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Estimation of the Yield Strength of Metals from Crystal Defect Energies

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<p>It has been found that the yield strength of a number of metals may be estimated by considering the contributions of various crystal defects to the strain energy per unit volume of a metal. It was found that for the metals in this study, the main contributions to the strain energy came from dislocations and grain boundaries. For high purity, well annealed metals, the contributions of solute atoms, self-interstitials, annealing twin boundaries and stacking faults are negligible. The calculations of the strain energy per unit volume at yield from crystal defect energies show good correlation to experimental data for high purity metals available in the open literature.</p>			
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ESTIMATION OF THE YIELD STRENGTH OF METALS FROM CRYSTAL DEFECT ENERGIES

INTRODUCTION

There is a growing need for new materials that are able to meet increasingly severe and complex performance criteria. The development of new materials often takes an empirical approach which forces designers to choose between several existing materials that meet only parts of a particular set of design requirements. A need, therefore, exists for a systematic approach to materials development so that "designer microstructures" may be produced to meet specific technological requirements. One of the purposes of this study is to take a first step towards relating microstructural variables to continuum scale material properties in order to provide a basis for the rational development of new materials.

Many metals and alloys exhibit a dependence of their yield strength on grain size as described by the Hall-Petch equation (1,2):

$$\sigma_y = \sigma_0 + kD^{-1/2} \quad (1)$$

where σ_y is the yield strength, D is the average grain diameter and σ_0 and k are empirical constants. Among the metals shown to follow this relationship are aluminum (3,4,5), silver (6), zinc (7), copper (8), nickel (9) and iron (10,11). Generally, σ_0 has been interpreted as the "friction" stress opposing dislocation motion within a grain (2,5,12) and k is termed the "unpinning constant" which is interpreted as a measure of the extent to which dislocations are piled up at barriers (5,11,13,14). However, some uncertainty still exists in the physical interpretations of these parameters (5) which is evidenced by the fact that the determination of the Hall-Petch constants for any particular material is generally dependent on running a series of tensile tests on specimens with various grain sizes and applying linear regression to a σ_y vs $D^{-1/2}$ plot.

Grain boundaries are regions of misorientation between adjacent grains in which the atoms are not aligned with the lattice of either grain. The displacement of these atoms from normal lattice positions creates a local increase in the energy of a polycrystal. This interfacial energy associated with grain boundaries may be measured by several methods including calorimetry (15) and thermal grooving (16). Similarly, characteristic energies are associated with other crystal defects such as vacancies, impurities, dislocations, stacking faults and twin boundaries. The purpose of this paper is to determine any relationships between these defect energies and Hall-Petch behavior in high purity metals.

PROCEDURE

Data relating the yield strength to the grain size of high purity metals have been generated in several previous investigations (3-11). In order to facilitate the comparison of these data to values of grain boundary energy, which are reported as energy per unit area, the σ_y vs $D^{-1/2}$ data were converted to elastic strain energy per unit volume at yield (w_e) vs grain boundary area per unit volume of material (S_v). The elastic strain energy per unit volume at yield is related to the yield strength by:

$$w_e = \frac{\sigma_y^2}{2E} \quad (2)$$

where E is Young's modulus of elasticity and all other terms are as previously defined. The grain boundary area per unit volume of material is related to the inverse of the average grain diameter by:

$$S_v = 2.25D^{-1} \quad (3)$$

where all terms have been previously defined (17). The w_e vs. S_v data were then plotted and analyzed using linear regression to obtain the slope and intercept of the data. The grain boundary energies for several metals and alloys have been previously measured. The grain boundary free energies of aluminum, silver and zinc were measured using calorimetry. Thermal etching was used to determine the grain boundary free energies of copper, nickel and iron. In all cases, the measurements were performed on high purity metals at temperatures high enough to insure that the metals were well annealed. These values have been gathered and tabulated in a review by Inman and Tipler (18).

RESULTS AND DISCUSSION

Figure 1 shows the observed variation between w_e and S_v for high purity zinc. It is apparent that a proportional linear relationship exists between these two quantities. This observation is physically and dimensionally consistent because grain boundaries have a characteristic energy expressed in terms of energy per unit area. When this energy per unit area is multiplied by S_v , the grain boundary area per unit volume, the product has the same units as w_e ; namely, energy per unit volume. This observation is also consistent with Hall-Petch behavior because the two terms, w_e and S_v , are proportional to the squares of σ_y and $D^{-1/2}$ respectively. Similar relationships were found for silver, aluminum, copper, iron and nickel. Linear regression was performed on the data in order to determine the slopes (dw_e/dS_v) and intercepts (w_0) for these relationships. The results of these calculations are given in Table 1. Whenever possible, handbook and textbook values (19,20) were used to insure that "typical" values of σ_0 were used for a given material. In the cases of silver and nickel, some discrepancy existed between the data, so the data was averaged. In the case of aluminum, the value range found (19) was used to choose the data which would best typify general behavior.

The grain boundary free energies (F_{gb}) of a number of metals are given in Table 2. A quick comparison between the values and the (dw_e/dS_v) values in Table 1, which are the grain boundary contributions to w_e , shows that a direct correlation of these two quantities may be drawn only for iron. However, among the metals being considered, iron is unique in that its body centered cubic crystal structure contains no close packed planes. It is the presence of these close packed planes in the hexagonal close packed structure of zinc and the face centered cubic structure of the remaining metals that accounts for the greater degree of cross-slip found in these metals. A parameter describing the relative abilities of metals to cross-slip may be assigned based on the crystal structure of that metal. Presently, this parameter is designated 'c' and is defined as the number of close packed slip systems

available for cross slip plus the one system on which slip is already occurring. In a face centered cubic crystal, there are twelve equivalent close packed slip systems. If slip is already occurring on one of these, that leaves eleven slip systems available for cross-slip. When the one operating system is added back, this yields a value of c equal to twelve for a face centered cubic metal. Similarly, values of c equal to three and one would be assigned to hexagonal close packed and body centered cubic metals respectively. In Table 3, the crystal structure and cross-slip parameter, c , are given for the metals being presently considered. Also in Table 3, the grain boundary free energy (F_{gb}) is compared to the quantity obtained by multiplying the (dw_e/dS_v) of each metal with its cross slip parameter. Very good agreement between these values is found for the metals in this study with a maximum difference of five percent.

These results may be rationalized by considering how grain boundaries inhibit dislocation motion. When a dislocation encounters a grain boundary, extra energy is required to continue deformation because the misorientation between adjoining grains interferes with slip processes. This extra energy is related to the grain boundary free energy. However, in face centered cubic and hexagonal close packed metals, there are multiple equivalent slip systems on which deformation may continue past the grain boundary. Therefore, the ability of a grain boundary to impede dislocation motion is reduced by a factor related to the ability of the metal to cross-slip. Consequently, the slope of the w_e vs S_v relation is related to the grain boundary free energy and the ability to cross-slip by:

$$\frac{dw_e}{dS_v} = \frac{F_{gb}}{c} \quad (4)$$

where all terms are as defined previously.

The Peierls stress (21,22) is the stress needed to move a dislocation through an otherwise perfect lattice. For most metals, the Peierls stress is on the order of 10^{-6} to 10^{-5} where G is the shear modulus of the metal. The stress calculated from the Peierls-Nabarro model, however, is much lower than the yield stress observed in even the highest purity metals. This difference between the observed yield strength and the stress predicted by the Peierls-Nabarro model is due to the strain energy caused by the presence of defects in the metals which impede dislocation motion. These defects include, in addition to grain boundaries, other dislocations, solute atoms, vacancies, interstitials, stacking faults and annealing twin boundaries. In this paper, high purity metals are being considered, so the consideration of solute atoms is not necessary. The effects of vacancies and self-interstitials may also be neglected because room temperature mechanical properties are being considered. Typical equilibrium volume fractions of these defects at 300 K are on the order of 10^{-15} for vacancies and 10^{-100} for interstitials (23). At this point the effects of dislocations, stacking faults and annealing twin boundaries are left to be considered.

The first of these defects to be considered will be other dislocations. The strain energy per unit length of dislocation line has been determined from elasticity theory (24) and may be expressed by:

$$U_{\perp} = \alpha G b^2 \quad (5)$$

where U_{\perp} is the elastic strain energy, G is the shear modulus of a material, b is the Burger's vector of the dislocation and α is a material constant with values ranging from 0.5 to 1.0. In order to calculate U_{\perp} , the constant α had to be determined. These values were not available for individual metals, so values based on the relationships between the magnitude of the unit Burger's vector and the lattice constant a_0 for each crystal structure were calculated. This approach was taken because much of the

strain energy associated with a dislocation is due to atoms in the vicinity of the dislocation being pushed or pulled out of their normal lattice positions. The strain energy resulting from the presence of a dislocation in a crystal, is therefore, going to depend on the equilibrium positions of the surrounding atoms. These equilibrium positions are defined by the crystal structure of a metal. In face centered cubic crystals, slip occurs in the $[110]$ direction; therefore, $\frac{a_0^2}{|b|^2} = 2$, where $|b|$ is the magnitude of the Burger's vector. Similarly, because slip occurs in the $[111]$ direction in body centered cubic crystals, $\frac{a_0^2}{|b|^2} = 4/3$. For basal slip in hexagonal close packed metals, $\frac{a_0^2}{|b|^2} = 1$. These relative values for the different crystal structures were then normalized to the range of 0.5 to 1.0. These values for α according to crystal structure are given in Table 4.

In order to calculate the elastic strain energy per unit volume due to dislocations, the dislocation line length per unit volume (dislocation density) is needed in addition to U_{\perp} . Because actual measurements of the dislocation densities (ρ_{\perp}) of the metal specimens in question were not made, a reasonable estimate of this value was necessary. Several sources (20,24,25) state that a typical value of the dislocation density of a well annealed metal is on the order of $10^{10}m^{-2}$. Because the specimens used in the cited studies (3-11) were in the annealed condition, this value of the dislocation density was used to calculate the strain energy per unit volume due to the presence of dislocations by multiplying it with U_{\perp} .

Annealing twins are most prevalent in face centered cubic metals (20,26) and are formed at the edges of grain boundary triple junctions as the junction migrates during recovery and grain growth at elevated temperatures (26). One explanation for this is that during grain growth, the possibility exists for a growing grain to meet another in such a way that the interface is near or at the coincidence boundary for a coherent twin, the $\{111\}$ plane (26). It has been calculated (27) that grains in face centered cubic metals meet in this manner about once per 16000 times. From this information, a rough estimate of the contribution of twin boundaries to the elastic strain energy of a face centered cubic metal may be made. The twin boundary energies (28) for the four fcc metals being considered are given in Table 5. From the calculation involving the probability of grains meeting in such a way to allow twin boundary formation, the twin boundary area per unit volume may be estimated by

$$A_{twin} = \frac{S_v}{16000} \quad (6)$$

where A_{twin} is the annealing twin boundary area per unit volume of metal and S_v is the grain boundary surface area per unit volume. In order to calculate the maximum possible contribution of twin boundaries to the elastic strain energy per unit volume, the calculation was made for the metal with the greatest twin boundary energy (Al) using the smallest grain size used in the grain boundary studies (5), which yielded the highest S_v and therefore, the highest A_{twin} . Using these values, the maximum contribution of annealing twin boundaries to the elastic strain energy was found to be about three orders of magnitude smaller than the contribution due to the presence of dislocations. The metals in this study have twin boundary energies (γ_{twin}) that are generally of the same order of magnitude as their grain boundary contributions to the elastic strain energy per unit volume (dw_e/dS_v). However, the occurrence of twin boundaries is over four orders of magnitude less than that of grain boundaries (Eq. 6). Consequently, twin boundary contributions to the equilibrium elastic strain energy of a pure metal will be considered negligible for the purposes of this study.

The contributions of stacking faults to the elastic strain energy should be of concern only in metals with low stacking fault energies such as copper and silver. In metals with high stacking fault

energies (Al, Ni, Zn), the stacking fault probability is much too low to be of consequence. The contribution of stacking faults to the elastic strain energy may be estimated by:

$$U_{sf} = \rho_{sf} d_{sf} \gamma_I \quad (7)$$

where U_{sf} is the elastic strain energy due to stacking faults, ρ_{sf} is the stacking fault density, d_{sf} is the stacking fault width and γ_I is the intrinsic stacking fault energy. Values for γ_I have been measured using weak beam electron microscopy. Values of ρ_{sf} have been measured using X-ray techniques for both copper (29) and silver (30). The stacking fault width may be calculated using an equation relating it to the stacking fault energy (31). Calculations of U_{sf} show that it is also three orders of smaller than the elastic strain energy due to dislocations for both copper and silver. Consequently, U_{sf} is considered negligible in this study.

The intrinsic stacking fault energies of these metals are of the same order of magnitude as their twin boundary energies as well as their grain boundary contributions to w_e . However, the stacking fault density of a metal is related to its dislocation density by:

$$\rho_{sf} = n \rho_{\perp} \quad (8)$$

where n is the measured ratio of the density of dissociated partial dislocations to the total dislocation density and all other parameters are as previously defined (29,30). The stacking fault density is about three orders of magnitude smaller than the total dislocation density. Also, the stacking fault width is generally no more than several atomic diameters (31). Therefore, the contributions of stacking faults to the elastic strain energy per unit volume at yield are negligible because the total stacking fault areas in the metals considered in this study are relatively small.

From the information given above, it may be concluded that for high purity metals, the contribution of defects other than grain boundaries, to the elastic strain energy may be estimated by calculating the elastic strain energy per unit volume due to dislocations. This quantity has been calculated for the metals considered in this study and are presented in Table 6. Also shown in Table 6 are the experimentally determined values for w_0 from Table 1. Fairly good agreement between these values is found with the average difference around ten percent. These results allow the following relation between w_0 and the strain energy per unit volume due to crystal defects in high purity metals to be drawn:

$$w_0 = U_{\perp} \rho_{\perp} \quad (9)$$

where w_0 is the contribution of defects other than grain boundaries to the elastic strain energy per unit volume, and all other terms are as previously defined.

Because actual dislocation density measurements were not made, it may be argued that the agreement between the experimental w_0 and the calculated strain energy per unit volume of defects is due to fortuitous selections of values for α in the calculation of U_{\perp} and of the dislocation density. However, it should be noted that when using reasonable values for these parameters, the results of the calculations give results that are of the correct order of magnitude which suggests that this concept may warrant more rigorous study involving the actual measurement of dislocation densities using transmission electron microscopy.

The results of the comparisons of data from grain size studies and of characteristic strain energies of crystal defects make it possible to define the elastic strain energy per unit volume in terms of

these characteristic energies and the quantities of these defects present in high purity metals. From Equations 4 and 9, the following may be derived:

$$w_e = U_{\perp} \rho_{\perp} + \frac{F_{gb}}{c} S_v \quad (10)$$

Equation 2 gave the relationship between the elastic strain energy per unit volume at yield and the yield strength as:

$$w_e = \sigma_y^2 / 2E \quad (2)$$

where all terms are as defined previously. Substituting Equation 2 into Equation 9 yields the following result:

$$\sigma_y = \sqrt{2E U_{\perp} \rho_{\perp} + 2E \frac{F_{gb}}{c} S_v} \quad (11)$$

thereby allowing the estimation of the yield strength from the characteristic energies and the volume fractions of dislocations and grain boundaries. Equation 11 shows that the yield strength of a metal increases as both the dislocation density and the grain boundary surface area per unit volume increase. This is in agreement with the general observations that the yield strength of a metal increases with cold working and with decreasing grain size.

CONCLUSIONS

(1) The elastic strain energy per unit volume at the yield point of high purity metals at room temperature may be accounted for by considering the strain energy introduced into a crystal lattice by the presence of dislocations and grain boundaries.

(2) The contributions of stacking faults, twin boundaries, vacancies and interstitials to the elastic strain energy at yield are negligible in high purity metals because of their relatively low volume fractions.

(3) The room temperature, quasi-static yield strength of high purity metals can be estimated by calculating the contributions of the appropriate crystal defects to the elastic strain energy of a metal.

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TABLE 1: Slopes and Intercepts of w_e vs S_v Data

Metal	Slope dw_e / dS_v (J/m^2)	Intercept w_0 (J/m^3)	References
Ag	0.0349	2123	6,20
Al	0.0284	2312	3,4,5,19
Cu	0.0539	3013	8
Fe	0.7800	3429	10,11
Ni	0.0560	5208	9,20
Zn	0.1190	1517	7

TABLE 2: Grain Boundary Free Energies for Pure Metals
(from Ref. 18)

Metal	Grain Boundary Free Energy, F_{gb} (J/m^2)
Ag	0.420
Al	0.340
Cu	0.625
Fe	0.780
Ni	0.690
Zn	0.340

TABLE 3: Crystal Structure, Cross-slip Parameter and Product of Cross-slip Parameter and Slope of w_e vs S_v

Metal	Crystal Structure	Cross-slip Parameter, c	$c(dw_e / dS_v)$ (J/m^2)	F_{gb} (J/m^2)
Ag	fcc	12	0.419	0.420
Al	fcc	12	0.341	0.340
Cu	fcc	12	0.647	0.625
Fe	bcc	1	0.780	0.780
Ni	fcc	12	0.672	0.690
Zn	hcp	3	0.357	0.340

TABLE 4: Values of Parameter α Assigned by Crystal Structure

Crystal Structure	α
hcp	0.5
bcc	0.67
fcc	1.0

TABLE 5: Twin Boundary Energies (from Ref. 28)

Metal	$\gamma_{twin} (J / m^2)$
Ag	0.008
Al	0.075
Cu	0.024
Ni	0.043

TABLE 6: Total Strain Energy per Unit Volume Due to Dislocations and w_0

Metal	$U_{\perp\rho_{\perp}} (J / m^3)$	$w_0 (J / m^3)$
Ag	2228	2123
Al	2125	2312
Cu	2878	3013
Fe	3193	3429
Ni	4827	5208
Zn	1289	1517

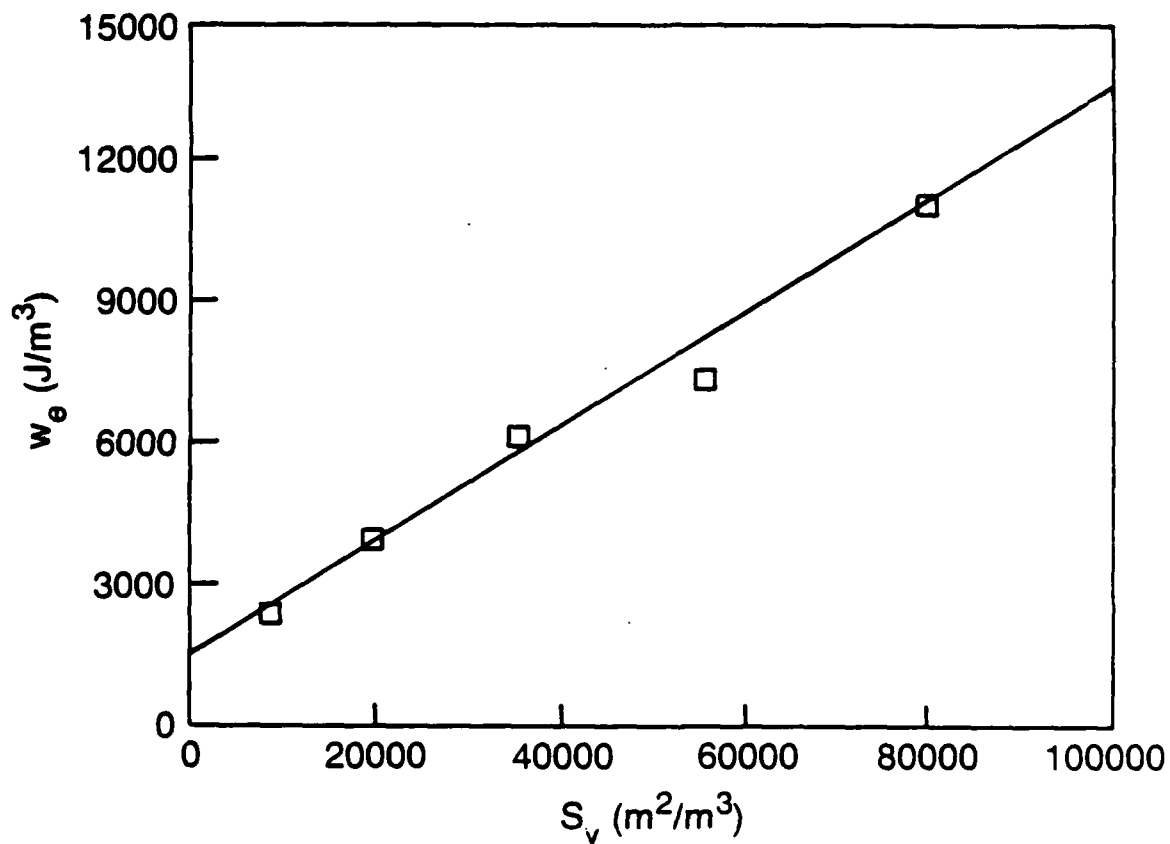


Fig. 1 — w_e vs. S_v for 99.99% pure zinc (original σ_y vs. $D^{-1/2}$ data from (7)).