.

### 1. Introduction

A new generalized form of the Hall – Petch relationship which takes into account the specific surface area (surface to volume ratio) of grain boundaries has recently been put forward [1] and is given as:

$$\sigma_f = \sigma_o + K_y S_v^m \quad (1)$$

In equation (1)  $\sigma_f$  is the flow stress,  $\sigma_o$  is the friction stress,  $m$  is a constant,  $K_y$  is the Hall - Petch slope and  $S_v$  is the surface to volume ratio of the grains.

Previous attempts [2,3], at the explanation of the flow stress - grain size dependence are based on the concept of grain boundaries acting as obstacles to dislocations. The recent approaches to the flow stress - grain size dependence employ the arguments of Ashby (4) for the generation of Statistically stored and Geometrically necessary dislocations (SSD & GND). The role of grain boundary regions as areas of high density of GND therefore, becomes substantial. With the above in mind, the surface to volume ratio of the grains  $S_v$ , which may be considered as a parameter for assessing the grain size, assumes an important physical meaning. The advantages in the adoption of  $S_v$ , as a parameter for the characterization of the grain size [5] instead of the grain diameter has been elaborated by other workers [6 – 8]. In the case of dual phase materials, the surface to volume ratio has even a wider application, since the work hardening of the material will reflect the geometrical arrangement of the phases.

### 2. The Ashby Model (4) of Work Hardening.

The classical Hall - Petch relationship relates the yield stress to the inverse square root of the grain diameter [2,3]:

$$\sigma_Y = \sigma_o + K_y d^{-1/2} \quad (2)$$

where  $\sigma_Y$  is the yield stress,  $d$  is the grain diameter, and  $K_y$  and  $\sigma_o$  are constants. The applicability of this equation to the flow stress has been well demonstrated (9). When eqn. (2) is applied to the flow stress,  $\sigma_o$  and  $K_y$  are functions of strain. Hall - Petch type relationship is obeyed by FCC metals (10), dual materials (11), ordered phases (12) as well, as lamellar structures [13]. The universality of equation (2) in the above form or the interpretation of its original conception has been questioned [14, 15]. Due to the fact that the Hall - Petch model was a description of statistical observation, physical basis for its formulation has been constantly sought and alternative models proposed (for review see ref. 5).

One of such models is the work hardening model [16 – 18]. The fundamental formulation of the work hardening model is the dependence of the flow stress on the square root of the dislocation density; expressed as follows:

$$\sigma_f = \sigma_o + \alpha G b \rho^{0.5} \quad (3)$$

Where  $\sigma_f$  and  $\sigma_o$  have their usual meanings,  $\alpha$  is a constant,  $b$  is the Burger's vector, and  $\rho$  is the dislocation density. Ashby's [4] modification of the work hardening model lies in the concept of the GNDs and SSDs. The GNDs are essential for the compatibility requirement deformation.

The grain size dependent part of the flow stress originates from the density of the GNDs,  $\rho_g$ . The geometrically necessary dislocations are largely confined to the grain boundary regions [1, 19]. Ashby [4] has predicted that the density of the GNDs will be directly proportional to the inverse of the grain diameter. This prediction has been disputed by Thompson, Baskes & Flanagan [20] on the grounds of texture formation. Dollar & Goryzyca [1] have also argued against a direct inverse proportionality between  $\rho_g$  and grain diameter. The latter post that the average dislocation density may be related to the grain size but not the local dislocation density.

On the other hand, the density of the SSDs,  $\rho_s$  should not be related to the compatibility conditions that lead to the generation of the GNDs but to the amount of deformation. Also, the lattice forces and the stacking fault energy (SFE) will play a role on the magnitude of  $\rho_s$ . Local order may equally contribute to the density of the SSDs. In another way, it could be said that  $\rho_s$  will surely depend on how easily recovery processes are proceeding. Interactions between the SSDs and the GNDs or an interrelationship between  $\rho_s$  and  $\rho_g$  may be anticipated since the GNDs generated earlier may act as obstacles to the generation and movement of later generated dislocations. Bearing in mind the number of factors involved and that the accumulation of SSDs is a result of chance encounters [4], a simple prediction of the density of the SSDs,  $\rho_s$ , will be impossible.

### 3. Modification of the Hall – Petch Equation

#### (A) Low Strain region

At low strains, the SSDs and GNDs are largely stored in different region of the grain. The total dislocation density may therefore be given as:

$$\rho_t = \rho_s + \rho_g \quad (4)$$

Following Thompson et al [20], the volume fraction occupied by the GNDs will be determined by the factor  $\lambda_s/d$ , where  $\lambda_s$  is the statistical slip distance and  $d$  is the grain diameter. Ashby [4] suggested that  $\rho_s$  is a function strain and grain size, i. e. our opinion,  $\rho_s$  will not be a function of grain size provided that  $\lambda_s$  is smaller than the grain diameter; thus providing a limiting case to the Ashby model. This is in agreement with Thompson et al [20],

whose statistical slip distance is an undetermined function of strain and grain diameter in the sense that the grain diameter is the upper limit for  $\lambda_s$ . The total dislocation density may therefore be written as:

$$\rho_t = \rho_s(1 - \lambda_s/d) + \rho_g \lambda_s/d \quad (5)$$

On the assumption that the sum of the volume fractions of the SSDs and GNDs is equal to unity, equation (3) then becomes;

$$\sigma_f = \sigma_o + \alpha Gb\{\rho_s(1 - \lambda_s/d) + \rho_g(\lambda_s/d)\}^{0.5} \quad (6)$$

For  $\lambda_s \approx d$ , a case in the low strain region, equation (6) may be simplified to:

$$\sigma_f = \sigma_o + \alpha Gb\{\rho_g\}^{0.5} \quad (7)$$

Dollar & Gorycryca [1] have given the density of the GNDs as:

$$\rho_g = \beta \varepsilon S_v \quad (8)$$

Where  $\varepsilon$  is strain and  $\beta$  is a constant. Substituting (8) in (7), we have;

$$\sigma_f = \sigma_o + \alpha Gb(\beta \varepsilon S_v)^{0.5}$$

or

$$\sigma_f = \sigma_o + \alpha' Gb(\varepsilon S_v)^{0.5} \quad (9)$$

Note that  $\alpha' = \alpha \beta^{0.5}$

Equation (9) is a Hall – Petch type equation. Recall that  $S_v \approx 1.73/d$ . An important point to note is that the equation predicts a strain dependent Hall – Petch slope at low strains. Also, the contribution of the dislocation density to the flow stress is determined solely by the density of the GNDs – a point predicted by Ashby [4]. It could be said that a strong influence of the SFE on the flow stress grain size dependence in the micro yield region (note that the GNDs are characteristic of the microstructure only) may not be expected.

Irvine, Gladman & Pickering [21] have considered the parameters affecting the flow stress of austenitic rat steels. The FFE which controls the work hardening rate has little or no influence at low strains. Meyers & Ashworth [22] have also concluded that the micro yields region is marked by the accommodation of GNDs.

#### (B) High strain region

Let us now consider the high strain region. Contrary to the low strain situation, both the GNDs and SSDs will be expected to play substantial roles. At not-too-low strain, the density of the GNDs will be swamped by that of the SSDs (i.e.  $\rho_s \geq \rho_g$ ), (see ref.[18]) and the square root of the total dislocation density by be

approximate as:

$$(\rho_s \rho_g)^{0.5} = \rho_s^{0.5} \{1 + \rho_g/2\rho_s - \rho_g^2/8\rho_s^2 + \rho_g^3/1(\rho_s^3 \dots)\} \quad (10)$$

Neglecting terms of order higher than two and substituting in equation (3), we arrive at:

$$\sigma_f = \sigma_o + \alpha Gb \{ \rho_s^{0.5} (1 + \rho_g/2\rho_s - \rho_g^2/8\rho_s^2) \}^{0.5} \quad (11)$$

or

$$\sigma_f = \sigma_o + A\rho_s^{0.5} + A'\rho_g/\rho_s^{0.5} - A''\rho_g^2\rho_s^{1.5} \quad (12)$$

Where  $\rho_o A = \alpha Gb$ ,  $A'' = \alpha Gb/2$ ,  $A''' = \alpha Gb/8$ .

The density of the SSDs may be approximated thus [23]:

$$\rho_s = \rho_o + C\varepsilon^n \quad (13)$$

Where  $\rho_o$  is the initial dislocation density,  $\varepsilon$  is strain,  $C$  &  $n$  are constants.

Substituting in equation (12) equations (8) and (13),

$$\sigma_f = \sigma_o + A(\rho_o + C\varepsilon^n)^{0.5} + A'\beta\varepsilon S_v / (\rho_o + C\varepsilon^n)^{0.5} - A''\beta\varepsilon S_v / (\rho_o + C\varepsilon^n)^{1.5} \quad (14)$$

For  $\rho_s \gg \rho_o$  which corresponds to the 2<sup>nd</sup> stage in the deformation of monocrystals, eqn (14) becomes:

$$\sigma_f = \sigma_o + A(C\varepsilon^n)^{0.5} + A'\beta\varepsilon S_v / (C\varepsilon^n)^{0.5} - A''(\beta\varepsilon S_v)^2 / (C\varepsilon^n)^{1.5} \quad (15)$$

On further simplification we may write

$$\sigma_f = \sigma_o + A_1\varepsilon^{n/2} + A_2\varepsilon^{1-n/2}S_v - A_3''\varepsilon^{2-1.5n/2}S_v^2 \quad (16)$$

Where

$$A_1 = \alpha GbC^{0.5}, A_2 = \alpha Gb\beta/2C^{0.5} \text{ and } A_3'' = \alpha Gb\beta/2C^{1.5}$$

For friction stress  $\sigma_i$   $\sigma_o + A_1\varepsilon^{n/2}$  where  $A_1\varepsilon^{n/2}$  is a grain size independent increase in the lattice friction stress, equation. (16) may be written as:

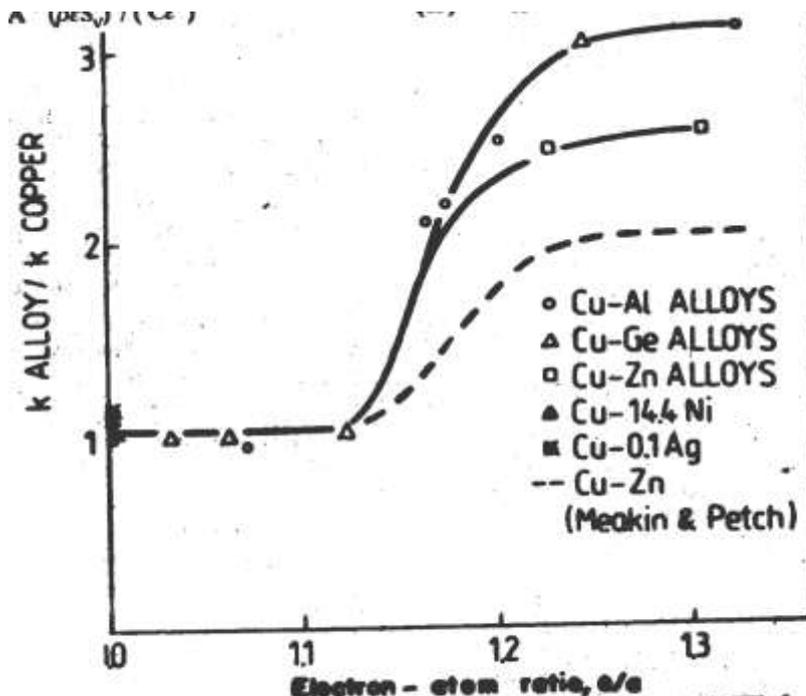
$$\sigma_f = \sigma_o + A_2\varepsilon^{1-n/2}S_v^2 - A_3''\varepsilon^{2-1.5n/2}S_v^2 \quad (17)$$

Equation (17) is a Hall – patch type equation. The 3rd term on the right hand side of equation (17) may be neglected. For the large grain sizes, the contribution of  $S_{v2}$  will be negligible when compared to that of  $S_v$ . When the grain size decreases, the Meyers and Ashworth [22], using the Ashby concept, have derived an equation similar to equation (17). They gave a flow stress – grain size relationship that includes both  $d^{-1}$  and  $d^{-2}$  terms.

On the assumption that the  $S_v^2$  term is unimportant, that Hall – Petch slope as determined from equation (15) is

$$K_y = \alpha(T\beta\beta\varepsilon^{1-n/2})/2C^{0.5} \quad (18)$$

In this case,  $n$  is a measure of the work hardening one may suggest that the value of  $n$  will be high for low SFE materials and lower with increasing SFE.



1: Dependence of Hall – Petch Slope on Stacking Fault Energy (SFE) for Cu– base alloys. SFE decreases as electron – atom ratio (e/a) increases. (Johnston and Feltner, 1970).

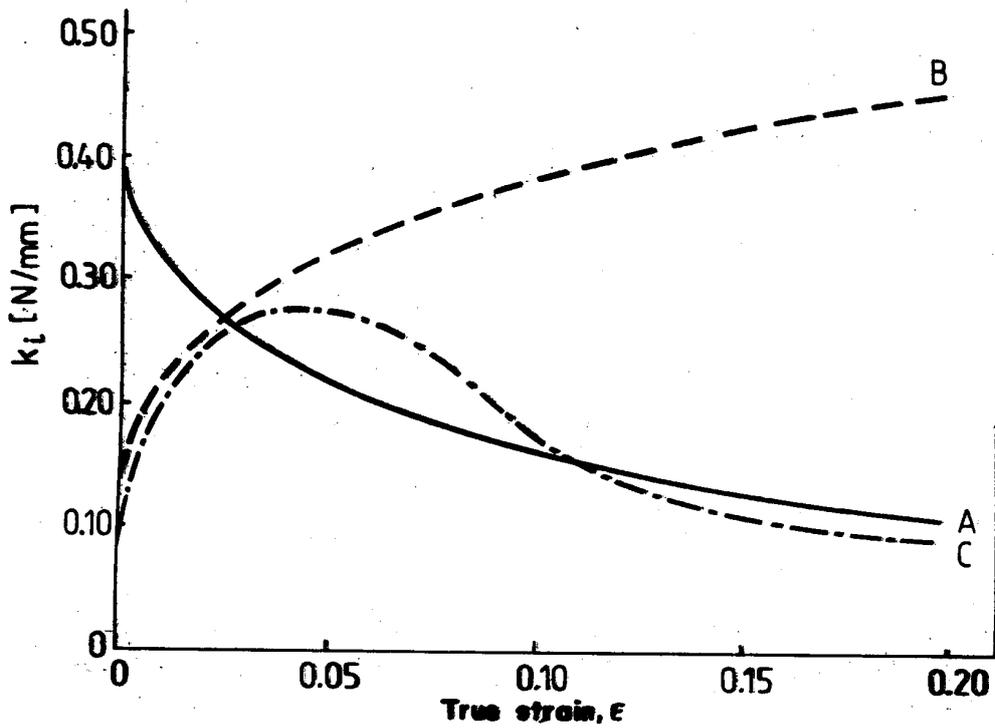


Figure 2a: Dependence of Hall - Petch Slope on Strain. A, B, C refer to austenitic steel of low, high and medium SFE respectively. (Dollar and Gorkczyka, 1985)

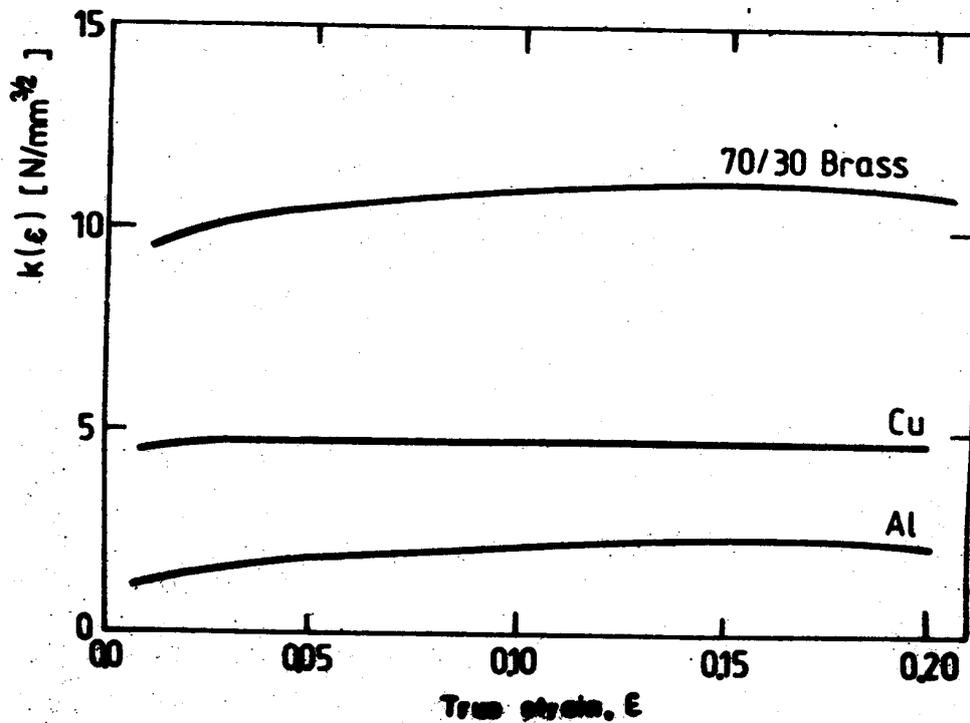


Figure 2b: Hall - Petch Slope versus True Strain (Hansen, 1985)

The strain hardening exponent of Cr - Ni suggests that the Hall -Petch slope  $K_v$ , is related to the SFE through the initial value of  $n$ . Johnston & Feltner [25] have summarized the results of other workers on the influence of the SFE on the Hall - Petch slope (see figure 1). The ratio of the Hall - Petch slopes ( $K_{Alloy}/K_{Cu}$  is the ratio of the Hall - Petch slope of Cu alloy to that of pure Cu whereas  $e/a$  is the electron to atom ratio) is seen to increase with increasing electron to atom ratio or decreasing SFE. For low SFE materials, one can predict an initial high value of  $K_y$  from equation (16) with increasing deformation, the value of  $K_y$  will tend to decrease. There is apparent agreement between this and the results. Presented by Dollar and Gorczyca [26] (figure 2a; Note that A, B, C refer to three austenitic steels of low, high, and medium SFE respectively and  $K_i$  refers to the Hall - Petch slope). The initial high value of  $K_y$  in a Cu - Zn alloy [6] which is a low SFE alloy, has been attributed to the blocking of slip (slip hardening). Rapid increase in the density of SSDs [27] for a high value of  $n$  may account for the normally observed  $K_y$  values for low SFE material. Equation (17) also predicts a non - dependence of  $K_Y$  on strain, on the assumption that  $n = 2$ . This is the case for medium SFE metals. Hansen [28] has published results for a strain - independent Hall - Petch slope or  $K(\epsilon)$  (figure 2b) for Cu. In the case of high SFE materials, the Hall - Petch slope is an increasing function of strain. One can reach that conclusion for values of  $n < 2$ . For 1020 steel and Fe, Hahn [23] has given the values of  $n$  as between 0.7 - 1.5.

Equation (17) may be criticized on the grounds that the value of  $n > 2$  assumed for low SFE materials has not been observed experimentally [29]. Explanation for this apparent discrepancy may lie with the constants  $\beta$  and  $C$ . Both constants may not be independent of strain. The accumulation of SSDs will strongly depend on the value of  $n$  since the density of the SSD is expected to dominate [4, 20, 22] over that of the GND. The assumption of a strain dependent  $n$  is in agreement with the generally acknowledged fact of dislocation saturation after high deformation. Equation (13) predicts an increasing density of SSDs,  $\rho_s$  with increasing strain. As has been discussed earlier, the density of the SSDs, will depend on how easily recovery

processes are proceeding. The occurrence of recovery processes, such as annihilation, remobilisation and cross slip which moderate the increase in  $\rho_s$  with strain [30] may lower the value of  $n$ . It is therefore plausible to suggest, that with increasing deformation, the value of  $n$  will decrease. The rate of decrease may be sensitive to temperature and strain rate.

#### 4. Conclusions

The model discussed above predicts a Hall - Petch type equation at low strains. In this region, the GNDs dominate. At higher strains, flow stress will depend on both  $S_v$  and  $S_v^2$ . The contribution of  $S_v^2$  will be significant mainly at very small grain sizes. It is also concluded that the SFE will affect the Hall- Petch slope through the value of the parameter.

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