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ON THE MECHANISM OF YIELDING
AND FLOW IN IRON

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ON THE MECHANISM OF YIELDING
AND FLOW IN IRON

By
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CONTENTS

	Page
Abstract	v
I. Introduction	1
II. Deformation Equations	5
III. Experimental Data	8
A. General	8
B. Evaluation of the Activation Volume v^*	10
C. Evaluation of the Activation Energy H	17
D. Evaluation of the Frequency Factor ν	22
IV. Discussion	25
V. Summary and Conclusions	31
References	32
Appendix I — References for Table I	35

TABLES

I. Summary of Data Considered	9
II. Comparison of Experiment With Theory of Dislocation Mechanisms Which Could Control Yielding and Flow in Iron	24

FIGURES

1. Schematic of the Model Proposed by Cottrell for Yielding in Iron and Steel (7519-4160)	2
2. Schematic of the Force-Distance Relationship for Yielding or Flow of Iron (7519-4148)	6
3. Variation of Upper Yield Stress σ_{uy} and Lower Yield Stress σ_{ly} With Strain Rate at 298°K (7519-4147)	11
4. Variation of Time to Yield With Stress at 298°K (7519-4149)	11
5. Effect of Shear Stress on the Activation Volume v^* for Initial Yielding in Iron and Steel (7519-4158)	12
6. Effect of Shear Stress on the Activation Volume v^* for the Lower Yield Point in Iron and Steel (7519-4159)	12
7. Effect of Shear Stress on the Activation Volume v^* for Flow Subsequent to the Lower Yield Stress (7519-4150)	14

FIGURES

	Page
8. Effect of Shear Stress on the Activation Energy for the Initiation of Yielding in Iron and Steel (7519-4151)	16
9. Variation of Stress for a Constant Delay Time With Temperature. (Values of stress at 78°K were obtained by extrapolating the initial lower stress region of the log delay time <u>vs</u> stress curve given in Reference 30) (7519-4152)	16
10. Variation of the Activation Energy for the Initiation of Yielding of Iron and Steel With Temperature (7519-4153)	18
11. Variation of the Activation Energy for the Lower Yield Stress of Iron and Steel With Temperature (7519-4154)	18
12. Variation of the Activation Energy for Dislocation Mobility With Temperature in 3.25% Silicon-Iron (7519-4155)	19
13. Variation of $\partial \ln t_d / \partial \ln \sigma$ With $1/T$ for a Mild Steel (7519-4156)	21
14. Variation of H for Yielding in Iron With the Ratio τ / τ^0 (7519-4157)	22
15. Multiplication of Dislocations by the Double Cross-Slip Mechanism of Koehler and Orowan (after Low and Guard ⁴⁴) (7519-4161)	28

ABSTRACT

The activation energy, activation volume, and frequency factor have been evaluated for yielding (delay time for yielding, upper yield stress, lower yield stress, and Lüders band propagation) and flow (friction stress, flow stress, and dislocation mobility) for various irons and steels from data in the literature. It was found that the values of these flow parameters and their stress dependence were the same, within experimental error, for both yielding and flow, and for all the materials considered. This suggests that either the same dislocation mechanism is controlling in every case, or that one or more mechanisms possess approximately the same values for these parameters. The dislocation mechanism for which there was closest agreement between theoretical calculations and experimental data was overcoming the Peierls stress.

On the basis of the available experimental data and the present analysis, it is suggested that the upper and lower yield stresses in iron and steel may represent the sudden generation of a large number of dislocations by the double cross-slip mechanism of Koehler and Orowan, rather than the breaking away from a Cottrell atmosphere.

I. INTRODUCTION

Experimental investigations on yielding and flow in iron have established that:

- a) Discontinuous yielding (i. e., the upper and lower yield points) is associated with the presence of carbon and nitrogen.^{1,2,3}
- b) The effect of grain size on the upper yield stress,[†] σ_{uy} , the lower yield stress, σ_{ly} , and the flow stress, σ_{fl} , subsequent to yielding is given by an equation of the form^{4,5,6,7,8}

$$\sigma = \sigma_i + k^* d^{-1/2} \quad , \quad \dots (1)$$

where d is the average grain diameter and k^* is a constant. σ_i is termed the friction stress and consists of two parts: an athermal component, $\sigma_i(st)$, which depends only on the structure st (e. g., precipitates, C + N in solution, etc.) and a thermal component, σ_i^* , which depends sensitively on temperature and strain rate. Equation 1 may thus be written

$$\sigma = \sigma_i^* + \sigma_i(st) + k^* d^{-1/2} \quad . \quad \dots (2)$$

Interpretation of the observed mechanical behavior during yielding and flow of iron in terms of dislocation theory is mainly due to Cottrell^{9,10} and Petch.^{5,11} Their explanation is as follows: Due to the elastic interaction between carbon and nitrogen and dislocations in iron, these interstitials segregate to the dislocations and lock them. During the initial loading of a specimen below the upper yield stress, some dislocations are torn from their interstitial atmosphere at regions of stress concentration (e. g., at S_1 in Figure 1) and act as sources for the generation of additional dislocations. The newly generated dislocations then move along the slip plane and pile up at some strong obstacle, such as a grain boundary, where they exert a stress concentration, whose value, a distance ℓ ahead of the pileup, is given by $(\sigma - \sigma_i) (d/2\ell)^{1/2}$. Here, σ is the applied stress, d is the grain diameter, and σ_i represents the resistance of the lattice to the motion of dislocations from S_1 to the grain boundary. Yielding occurs at S_2 (the

[†]In the present paper, σ indicates the tensile stress. The shear stress along the slip plane will be designated by τ , and it will be assumed that $\tau = \sigma/2$.

Figure 1. Schematic of the Model Proposed by Cottrell for Yielding in Iron and Steel

location of another locked dislocation) when the total stress there is sufficient to tear the dislocation from its atmosphere. If σ_l is the unlocking stress at S_2 , one may write

$$(\sigma - \sigma_i) (d/2l)^{1/2} + \sigma = \sigma_l ; \quad \dots (3)$$

and, if $d \gg l$, this becomes

$$\sigma = \sigma_i + (2l)^{1/2} \sigma_l d^{-1/2} , \quad \dots (4)$$

which is identical to Equation 1, with $k^* = (2l)^{1/2} \sigma_l$.

The motion of dislocations from S_1 to the grain boundary can then account for the commonly observed pre-yield microstrain,^{12,13,14} and the yielding at S_2 is identified with the upper yield stress (i. e., the formation of the initial Lüders band).[†] The lower yield stress is then a propagation of the Lüders band, and in essence is a repetition of the above process along the band front. To explain that a lower stress is required to propagate a Lüders band, as compared

[†]The initial Lüders band generally occurs in the vicinity of the grips or other regions of stress concentration. Hence, the experimental values of σ_i and σ_l of Equation 4 for the upper yield stress may be lower than the true values, by a factor representing the stress concentration.

to its initiation, it is assumed that a higher stress concentration[†] occurs at the band front than existed at the site of initial yielding, and that there are more places where the unlocking can occur.

The flow stress, for strains beyond the Lüders strain, is associated with the motion of dislocations free of their atmosphere. It is anticipated that this motion is governed by the same mechanism as that giving the friction stress, σ_i , in yielding.

Strain-aging occurs when a strained specimen is heated to a sufficiently high temperature that interstitial diffusion reforms atmospheres about the "free" dislocations. Serrated stress-strain curves result when strain-aging occurs during deformation. This will occur when the strain rate and temperature are such that initially a dislocation is torn from its atmosphere, only to regain it later as the dislocation is temporarily held up at some obstacle.

Equations 1 and 4 require that the temperature dependence of the yield stress represents the combined temperature dependence of the friction stress, σ_i , and locking stress, σ_l . Cottrell and Bilby,¹⁵ Fisher,¹⁶ and Cottrell¹⁷ have shown that one can expect a strong temperature dependence for σ_l , comparable to that observed for the lower yield stress. No complete theoretical evaluation has as yet been made for the temperature dependence of σ_i^* . However, a strong temperature dependence is observed experimentally for this parameter, and it has been suggested that σ_i^* may be due to a high Peierls stress¹⁸ or due to the movement of jogs in screw dislocations.¹⁹

The above discussion suggests considerable agreement between the experimental observations and the theoretical model. However, there exist certain experimental facts which are not in complete accord with the theory. These are:

- a) The constant, k^* , of Equation 1 for the lower yield stress is relatively independent of temperature, from 300°K to approximately 120°K.^{8,20,21} Since k^* is a measure of the unlocking stress, this is not expected from the theoretical analyses^{15,16,17} of the breaking-away from an atmosphere.
- b) The value of k^* is approximately the same for the flow stress, representing the motion of "free" dislocations, as for the lower yield stress.^{7,8}

[†]Consequently, the experimental values of σ_i and σ_l for the lower yield stress will be even less than the corresponding values for the upper yield stress.

- c) The friction stress, σ_i , obtained for mild steel by extrapolation to zero concentration of carbon plus nitrogen in solution¹⁸ has a stronger temperature dependence than the flow stress for zone refined iron.^{22,23}
- d) For a given total carbon-plus-nitrogen concentration, the temperature dependence of the lower yield stress for polycrystalline samples extrapolated to infinite grain size is stronger than that for single crystals.²³

These discrepancies between theory and experiment indicate that our understanding of the dislocation mechanisms which control yielding and flow in iron is still inadequate. One aspect which has not been previously explored in detail is to evaluate such atomic parameters as the frequency factor, the activation energy, and the activation volume for yielding and flow from mechanical test data and compare these with predictions of specific dislocation models. Consequently, this was undertaken in the present paper. Since considerable mechanical test data of value could be found in the literature, it was decided to use these data rather than initiate a new experimental program.[†]

[†]Some unpublished data by the author are also included.

II. DEFORMATION EQUATIONS

The deformation of metals may be thermally activated and, if a single deformation mechanism is controlling, the strain rate, $\dot{\gamma}$, is given by

$$\dot{\gamma} = \nu \exp(-H/kT) \quad , \quad \dots (5)$$

where ν is a frequency factor which includes essentially the frequency of vibration, the number of places where activation can take place, and the strain per successful fluctuation. H is the enthalpy of activation, which may be a function of stress and/or temperature, and can be obtained from yield and flow stress data by the following equations:²⁴

$$H = -kT^2 \left[\frac{\left(\frac{\partial \tau^*}{\partial T} \right) \dot{\gamma}}{\left(\frac{\partial \tau}{\partial \ln \dot{\gamma} / \nu} \right)_T} \right] \quad \dots (6)$$

or

$$H = k \left(\frac{\partial \ln \dot{\gamma} / \nu}{\partial 1/T} \right)_{\tau^*} \quad , \quad \dots (6a)$$

where $\tau^* = \tau - \tau_\mu$ is the effective shear stress; i. e., τ^* is the difference between the applied shear stress, τ , and the long range internal shear stress, τ_μ , the latter being proportional to the shear modulus μ . τ^* is frequently termed the thermal component of the stress.

One expects that the force-distance relationship for thermally-activated yielding or flow is of the general form shown in Figure 2. Hence, for a given value of stress, τ^* , the dislocation will take the position x_1 and the energy H which must be supplied by thermal fluctuations is given by the shaded area. One can therefore write Equation 5 as:

$$\dot{\gamma} = \nu \exp \left(- \frac{H^* - v^* \tau^*}{kT} \right) \quad , \quad \dots (7)$$

where H^* is the total area under the force-distance curve between x_1 and x_2 , and $v^* \tau^* = b L (x_2 - x_1) \tau^*$ is the work done by the stress during the thermal activation.

Figure 2. Schematic of the Force-Distance Relationship for Yielding or Flow of Iron

b is the Burgers vector, and L^* is the length of the dislocation segment involved in the activation. v^* is the "activation volume."

If the total energy to overcome the obstacle to flow (i. e. the total area under the force-distance curve) is not a function of stress, one can obtain the value of v^* in the following manner: From Figure 2 we note that H can be expressed as

$$H = \int_{F = \tau^* b L}^{F_{\max}} (x_2 F - x_1 F) dF, \quad \dots (8)$$

which gives, upon differentiation with respect to τ^* ,

$$-\left(\frac{\partial H}{\partial \tau^*}\right)_T = (x_2 - x_1) b L = v^*. \quad \dots (9)$$

Furthermore, from Equation 5 we obtain

$$-\left(\frac{\partial H}{\partial \tau^*}\right)_T = kT \left(\frac{\partial \ln \dot{\gamma} / \nu}{\partial \tau^*} \right)_T, \quad \dots (10)$$

and combining Equations 9 and 10 gives[†]

$$v^* = kT \left(\frac{\partial \ln \dot{\gamma} / \nu}{\partial \tau^*} \right)_T \quad \dots (11)$$

In the above, we have derived equations for the activation energy and the activation volume for a particular deformation mechanism. Of additional interest is an evaluation of the frequency factor, ν , of Equation 5. This can be obtained from the slope of a plot of H vs temperature; for, upon taking the logarithm of Equation 5 and rearranging, one obtains:

$$H = kT \ln(\nu / \dot{\gamma}) \quad \dots (12)$$

Equation 12 indicates that, when $\nu = \text{const.}$, H is proportional to the temperature for a constant strain rate.

[†]If the total energy is a function of the stress, then the quantity $[(\partial \ln \dot{\gamma} / \nu) / \partial \tau^*]_T$ is not the "true" activation volume, but rather simply represents $(\partial H / \partial \tau^*)_T$

III. EXPERIMENTAL DATA

A. GENERAL

The values of H , v^* , and ν were determined by Equations 6, 6a, 11, and 12, for the materials and testing conditions listed in Table I. To study the effect of stress on H and v^* , comparisons between the various materials had to be made at the same value of τ^* . Since τ_μ could not be obtained directly from the available data, it was decided to eliminate the athermal component of the stress by subtracting a reference stress, τ° , from the applied stress. For example, since the yield stress is given by

$$\tau(T, \dot{\gamma}) = \tau^*(T, \dot{\gamma}) + \tau_\mu \quad , \quad \dots (13)$$

then, for a constant value of τ_μ ,

$$\tau(T, \dot{\gamma}) - \tau^\circ(T, \dot{\gamma}) = \tau^* - \tau^{\circ*} \quad , \quad \dots (14)$$

and the athermal component is eliminated. Here, it is assumed that the change in τ_μ with temperature, due to the change in shear modulus with temperature, is small compared to the change in τ^* with temperature. In view of the strong temperature dependence of the yield and flow stress in iron, this assumption is justified.

The choice of τ° is somewhat arbitrary. In the present analysis, τ° was chosen as either: (1) the stress at 300°K associated with a time of yielding of ~ 1 sec, or (2) the stress at 300°K for a strain rate of $\sim 10^{-1}$ sec. The reason for this choice of τ° can be seen by referring to Figures 3 and 4, in which the stress for yielding is plotted vs the logarithm of the strain rate and vs the logarithm of the time of yielding. From these plots, it is seen that sharp changes in slope occur at strain rates of 10^{-1} to 1 sec^{-1} , or time of yielding of 1 to 10 sec. Additional support for the equivalence of these two definitions of τ° will become evident subsequently.

TABLE I
SUMMARY OF DATA CONSIDERED

Author†	Material	Grain Size ASTM Number	Type of Test
H. G. Baron	Armco Iron (0.021 C) Mild Steel (0.20 C) 0.34 C Steel Quench and Temper		T- ϵ
P. E. Bennett and G. M. Sinclair	Ingot Iron (0.012 C)	4	S- ϵ
H. Conrad	Electrolytic Iron (0.014 C)	8	T- ϵ
J. C. Fisher and H. C. Rogers	SAE 1010 Steel	8	T- c_L
J. A. Hendrickson, D. S. Wood, and D. S. Clark	Mild Steel (0.12 C)	6.7	T- σ
J. A. Hendrickson and D. S. Wood	Mild Steel (0.17 C)	6.5	T- P_m
J. A. Hendrickson, D. S. Wood, and D. S. Clark	Mild Steel (0.17 C)	6.5	T- σ
J. Heslop and N. J. Petch	Mild Steel (0.11 C)	4 - 7	T- ϵ
J. M. Krafft and A. M. Sullivan	Low Carbon Iron (0.01 C) 1010 Steel (0.11 C) Mild Steel (0.16 C) Mild Steel (0.22 C) Mild Steel (0.22 C) 0.31 C Steel	6 7.5 8 9 8 8	C- P_t C- P_t C- P_t C- P_t C- P_t C- P_t
C. W. MacGregor and J. C. Fisher	SAE 1020 Steel SAE 1045 Steel		T- ϵ T- ϵ
M. J. Manjoine	Mild Steel		T- ϵ
J. L. M. Morrison	0.2 C and 0.6 C Steel		T- ϵ
H. Quinney	Yorkshire Iron		T- ϵ
D. F. Stein and J. R. Low	Silicon-Iron (3.25 Si, 0.005 C)	Single Crystal	B- P_d
J. Winlock and R. Leiter	Low Carbon Steel Low Carbon Steel	20/in. ² 200/in. ²	T- ϵ T- ϵ
J. Winlock	0.06 C Steel 0.21 C Steel 0.34 C Steel 0.48 C Steel		T- ϵ T- ϵ T- ϵ T- ϵ

†References are listed in Appendix I.

TABLE I (Continued)

Author†	Material	Grain Size ASTM Number	Type of Test
D. S. Wood and D. S. Clark	Mild Steel (0.17 C)	6.5	T-P _t
	Mild Steel (0.12 C)	6.7	T-P _t
	Mild Steel (Decarb)	6.1	T-P _t
	Mild Steel (Decarb and Recarb)	6.1	T-P _t
	Mild Steel (Decarb plus Renitride)	6.1	T-P _t
T. Vreeland, D. S. Wood, and D. S. Clark	Mild Steel (0.12 C)	6.7	T-P _m
C. Zener and J. H. Hollomon	0.25 C Steel (Tempered Bainite)		T- $\dot{\epsilon}$

Significance of Symbols

T = tension

C = compression

S = torsion

B = bending

 $\dot{\sigma}$ = constant stress rate $\dot{\epsilon}$ = constant strain rateP_t = stress pulse – delay time studiesP_m = stress pulse – microstrain studiesP_d = stress pulse – dislocation mobility studiesc_L = creep – Lüders band propagation

†References are listed in Appendix I.

B. EVALUATION OF THE ACTIVATION VOLUME v^*

The activation volume, v^* , was obtained by Equation 11, § from data on the variation of time to yield with stress and from the effect of strain rate on stress. In the present analysis, $\partial \ln \dot{\gamma} / \partial \tau^*$ was taken from the slope of a semilog plot of strain rate or delay time vs stress. Generally, when a curvature occurred in such a plot, three slopes were taken, that for the lowest stress, the median stress, and the highest stress. In those cases where the stress range was insufficient to indicate a curvature on the semilog plot, the average slope of the straight line was identified with the average value of the stress over the range for which the data were given.

§It was assumed that $\nu = \text{const.}$, independent of stress and temperature. The justification for this assumption will be given in a subsequent section.

Figure 3. Variation of Upper Yield Stress σ_{uY} and Lower Yield Stress σ_{lY} With Strain Rate at 298°K

Figure 4. Variation of Time to Yield With Stress at 298°K

Figure 5. Effect of Shear Stress on the Activation Volume v^* for Initial Yielding in Iron and Steel

Figure 6. Effect of Shear Stress on the Activation Volume v^* for the Lower Yield Point in Iron and Steel

The values of v^* obtained for yielding and flow in iron[†] are given as a function of stress in Figures 5, 6, and 7. In Figure 5, it is seen that the various data for both the delay time and the upper yield stress fall within one scatter band, indicating that both types of test measure the same phenomenon, i. e., the initiation of yielding. The values of v^* for the initiation of yielding decreases from about $30b^3$ at $\tau = \tau^0$ to about $8b^3$ at $\tau - \tau^0 = 38 \text{ kg/mm}^2$, and is independent of carbon content over the range from wet-hydrogen-treated material to 0.6% carbon. For stresses below τ^0 , the activation volume increases quite rapidly, to values in excess of $100b^3$. This rapid increase in v^* is associated with the low stress region in Figures 3 and 4, where the stress is relatively insensitive to the strain rate or delay time. For the range $(\tau - \tau^0) > 1$, a straight line is obtained when v^* is plotted vs the logarithm of $\tau - \tau^0$, and one obtains $v^* = 26b^3 - 5.2b^3 \ln(\tau - \tau^0)$.

Figure 6 gives v^* as a function of the stress for the lower yield stress. For comparison, the average curve of Figure 5 for initial yielding is included. It is seen, from Figure 6, that the variation of v^* with stress for the lower yield stress shows the same general trend as for the upper yield stress (or delay time for yielding). The values of v^* for the lower yield at a given stress are approximately 1.2 to 1.3 times that for the upper yield, i. e., $v_{ly}^*/v_{uy}^* = 1.2$ to 1.3. Of significance in this regard is that the difference between the upper yield stress and the lower yield stress at a given temperature also corresponds approximately to $\sigma_{uy}/\sigma_{ly} = 1.2$ to 1.3.⁸ This suggests that the difference between the upper and lower yield stresses is the difference in stress concentration, q , existing at a Lüders band front, compared to that existing at the site of the formation of the initial band, rather than the operation of different mechanisms, as indicated earlier.⁸ The present results on v^* , and those on the variation of the upper and lower yield stress with temperature,⁸ would thus indicate that $q_{ly}/q_{uy} = 1.2$ to 1.3.

A further point of interest, in regard to Figure 6, is that v^* obtained from measurements of the rate of Lüders band propagation²⁵ agrees with the value obtained from the effect of strain rate on the lower yield stress.

[†]The values of v^* obtained by using the measured stress values will be too large, by a factor q , which represents the stress concentration factor. Hence, they represent an upper limit to the true values.

Figure 7. Effect of Shear Stress on the Activation Volume v^* for Flow Subsequent to the Lower Yield Stress

Figure 7 gives the effect of stress on v^* for flow beyond the Lüders strain. Included in this figure are values of v^* obtained from measurements of pre-yield microcreep,¹² and of dislocation velocities in silicon-iron determined by etch-pit technique.²⁶ The dashed curve in this figure is the average curve for the lower yield stress, taken from Figure 6.

It is seen, from Figure 7, that the values of v^* for microcreep, the flow stress, and dislocation mobility fall, for the most part, about the curve for the lower yield stress. However, in the range of $\tau - \tau^0 = 2$ to 8 kg/mm^2 , two sets of data, that by MacGregor and Fisher²⁷ for the flow stress in steel, and that by Stein and Low²⁶ for the dislocation mobility in silicon-iron, lie somewhat above the curve for the lower yield stress. In the case of the data by MacGregor and Fisher, this may represent an effect of strain rate on structure, for the value of $\partial \ln \dot{\gamma} / \partial \tau^*$ was evaluated by comparing the stresses at a constant strain on the stress-strain curves obtained at different strain rates. The possible effect of strain rate on structure was eliminated in tests by the author,²⁸ where the strain-rate was changed during deformation (i. e., by employing so-called "differential" tests). The values of v^* obtained in this manner are in good agreement with the curve for the lower yield stress (See Figure 7).

In the case of the data for the mobility of dislocations in silicon-iron, the higher values of v^* , in the range of $\tau - \tau^0 = 2$ to 8 kg/mm^2 , can be due to the difficulty of identifying τ^0 exactly from the data given by Stein and Low. For these data, τ^0 was taken as 14.5 kg/mm^2 . This is approximately the shear stress for a dislocation velocity of 10^{-4} cm/sec at 298°K .

There are two additional points, in regard to v^* for flow, worthy of mention. First, v^* for the pre-yield microstrain, obtained from the data by Hendrickson et al.,¹² falls near the curve of Figure 7 only if the total applied stress is considered, rather than $\tau - \tau^0$. Second, since k^* of Equation 1 for the lower yield stress at 194°K was found by Heslop and Petch²⁹ to be independent of strain rate, the values of v^* obtained from their data for the lower yield stress also apply to the friction stress, σ_i , at this temperature. Hence, one expects that v^* for the friction stress also lies along the dashed curve of Figure 7.

Figure 8. Effect of Shear Stress on the Activation Energy for the Initiation of Yielding in Iron and Steel

Figure 9. Variation of Stress for a Constant Delay Time With Temperature (Values of stress at 78°K were obtained by extrapolating the initial lower stress region of the log delay time vs stress curve given in Reference 30)

C. EVALUATION OF THE ACTIVATION ENERGY H

The value of H can be obtained from the experimental data by employing Equations 6 and 6a.[†] Further, by combining Equations 6 and 11, one obtains

$$H = -v^* T \left(\frac{\partial \tau^*}{\partial T} \right) \dot{\gamma} \quad \dots (15)$$

Figure 8 gives the effect of stress on the activation energy for the initiation of yielding, as determined from Equations 6a and 15.[§] From this figure, it is seen that H decreases from approximately 0.5 to 0.6 ev at $\tau = \tau^0$ to approximately 0.06 ev at $\tau - \tau^0 = 46 \text{ kg/mm}^2$.

Equation 12 indicates that, if ν is a constant, H will be proportional to the temperature if temperature is substituted for stress in Figure 8. The relationship between stress and temperature can be obtained from constant strain rate tests, or by plotting the stress for a given delay time vs the temperature (See, for example, Figure 9, derived from data by Clark³⁰). The proportionality between H and the temperature is shown, in Figure 10, for the two materials (ingot iron and mild steel) for which sufficient data were available for the evaluation. The value of H_0 for $T = T_0$ ($\tau = \tau^0$) is 0.53 ev for both materials.

A plot of H vs temperature for the lower yield stress is given in Figure 11, where $H_0 = 0.60 \text{ ev}$. The data points for this figure were derived by taking the values of v^* from the average curve, given in Figure 6, and the values of $\partial \tau^* / \partial T$ from the average curve for the effect of temperature on the lower yield stress of various irons and steels with a total carbon-plus-nitrogen content greater than 0.01% by weight. (Curve A in Figure 2 of Reference 23).

Since the temperature dependence of the friction stress, σ_i , and the flow stress, σ_{fl} , is practically the same as that for the lower yield stress,⁸ and since the values of v^* are practically the same (See Figure 7), the variation of H with temperature for the friction stress and the flow stress will be the same as that given in Figure 11 for the lower yield stress. Similarly, the value of H_0 ($\sim 0.6 \text{ ev}$) will be the same for all three parameters.

[†]Here, also, it is assumed that $\nu = \text{const.}$

[§]The values of H derived from these equations do not include a stress concentration factor, and hence can be considered as "true" values.

Figure 10. Variation of the Activation Energy for the Initiation of Yielding of Iron and Steel With Temperature

Figure 11. Variation of the Activation Energy for the Lower Yield Stress of Iron and Steel With Temperature

Of special significance is an evaluation of H_0 for the mobility of dislocations in silicon-iron, for here one deals directly with the motion of free dislocations. The variation of H with temperature, obtained from the data given by Stein and Low²⁶ in their Figure 9, is presented in Figure 12 of this paper for two dislocation mobilities, namely 10^{-2} cm/sec and 10^{-6} cm/sec. It is noted, in Figure 12, that $H_0 = 0.55$ to 0.59 ev, in agreement with the values for the upper yield, lower yield, and flow stresses of iron and steel.

Figure 12. Variation of the Activation Energy for Dislocation Mobility With Temperature in 3.25% Silicon-Iron

Finally, it is of interest to interpret the significance of the values of the activation energy, $Q = 0.44$ to 0.61 ev, obtained by Zener and Hollomon³¹ for yielding and flow of various irons and steels. They found that the yield and flow stress could be expressed as a function of the parameter $P = \dot{\epsilon} \exp(Q/kT)$ so that

$$\sigma \propto P^n \propto \left[\dot{\epsilon} \exp(Q/kT) \right]^n, \quad \dots(16)$$

where $\dot{\epsilon}$ is the tensile strain rate and n is a constant, of value between 0.01 and 0.02. It will now be shown that Equation 16 can be developed from Equation 5. Referring to Figure 2, we can write, for H ,

$$H = H_0 - v \tau^* , \quad \dots(17)$$

where H_0 is the total area under the curve from $x = 0$ to $x = a$ (i. e., the value of H for $\tau^* = 0$) and $v \tau^*$ represents the total work done by the stress when the dislocation moves from $x = 0$ to $x = a$. Here, v does not have the physical significance of v^* of Equation 11, but merely represents a volume term by which the stress is multiplied to give the total work done by the stress in overcoming the obstacle to flow.[†] Substituting the H , given by Equation 17, into Equation 5 and rearranging, we have

$$\frac{\dot{\gamma} \exp(H_0/kT)}{\nu} = \exp \left[\frac{v(\tau^*) \tau^*}{kT} \right] . \quad \dots(18)$$

Since one obtains a straight line when the logarithm of the experimental tensile strain rate $\dot{\epsilon}$ is plotted vs the logarithm of the tensile stress σ (See, for example, References 31 and 32), it appears that, for the stress range considered,

$$\exp \left[\frac{v(\tau^*) \tau^*}{kT} \right] \approx (\sigma/\sigma^0)^m , \quad \dots(19)$$

or

$$\ln(\sigma/\sigma^0) \approx \frac{v(\tau^*) \tau^*}{mkT} \approx \frac{v(\tau^*) \tau^*}{c} , \quad \dots(19a)$$

where σ^0 is a constant (e. g., the reference stress at $T = 300^\circ\text{K}$ and $\dot{\epsilon} = 10^{-1} \text{sec}^{-1}$) and $m = \partial \ln \dot{\epsilon} / \partial \ln \sigma = 1/n$. Since v is primarily a function of stress alone,[§] and since the left hand side of Equation 19a is only a function of the stress, c must be a constant for a given material (i. e., m must be proportional to $1/T$). That this is essentially the case is shown in Figure 13, where m for both delay time data and upper yield stress data for a mild steel (0.17 C) is plotted vs the reciprocal of the temperature.

If Equation 19 is valid, the values of Q obtained by Zener and Hollomon³¹ should be approximately equal to H_0 of Equation 17. The agreement between the present values of H_0 (0.5 to 0.6 ev) and those obtained by Zener and Hollomon

[†]If the total energy to overcome the obstacle to flow varies with the stress, then $H_0 - v \tau^*$ is merely an empirical approximation for $H(\tau^*)$, and $v \tau^*$ does not represent the total work done by the stress.

[§]The data of Figures 5, 6, and 7 support this, for the values of v^* for a given stress were obtained at various temperatures.

Figure 13. Variation of $\partial \ln t_d / \partial \ln \sigma$ With $1/T$ for a Mild Steel

(0.44 to 0.61 ev) lend support to this interpretation. Also, by substituting Equation 19a into Equation 17, we obtain

$$H = H_0 - c \ln(\sigma/\sigma^*) \quad , \quad \dots (20)$$

indicating that the activation energy decreases approximately with the logarithm of the stress, which has been shown to be the case for yielding in iron and steel by Yokobori³³ and Campbell.^{34,35}

Plots of H vs $\log_{10}(\tau/\tau^*)$ (data taken from the curve of Figure 5) are given in Figure 14, for values of τ^* of 1, 5, 10, and 15 kg/mm², which is the range of τ^* for the materials considered in the present paper. From this figure, it is seen that Equation 20 is approximated over a relatively large part of the stress range considered. Further, it is evident that c increases as τ^* increases. An approximation to this variation of c with τ^* was found to be $c = 1.5(\tau^*)^{1/4}$, when c is expressed in electron volts and τ^* in kg/mm².

As a check on the consistency of the above relationships, it is interesting to compare the value of c for mild steel ($\tau^* \approx 14$ kg/mm²), obtained from the slope ($= c/k$) of Figure 13, with that from the slope ($= c$) of Figure 14. From the

Figure 14. Variation of H for Yielding in Iron With the Ratio τ/τ^0

former, one obtains $c = 0.35$ eV; while, from the latter, $c = 0.30$ eV. This represents rather good agreement, considering the scatter in H , and suggests that Equation 20 [or the equivalent empirical expression by Yokobori,³³ $H = -a \log(\sigma/\sigma_0)$, where σ_0 is the stress at 0°K] is a good approximation for the effect of stress on the activation energy for yielding and flow in iron and steel.

D. EVALUATION OF THE FREQUENCY FACTOR ν

One can obtain ν of Equation 5 from the slopes of the plots of H vs temperature, such as those of Figures 10 and 11. These yield $\nu = 10^8$ to 10^9 sec^{-1} for the upper and lower yield stress, when the shear strain rate, $\dot{\gamma}$, is taken to be $3/2$ the tensile strain rate, $\dot{\epsilon}$. Since the flow stress beyond yielding exhibited the same ν^* , H , and temperature dependence as the lower yield stress, ν for flow is also $\approx 10^8$ to 10^9 sec^{-1} . Further, writing, for the delay time, t_d :

$$t_d = t_0 \exp(H/kT) \quad , \quad \dots(21)$$

one obtains, from Figure 10, $t_0 = 1.9 \times 10^{-9} \text{ sec}$ for the initial yielding of a mild steel, indicating that $t_0 \approx 1/\nu$. Finally, writing, for the dislocation velocity, $\dot{s}$, studied by Stein and Low,²⁶

$$\dot{\epsilon} = \nu' \exp(-H/kT) \quad , \quad \dots(22)$$

one obtains, from Figure 12, $\nu' = 10^5$ to 10^6 cm/sec⁻¹.

From a knowledge of ν' , one can obtain an estimate of the dislocation density, ρ , involved in yielding and flow for

$$\nu = \rho b \nu' \quad . \quad \dots(23)$$

Using the above values of ν and ν' , one obtains $\rho \approx 10^{10}$ cm⁻², which is compatible with the dislocation density obtained by Harper³⁶ from internal friction studies on cold-worked iron. Further, from the data on the initial creep rate in pre-yielding microcreep,¹² one obtains $\nu = 1$ sec⁻¹. Using this value in Equation 23 gives $\rho \approx 10^2$ cm⁻², indicating that only a small fraction of the initial dislocation density (estimated to be $\sim 10^8$ cm⁻²) is involved in microcreep.

Several factors suggest that ν (or t_0) is relatively independent of stress and temperature.[†] First, the fact that the derived values of H are proportional to the temperature strongly suggests that $\nu \approx \text{const}$. If this is so, then either ν is independent of stress and temperature or the combined effect of stress and temperature is such as to maintain ν constant. In the latter case, if ν is independent of either stress or temperature, then it must be independent of both. The fact that, ingeneral, when the logarithm of the strain rate at a constant stress is plotted vs the reciprocal of the temperature, one obtains a straight line, suggests that ν is relatively independent of temperature, and hence of stress as well. Also, the fact that the activation volume, obtained from Equation 12, was primarily a function of stress alone, over a wide temperature range, supports the assumption that ν is independent of stress and temperature.

[†]Unless the effects of stress and temperature on ν are very strong (e. g., an exponential or power effect), they will be overshadowed by the role stress and temperature play in the Boltzmann exponential.

TABLE II
COMPARISON OF EXPERIMENT WITH THEORY OF DISLOCATION MECHANISMS WHICH COULD
CONTROL YIELDING AND FLOW IN IRON

Mechanism	Theoretical Estimates†		Experimental Data	
	Equation and Value	Ref	Equation and Value	Ref
Breaking away from Cottrell Atmosphere	$H_1 = 0.9(1 - \tau/\tau_0)^3$, $H_1(\tau/\tau_0 = 0.25) = 0.38 \text{ ev}$	17	$H_1(\tau/\tau_0 = 0.25) = 0.5 \text{ to } 0.6 \text{ ev}$	1-3
	$\tau_0 = \frac{H_1(\tau=0)}{4.5 b^3} = 200 \text{ kg/mm}^2$	17	$\tau_0 = 55 \text{ kg/mm}^2$	
	$t_0 \approx \frac{10^2}{\nu_d} = 10^{-11} \text{ sec}$	17	$t_0 = 10^{-8} \text{ to } 10^{-9} \text{ sec}$	
	$H_1 = -\alpha \ln(\tau/\tau_0)$, $H_1(\tau/\tau_0 = 0.25) = 0.4 \text{ to } 0.6 \text{ ev}$	15, 33	$H_1 = H_0 - c \ln(\tau/\tau^*)$ Upper and lower yield points are associated with the presence of C and N	
Overcoming Peierls Stress	$\tau_p = \frac{2\mu}{1-\nu^*} \exp\left[-\frac{2\pi a}{b(1-\nu^*)}\right] = 2 \times 10^{-3} \mu$	38	$\tau_p = 5 \times 10^{-3} \mu$	12, 16 44
	$E_m - E_0 = \frac{b^2 \tau_p}{\pi} = 1 \times 10^{-3} E_m$	39, 40	$E_m - E_0 = 3 \times 10^{-3} E_m$	
	$\nu = \frac{\rho^{1/2} b^3 \nu_d}{f^2} \approx 10^8 \text{ sec}^{-1}$		$\nu = 10^8 \text{ to } 10^9 \text{ sec}^{-1}$ Dislocations in silicon-iron lie along close-packed directions	
Cross-slip	$H = H_Q - c \ln(\tau/\tau^*)$, $H_Q(\text{Al}) \approx 1 \text{ ev}$ $c(\text{Al}) \approx 0.35 \text{ ev}$	41	$H = H_Q - c \ln(\tau/\tau^*)$, $H_Q(\text{Fe}) = 0.5 \text{ to } 0.6 \text{ ev}$ $c(\text{Fe}) = 0.2 \text{ to } 0.35 \text{ ev}$	
	$\gamma_{\text{Al}} = \left[\frac{H_Q(\text{Cu})\mu(\text{Al})}{H_Q(\text{Al})\mu(\text{Cu})} \right] \gamma_{\text{Cu}} \approx 140 \text{ ergs/cm}^2$	42	$\gamma_{\text{Fe}} = 150 \text{ to } 250 \text{ ergs/cm}^2$	
	$\nu = \frac{b^2}{f^2} \nu_d \approx 10^{10} \text{ sec}^{-1}$		$\nu = 10^8 \text{ to } 10^9 \text{ sec}^{-1}$ Copious cross-slip occurs during deformation of iron	
Movement of jogs in screw dislocations	$H = H_f^v - f b d \tau^*$, $H_f^v \approx 1.5 \text{ ev}$	43	$H_f^v = 0.5 \text{ to } 0.6 \text{ ev}$	
	$l_j = 50b$ $\nu = \frac{\rho b^3 \nu_d}{f} \approx 10^8 \text{ sec}^{-1}$	19	$l_j = 30b$ $\nu = 10^8 \text{ to } 10^9 \text{ sec}^{-1}$	

†Significance of Symbols

H_1 = Energy for unlocking
 H_Q = Energy for cross-slip
 H_f^v = Energy to form a vacancy
 E_m = Maximum dislocation line energy
 E_0 = Minimum dislocation line energy
 μ = Shear modulus
 ν^* = Poissons ratio

ν_d = Debye frequency
 b = Burgers vector
 a = Spacing between slip planes
 ν = Frequency factor
 γ = Stacking-fault energy
 ρ = Dislocation density
 l = Length of dislocation segment
 l_j = Distance between jogs

d = Activation distance
 τ = Applied shear stress
 τ^* = Effective shear stress
 τ_0 = Applied shear stress at 0°K
 τ_p = Peierls shear stress at 0°K
 τ^* = Yield stress at 300°K for a strain rate of 10^{-1} sec^{-1}
 a, c, t_0 = Constants

IV. DISCUSSION

In the preceding section, it was found that, at low temperatures, the initiation of yielding (delay time for yielding and the upper yield stress), the propagation of yielding (Luders band propagation and the lower yield stress), and subsequent flow (dislocation mobility and the flow stress beyond the Luders strain) all exhibit essentially the same values of the activation volume, v^* , and the activation energy, H , as a function of stress. Also, wherever comparison was possible, there was good agreement in the values of the frequency factor, ν . This suggests that either these phenomena are controlled by the same dislocation mechanism, or by different mechanisms which are characterized by nearly the same values of v^* and H . In this section, a comparison will be made between the experimental values of these parameters and those predicted by specific dislocation models, to see if the controlling mechanism (or mechanisms) can be identified.

Dislocation mechanisms which might control yielding or flow in iron at low temperatures are:

- a) Breaking away from a Cottrell atmosphere
- b) Overcoming the Peierls stress
- c) Intersection of dislocations ("cutting the forest")
- d) Cross slip
- e) Production of vacancies or interstitials at jogs in dislocations with a screw component.

Of these, the intersection of dislocations can be immediately eliminated for two reasons: (a) the experimental activation volume (10 to $30b^3$) is several orders of magnitude smaller than one expects for this mechanism,³⁷ and (b) the measured activation volume does not decrease with strain,^{8, 28} as is expected for a metal such as iron, where slip occurs on several planes. These limitations do not apply to the four remaining mechanisms, and a detailed comparison between experiment and theory was made, which is summarized in Table II. From this table, it is seen that there is some agreement between theory and experiment, for all four mechanisms, making it difficult to identify the one which is controlling.

Initially, let us consider the movement of "free" dislocations, as given by the mobility determined by etch pits or by the flow stress beyond the Luders strain. Here, we can eliminate the breaking-away from a Cottrell atmosphere as the controlling mechanism, leaving overcoming the Peierls stress, cross-slip, and the movement of jogs in screw dislocations as possible mechanisms. For each of these mechanisms, the estimated activation volume[†] (~ 10 to $50b^3$) and frequency factor ($\sim 10^8$ to 10^{10} sec⁻¹) are in accord with the experimental values. Referring to Table II, further comparison between theory and experiment indicates that, for the motion of jogs in screw dislocations, the activation energy is only about one-third that expected for the formation of vacancies in iron, on the basis that the energy to form a vacancy is about one-half of the energy for self-diffusion (~ 3 ev). In the case of the Peierls mechanism, the experimental Peierls stress and energy are about three times that estimated theoretically. However, in view of the approximations involved in calculating the Peierls stress, this is not a serious disagreement. Since no theoretical calculations have been made for cross-slip in iron, the present experimental values are compared with calculations on aluminum, which also exhibits considerable cross-slip. From Table II, it is seen that the experimental activation energy, its stress dependence, and the derived stacking-fault energy for iron are in agreement with those for cross-slip in aluminum.

The above comparisons do not permit a positive choice between the three mechanisms. However, on the basis of Stein and Low's²⁶ observation that the yield stress in silicon-iron exhibits the same temperature dependence as the mobility of edge dislocations, which cannot cross-slip,[§] one is inclined to favor the Peierls or dragging of jogs over the cross-slip mechanism.

[†]For the movement of jogs in screw dislocations, Schoeck¹⁹ has calculated the density of jogs which will be frozen-in, as a result of cooling from above one-half the melting temperature in °K. This gives a spacing between jogs, l_j , of $\sim 50b$ and hence an activation volume, v_0 , of $\sim 50b^3$. Likewise, Seeger's treatment³⁹ of the Peierls mechanism, and Schoeck and Seeger's treatment⁴¹ of cross-slip, suggest that the length, l , of dislocation segment involved in the thermal activation is ~ 10 to $50b$, and hence $v_0 \approx 10$ to $50b^3$. The total energy may vary with stress for the Peierls and cross-slip mechanisms; hence v^* , as given by Equation 11, may not represent the "true" activation volume.

[§]However, vacancies can be produced at jogs in mixed dislocations of predominantly edge character.

For further comparison, it is of interest to determine, from the data of Stein and Low,²⁶ the value of the average distance, s , an edge dislocation moves per successful thermal fluctuation. This can be obtained from the value of the frequency factor, ν' , given in Figure 12. For the Peierls mechanism

$$s = \frac{L^{*2} \nu'}{Lb \nu_d} \approx b \quad ; \quad \dots (24)$$

while, for the dragging of a jog,

$$s = \frac{L^* \nu'}{b \nu_d} \approx 100 b \quad , \quad \dots (25)$$

where L is the average length of an edge dislocation[†] ($\sim 10^{-4}$ cm), b is the Burgers vector, L^* is the length of dislocation segment involved in thermal activation ($\sim 30 b$), and ν_d is the Debye frequency ($\sim 10^{13}$ sec⁻¹). The values of s obtained by Equations 24 and 25 are in accord with the respective mechanisms, and hence a separation cannot be made on this basis.

However, two additional facts favor the Peierls mechanism over cross-slip: (a) the dislocations in silicon-iron lie along close-packed directions, suggesting a high Peierls stress; and (b), if the dragging of jogs were controlling, one would expect a change in v^* with strain, which is not observed. These factors, plus the fact that the observed activation energy of 0.5 ev is somewhat low for the production of vacancies, suggest that the controlling mechanism for the motion of free dislocations in iron is the overcoming of the Peierls stress hills. Further, since the values of ν , H , and v^* for the lattice friction stress are the same as for the flow stress, one can conclude that overcoming the Peierls stress is also the controlling mechanism here.

Since k^* of Equation 1 is independent of temperature, and since its value is the same for both yielding and flow beyond the ^{||}Luders strain, Conrad and Schoeck⁸ have suggested that perhaps it represents a stress other than the Cottrell locking stress. If this is the case, then the upper and lower yield stress must represent the sudden generation of a large number of dislocations, by some mechanism other than the breaking-away from a Cottrell atmosphere. One mechanism which could produce large numbers of dislocations, and would be in accord with observations on silicon-iron,⁴⁴ is the double cross-slip mechanism,

[†]The value of L was taken as 1/20 of the distance moved by the edge dislocation, for Low and Guard⁴⁵ found that the edge components in silicon-iron moved, on the average, about 20 times farther than the screw components.

originally proposed by Koehler⁴⁵ and Orowan,⁴⁶ and discussed by Low and Guard⁴⁴ and Johnston and Gilman⁴⁷ (See Figure 15). The operation of this double cross-slip could be controlled by the mobility of the edge component in two ways:

- a) From a purely geometric standpoint, the farther the edge component moves, the greater is the length of screw component formed, and hence the greater is the probability that cross-slip will occur.
- b) Johnston and Gilman^{47, 48} have shown, in LiF, that new dislocations are created out of the wake of a moving dislocation, and that the number of new dislocations is proportional to the distance traveled by the original dislocation loop.

Figure 15. Multiplication of Dislocations by the Double Cross-Slip Mechanism of Koehler and Orowan (after Low and Guard⁴⁴)

The stress-strain behavior of iron and steel may thus represent the following: During the initial loading of the specimen below the upper yield stress, some dislocations are torn from their Cottrell atmosphere at regions of stress concentrations, such as inclusions or precipitates. As the stress is increased,

their mobility increases and some multiplication occurs by the double cross-slip mechanism. This gives the pre-yield microstrain. At a critical stress, first reached near the specimen grips, and representing the upper yield stress, sudden, profuse multiplication occurs by the double cross-slip mechanism, giving a Luders band with a dislocation density of approximately 10^{10} cm^{-2} . At the lower yield stress, this multiplication continues at the stress concentration existing at the band front. Once the Luders band has traversed the specimen, very little additional dislocation multiplication occurs, and the deformation is essentially a movement of existing dislocations. In this picture, the three phenomena: microstrain, yielding, and flow, are associated with the movement of free dislocations. Furthermore, the above analysis suggests that the controlling mechanism is the overcoming of the Peierls stress by the edge components.

At present, there is insufficient data on single crystals and high purity polycrystals of iron to ascertain the reason for the weaker temperature dependence of the yield stress of these materials, compared to impure polycrystalline specimens. It may be that the frequency factor is larger (e.g., the number of dislocations involved in the deformation or the total strain associated with a thermal fluctuation[†] is larger) for the materials which show the weaker temperature dependence of the yield stress. If this were the case, the value of the stress at 0°K should be the same for both classes of materials, and a sudden rise in the yield stress should occur at very low temperatures in those materials which exhibit the weaker temperature dependence. Some evidence for such a sudden rise is indicated by the yield stress data of Allen, Hopkins, and McLennan⁴⁹ on iron single crystals. However, this rise was not observed by Smith and Rutherford²² for zone-refined polycrystals tested as low as 4°K. It may be that, in this latter case, the steep rise was prevented by the occurrence of twinning and the erratic deformation which was always observed at these very low temperatures.

The data of Figures 3 and 4, and the present analysis, suggest that a different mechanism is controlling in the range where $\tau < \tau^\circ$, as compared to that where $\tau > \tau^\circ$. Since the stress is relatively independent of temperature in this region, Schoeck and Seeger⁵⁰ have proposed that the governing mechanism is the escape of dislocations from dilute atmospheres formed by a Snoek-type ordering of interstitials in the stress fields of the dislocations. Since both the strength

[†]The total strain will include that due to the cross-slip of the screw components, as well as that due to the movement of the edge components.

and radius of such an atmosphere are inversely proportional to the temperature, the yield stress, which is given by the ratio of the two, is independent of temperature. Support for this mechanism is provided in the present analysis by the large values of the activation energy and activation volume when $\tau < \tau^\circ$ (e.g., see Figures 5 to 8).

V. SUMMARY AND CONCLUSIONS

The values of the frequency factor, ν , the activation energy, H , and the activation volume, v^* , were determined for low temperature yielding and flow of iron, from data available in the literature; and an attempt was made to evaluate the controlling mechanism, by comparing the experimental results with theoretical predictions. The following is a summary of the results of this work:

- a) The data for materials with different carbon-plus-nitrogen contents and thermal histories were correlated by considering an effective stress, given by the difference between the applied stress, τ , and a reference stress, τ° , defined by the stress at 300°K and a strain rate of 10^{-1} sec^{-1} (or a delay time for yielding of 1 sec).
- b) Within the scatter of the experimental data, the values of H , v^* , and ν were the same for yielding and flow, suggesting that either the same dislocation mechanism is controlling in all cases, or that different mechanisms exhibit approximately the same values of these parameters. The values of ν , H , and v^* for $\tau = \tau^\circ$ were: $\nu = 10^8$ to 10^9 sec^{-1} , $H = 0.5$ to 0.6 ev , and $v^* = 25$ to $30b^3$.
- c) The dislocation mechanism for which there was closest agreement between theoretical calculations and experimental data was overcoming the Peierls stress hills. However, due to the inexactness of the theories and the incompleteness of the experimental data, one cannot rule out the possibility that other mechanisms may be controlling.
- d) It is suggested that the upper and lower yield points in iron may represent the sudden generation of a large number of dislocations by the double cross-slip mechanism of Koehler and Orowan.
- e) Additional investigations, on the effect of strain rate and temperature on yielding, and flow in single crystals and high purity polycrystals, are needed to ascertain the reason for the weaker temperature dependence of the yield stress of these materials, compared to that for polycrystalline specimens with carbon-plus-nitrogen contents greater than 0.01%.

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APPENDIX I.
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