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NUCLEATION OF KINK PAIRS

AND THE PEIERLS' MECHANISM OF PLASTIC DEFORMATION

by

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ABSTRACT

The saddle-point activation energy for the nucleation of a pair of kinks is found as a function of the applied stress, the lattice constants, the height and shape of the Peierls' hill and the line energy of a dislocation. The kinetics of dislocation motion when the Peierls' mechanism is controlling are investigated and the microscopic dislocation velocities and macroscopic strain rates are formulated in terms of the activation energy for the formation of pairs of kinks by an Arrhenius type equation. The log of the dislocation velocity is found to be approximately proportional to the log of the local applied stress. It is shown that the low temperature mechanical properties of several BCC metals can be explained in terms of the Peierls' mechanism and excellent agreement is obtained between theory and experiment for the flow stress vs. temperature, activation energy vs. stress and activation volume vs. stress curves for these metals.

I. INTRODUCTION

Peierls¹ was the first investigator to illustrate that a straight dislocation line has its lowest energy when it lies exclusively in a potential valley parallel to lines of closest packing of atoms on the slip plane. When such a straight dislocation is moved en mass from one valley toward the next, the atoms in the vicinity of the core of the dislocation change their positions and bond angles, causing the energy of the dislocation to increase. At the top of the Peierls' hill, midway between two adjacent valleys, the dislocation energy reaches a maximum value and any additional small displacement will cause the dislocation to fall down the hill into the next valley. The maximum shear stress necessary to promote such forward motion of the dislocation at the absolute zero, is known as the Peierls' stress, τ_p^0 .

In some crystals (e.g. FCC metals) the Peierls' hill is so low, that the motion of dislocations can be effected by very small Peierls' stresses. In these cases the low temperature deformation is controlled by the then more difficult mechanism of intersection of dislocations. However in other crystals (e.g. covalently bonded materials and BCC metals) the Peierls' hills may be so high, that the Peierls' process is the more difficult, and therefore becomes the controlling mechanism of plastic deformation.

When a stress, τ^* , is applied to the slip plane in the direction of the Burgers' vector, b , such that $\tau^* < \tau_p$ for the temperature T , the straight dislocation segment lying originally along the Peierls' valley at $A_0B_0C_0$ will move part way up the Peierls' hill to ABC , as shown in Fig. 1. At temperatures, T , above the absolute zero, thermal fluctuations will cause loops, such as $AB'C$, to form along the length of the dislocation. Most of such loops will collapse because, being longer, they have higher energies than the straight dislocation line. With larger fluctuations in energy, however,

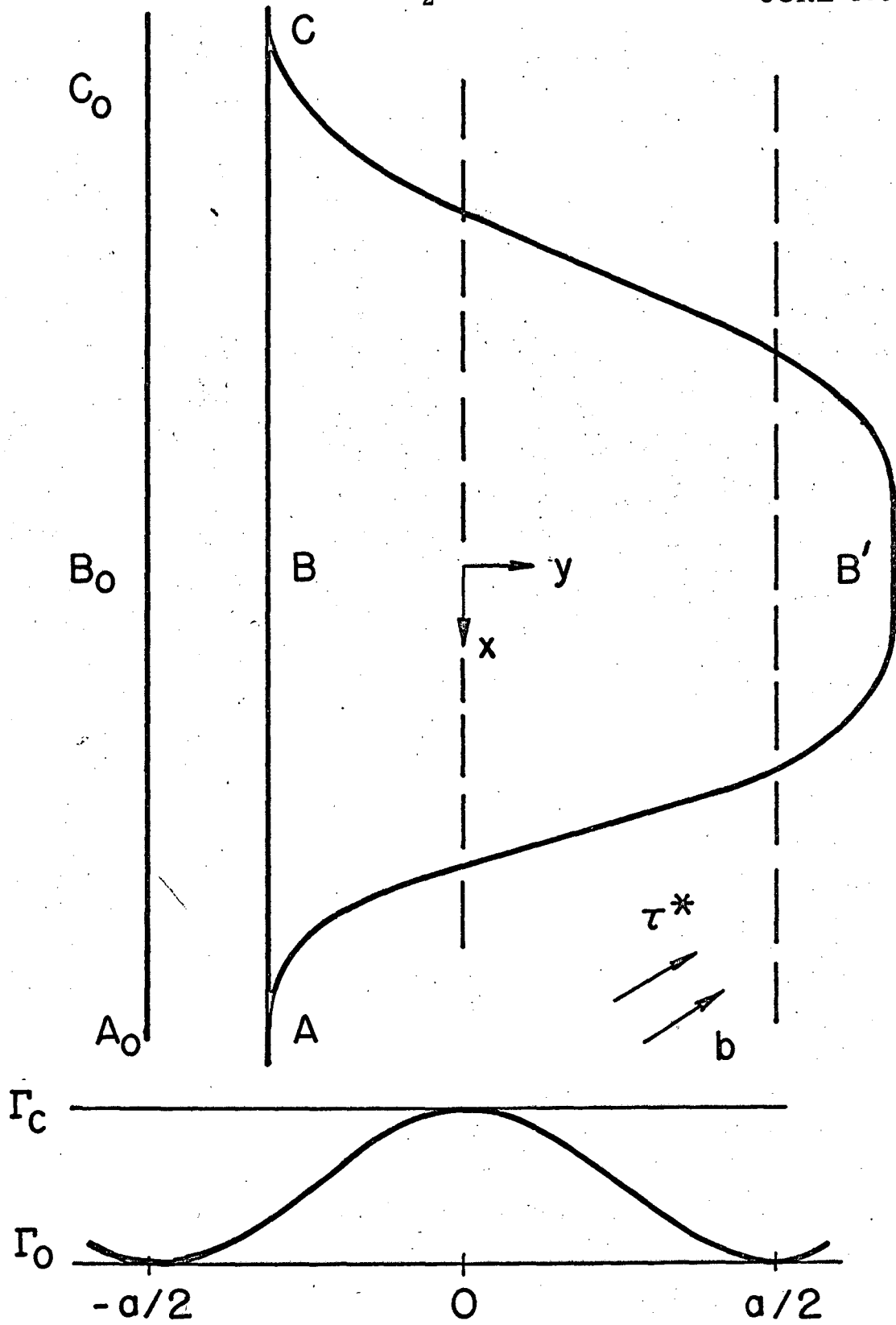


Fig. 1 Nucleation of a Pair of Kinks.

larger loops are formed and more work will be done by the applied stress in helping produce the loop. For sufficiently high local fluctuations in energy the effect of the applied stress becomes dominant, and loops of a "critical" size are produced which cannot collapse. The two kink segments AB' and B'C will then move away from each other under the action of the applied stress, resulting in the forward motion of the dislocation by a displacement a , equal to the periodicity of the rows of closely spaced atoms on the slip plane.

There are two major problems associated with the analytical formulation of plastic deformation by the Peierls' mechanism: The first is concerned with the calculation of the saddle-point free energy for the successful nucleation of a pair of kinks as a function of the applied stress so as to enable the determination of the frequency of formation of kink pairs along a dislocation segment; the second is associated with the formulation of the macroscopic strain rate in terms of the kinetic details of nucleation and migration of kink pairs. Other problems associated with the effect of interstitials on these details will be neglected for the present.

Several significant approaches to the analytical description of the Peierls' mechanism have already been formulated. Most of these have been directed primarily toward the rationalization of Bordoni peaks,² where the simplifying assumption of very small oscillating stresses ($\tau^* \ll \tau_p$) is justified. In contrast we will be interested here in the entire range of stresses from 0 to τ_p of significance to macroscopic plastic deformation. Lothe and Hirth³ assumed that the static equilibrium number of pairs of kinks were present and that these kinks separated as a result of stress-aided diffusion. Their deductions are probably useful for extremely high Peierls' hills and low applied stresses but they cannot be expected to be generally applicable. Seeger⁴⁻⁵ based his approximate analysis on kink-kink interactions as deduced from the continuum dislocation

theory. His formulation of the problem gives results that are almost correct for low stresses but, in terms of the assumptions that were made, will deviate from the correct solution at higher stress levels. These approaches have been critically reviewed by Jøssang, Skylstad and Lothe.⁶ More recently Friedel⁷ suggested a more attractive and realistic approach to the solution of the Peierls' process. He pointed out that the major factor involved in the kink-kink interaction arises from the extra dislocation line energy involved in the nucleation of a pair of kinks and therefore the Peierls' mechanism can be quite accurately formulated in terms of the dislocation line energy in lieu of the kink-kink interaction type of analysis used by Seeger. On the other hand several admittedly crude approximations were introduced that serve, as will be shown, to disqualify the conclusions arrived at by Friedel.

It is the purpose of the present paper to determine to a rather high degree of precision the true saddle-point free energy required to nucleate a pair of kinks as a function of the applied stress. The role of the frequency of nucleation of pairs of kinks and the frequency of annihilation of kinks in the Peierls' mechanism will be formulated to give the critical shear stress for flow as a function of the temperature and the shear strain rate. Finally the validity of the theory will be established by direct comparison of several deductions of the theory with some of the best experimental data that are currently available.

II. KINK ENERGY

Although Seeger has already calculated the energy of an isolated kink, we will again evaluate this energy, principally to illustrate the basis of the analytical techniques that will be subsequently used to calculate the saddle-point free energy for the nucleation of a pair of kinks. We will assume that the energy, $\Gamma\{y\}$, per unit length of a dislocation line is periodic in the y direction with a period, a , the spacing between parallel rows of closely spaced atoms on the slip plane, as shown in Fig. 1. The minor variations of the energy of the dislocation line with x and with its slope will be neglected. Furthermore, since the exact shape of the Peierls' hill is not yet known, we will assume that it can be approximated by

$$\Gamma\{y\} = \frac{\Gamma_c + \Gamma_0}{2} + \frac{\Gamma_c - \Gamma_0}{2} \left(\frac{\alpha}{2} + \cos \frac{2\pi y}{a} - \frac{\alpha}{4} \cos \frac{4\pi y}{a} \right), \quad (1)$$

where Γ_c and Γ_0 are the energies per unit length of a dislocation lying at the top and bottom of the Peierls' hill respectively and α is a factor that varies between -1 and 1. This perturbs the shape of the Peierls' hill from the purely sinusoidal variation that is obtained when $\alpha = 0$, and yet admits no additional extremal values of the line energy excepting those at $y = \pm a/2$ and $y = 0$. On this basis, the stress, Υ , that is needed to move the dislocation to a position, y_0 , in the absence of thermal fluctuations is given by

$$\Upsilon_b = \left. \frac{\partial \Gamma\{y\}}{\partial y} \right|_{y=y_0} = -\frac{\pi}{a} (\Gamma_c - \Gamma_0) \sin \frac{2\pi y_0}{a} \left(1 - \alpha \cos \frac{2\pi y_0}{a} \right). \quad (2)$$

The range of shapes of the Peierls' hills that are being considered here, and the effect of α on the Υ versus y_0 curves are illustrated in Fig. 2. The Peierls'

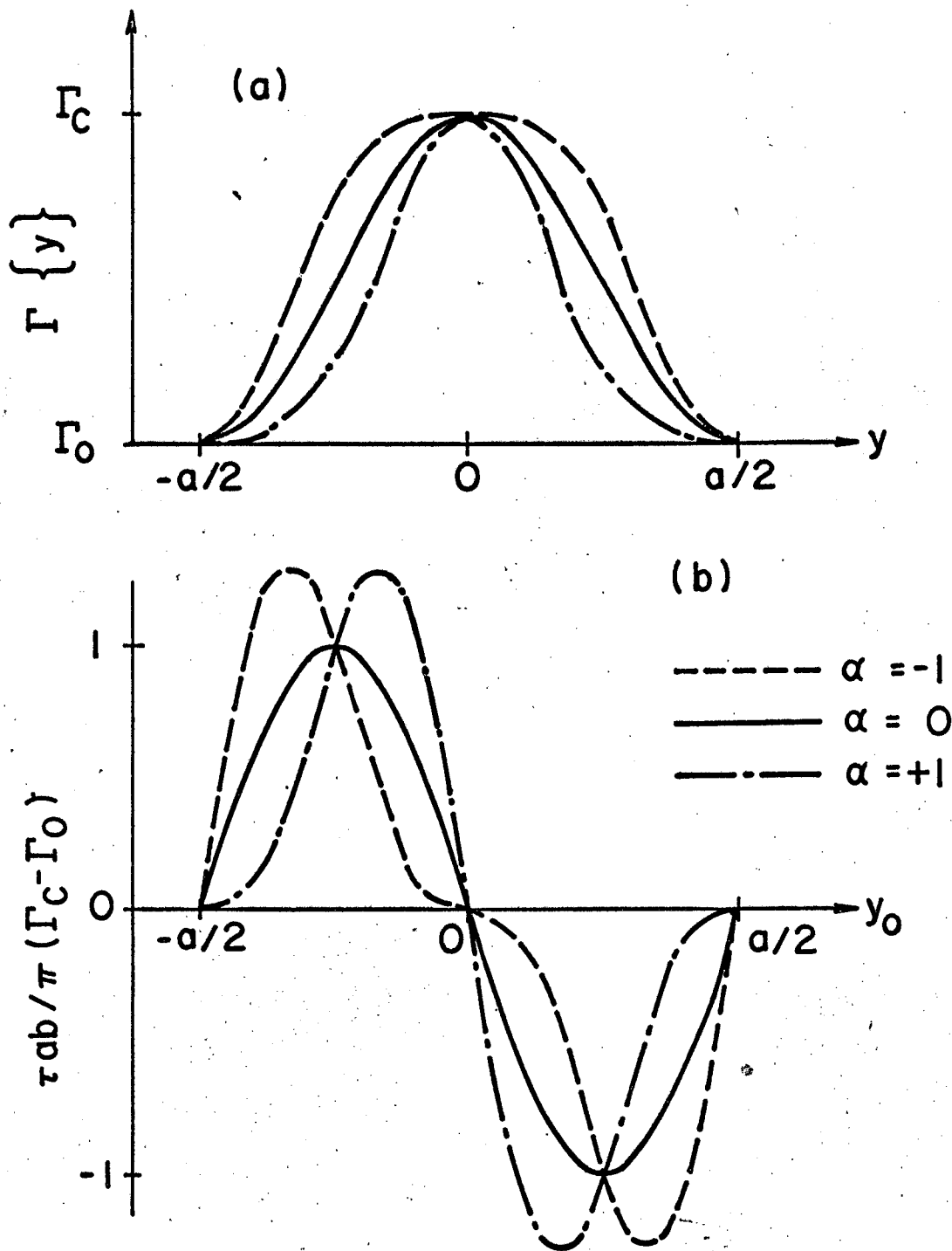


Fig. 2 Peierls' Hills and Stresses.

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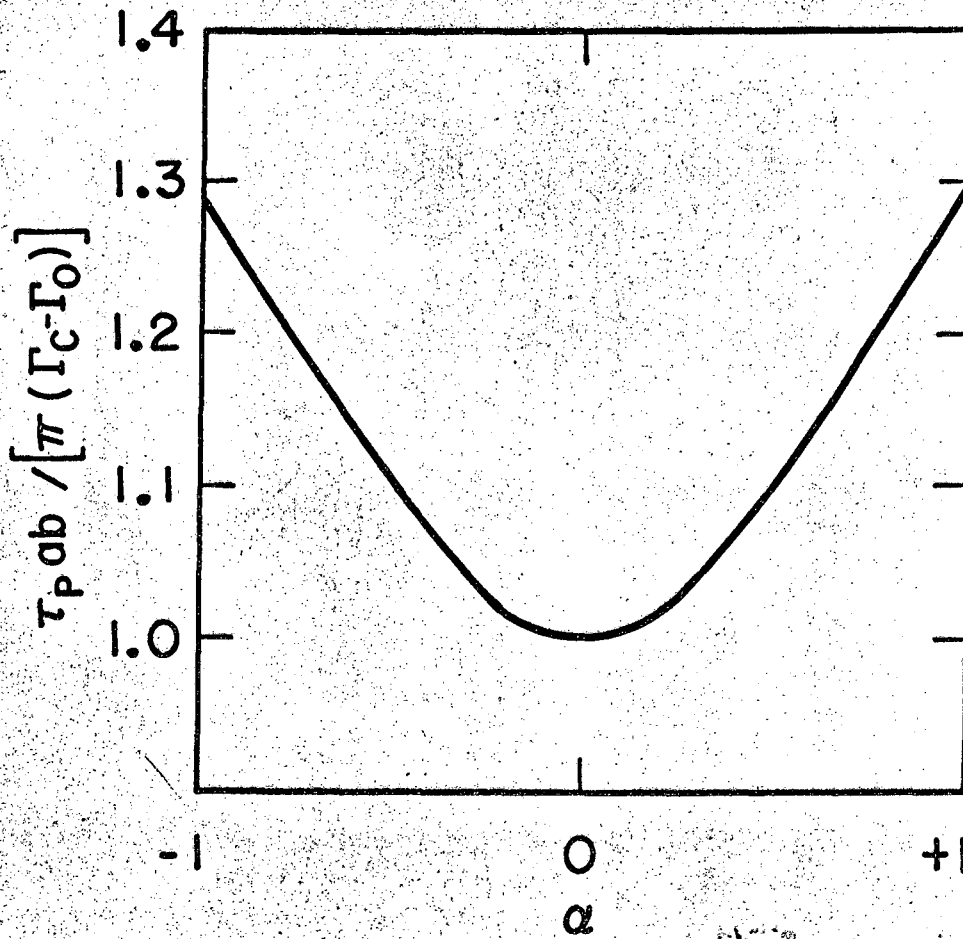


Fig. 3 Effect of α on the Peierls' Stress.

stress, Γ_p , is given by

$$\Gamma_p b = \frac{\Gamma_c - \Gamma_0}{|a|a} \frac{\pi}{16} (3 + \sqrt{1 + 8d^2}) \sqrt{8d^2 - 2 + 2\sqrt{1 + 8d^2}} \quad (3)$$

This function is plotted in Fig. 3; variations in the shape of the Peierls' hill can have pronounced effects on the Peierls' stress even though the height of the Peierls' hill, $\Gamma_c - \Gamma_0$, is fixed.

A stable isolated kink under zero stress is shown in Fig. 4. The energy of a kink, U_k , is defined as the excess line energy of the dislocation having a kink above that of a dislocation traversing the same distance x but lying exclusively in a single Peierls' valley. Therefore

$$U_k = \int_{-\infty}^{\infty} \Gamma\{y\} ds - \Gamma_0 dx \quad (4)$$

where ds is an element of length of the kinked dislocation. Since

$$ds = \sqrt{dx^2 + dy^2} \quad (5)$$

$$U_k = \int_{-\infty}^{\infty} \left(\Gamma\{y\} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} - \Gamma_0 \right) dx \quad (6)$$

For the equilibrium shape of a kink, U_k must be a minimum. Therefore the kink shape, $y(x)$, must satisfy Euler's condition, which is

$$0 = \frac{\partial}{\partial y} \left(\Gamma\{y\} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} \right) - \frac{d}{dx} \frac{\partial}{\partial \left(\frac{dy}{dx}\right)} \left(\Gamma\{y\} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} \right) \quad (7)$$

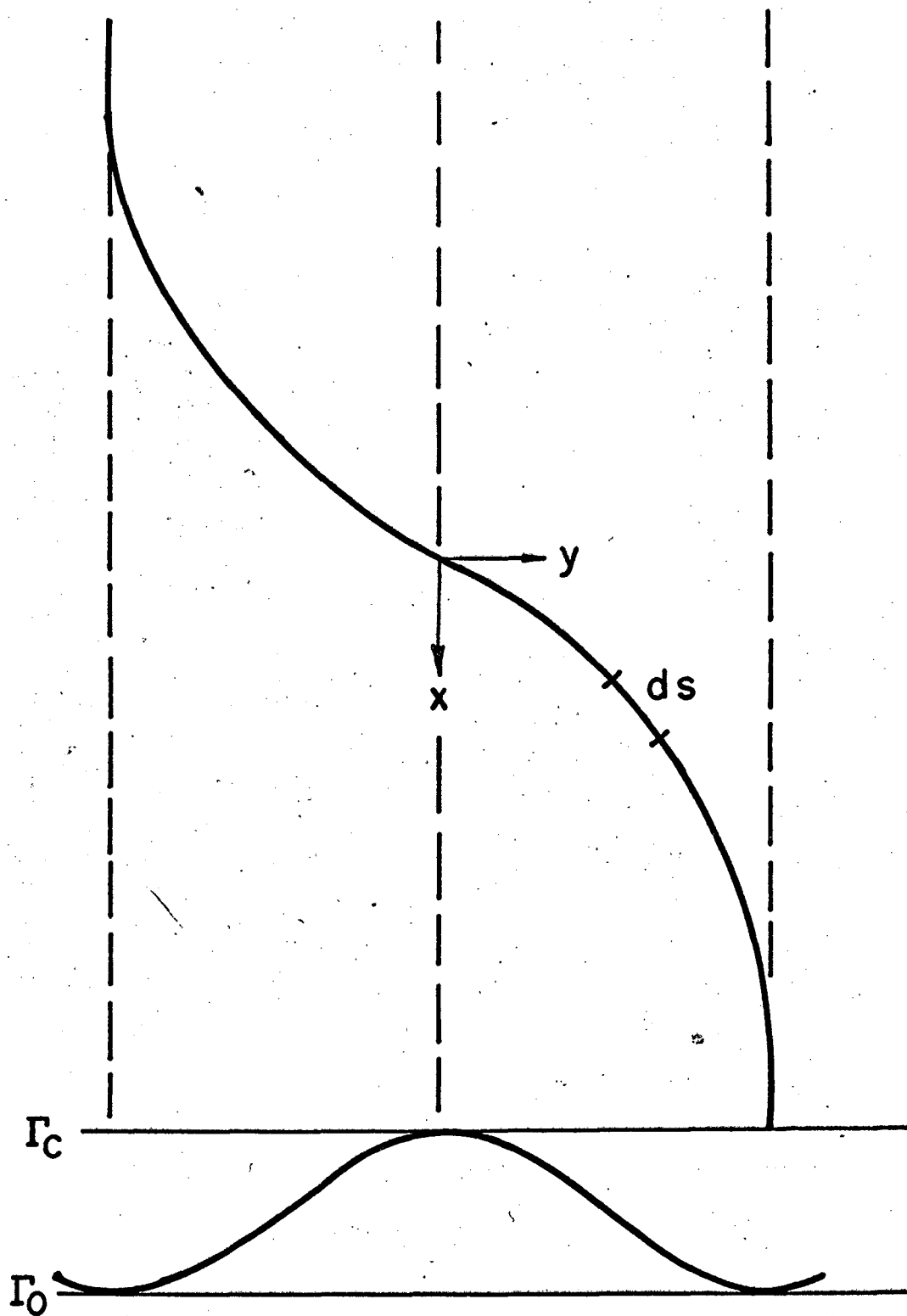


Fig. 4 An Isolated Kink.

This simplifies to

$$\frac{d}{dy} \left(\frac{\Gamma\{y\}}{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}} \right) = 0 \quad (8)$$

and may be immediately integrated once to give

$$\frac{dy}{dx} = \pm \sqrt{\left(\frac{\Gamma\{y\}}{K}\right)^2 - 1} \quad (9)$$

where K is the constant of integration. Using the boundary conditions

$$y = \pm \frac{a}{2} \quad \text{at} \quad x = \pm \infty,$$

$$y = 0 \quad \text{at} \quad x = 0,$$

and $\frac{dy}{dx}$ is continuous at $x = 0$,

$$(10)$$

gives

$$K = \Gamma_0 \quad (11)$$

Since major interest concerns only the value of the kink energy, Eqn. 9 need not be further integrated and can be introduced directly into Eqn. 6. It is convenient, however, to express Eqn. 6 in terms of y instead of x as the independent variable. Carrying out the substitution and the change of variables gives

$$U_k = \Gamma_0 \int_{-a/2}^{+a/2} \sqrt{\left(\frac{\Gamma\{y\}}{\Gamma_0}\right)^2 - 1} dy \quad (12)$$

The analytical integration of Eqn. 12 for $\delta = 0$, gives

$$U_k = \frac{\Gamma_0 a}{\pi} \left(\sqrt{2(R-1)} + (R+1) \tan^{-1} \sqrt{\frac{R-1}{2}} \right) \quad (13)$$

where

$$R = \rho_c / \rho_o .$$

(14)

For the general case, the results are given in Table I.

Table I

Peierls' Stress and Kink Energies

d	R^{-1}	$\frac{\tau_p ab}{\pi b_0}$	$\frac{2 u_k \pi}{a b_0}$
0	10^{-4}	10^{-4}	.05657
0	10^{-2}	10^{-2}	.56672
0.25	10^{-4}	1.03×10^{-4}	.05884
0.25	10^{-2}	1.03×10^{-2}	.58946
0.50	10^{-4}	1.10×10^{-4}	.06097
0.50	10^{-2}	1.10×10^{-2}	.61090
0.75	10^{-4}	1.19×10^{-4}	.06299
0.75	10^{-2}	1.19×10^{-2}	.63121
1.00	10^{-4}	1.30×10^{-4}	.06492
1.00	10^{-2}	1.30×10^{-2}	.65056
-0.25	10^{-4}	1.03×10^{-4}	.05410
-0.25	10^{-2}	1.03×10^{-2}	.54201
-0.50	10^{-4}	1.10×10^{-4}	.05140
-0.50	10^{-2}	1.10×10^{-2}	.51496
-0.75	10^{-4}	1.19×10^{-4}	.04833
-0.75	10^{-2}	1.19×10^{-2}	.48416
-1.00	10^{-4}	1.30×10^{-4}	.04441
-1.00	10^{-2}	1.30×10^{-2}	.44498

III. ENERGY TO NUCLEATE A PAIR OF KINKS

In order to calculate the energy required to nucleate a pair of kinks, we assume that a segment of a dislocation under zero stress, lies in the Peierls' valley as shown by $A_0B_0C_0$ of Fig. 1. When a local stress $\tau^* < \tau_p$ is applied, the dislocation moves in the positive Y direction as shown by ABC; its position, y_0 , is then given by Eqn. 2. The excess energy of a dislocation having any shape $y = y(x)$, (e.g. ABC in Fig. 1), above that for one that lies along $y = y_0$, is given by

$$U = \int_{-\infty}^{+\infty} \left(\Gamma\{y\} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} - \Gamma\{y_0\} - \tau^* b (y - y_0) \right) dx, \quad (15)$$

where the first term of the integrand is the line energy of the displaced dislocation, the second is its line energy when it lies along $y = y_0$ and the third term refers to the extra work done mechanically by the stress τ^* in displacing the dislocation from y_0 to y . Since we are looking for the minimum energy, U_n , necessary to nucleate a pair of kinks, it is reasonable to assume that U_n is a stationary value of Eqn. 15 associated with a "critical" shape of the dislocation $y(x)$. If this is the case, then y will satisfy the Euler's equation associated with Eqn. 15 which is

$$\left(\frac{\partial}{\partial y} - \frac{d}{dx} \frac{\partial}{\partial \left(\frac{dy}{dx}\right)} \right) \left(\Gamma\{y\} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} - \Gamma\{y_0\} - \tau^* b (y - y_0) \right) = 0. \quad (16)$$

This immediately simplifies to

$$\tau^* b = \frac{d}{dy} \left(\Gamma\{y\} / \sqrt{1 + \left(\frac{dy}{dx}\right)^2} \right). \quad (17)$$

Integrating once and solving for dy/dx gives

$$\frac{dy}{dx} = \pm \sqrt{\left(\frac{\Gamma\{y\}}{\tau^*by + K}\right)^2 - 1} \quad , \quad (18)$$

and integrating again gives

$$x = \pm \int_y^\lambda \left[\left(\frac{\Gamma\{y\}}{\tau^*by + K}\right)^2 - 1 \right]^{-1/2} dy \quad , \quad (19)$$

where K and λ are constants of integration. The boundary conditions that $x \rightarrow \pm\infty$ as $y \rightarrow y_0$ imply that the integrand on the right of Eqn. 19 must go to ∞ as $y \rightarrow y_0$. This implies

$$K = \Gamma\{y_0\} - \tau^*by_0 \quad , \quad (20)$$

and that the $+$ sign be taken for $x > 0$ and the $-$ sign for $x < 0$. λ is the value of y at $x = 0$.

Clearly one solution of Eqn. 17 is given by $y\{x\} = y_0 = \text{constant}$. This corresponds to $\lambda = y_0$. As λ is increased from y_0 to λ_A , λ_B and λ_C , the curves given by Eqn. 19 take the shapes shown schematically in Fig. 5. The curves are smooth except for a jump in the derivative at $x = 0$ which corresponds to a point force $F = 2\Gamma(\lambda)\cos\theta$ acting on the dislocation at $x = 0$ in the positive y direction. This force is necessary to hold the dislocation at the point $(0, \lambda)$. At $\lambda = \lambda_c$, where λ_c is given by

$$\Gamma\{\lambda_c\} = \tau^*b(\lambda_c - y_0) + \Gamma\{y_0\} \quad , \quad (21)$$

the discontinuity in $\frac{dy}{dx}$ and consequently the point force go to zero, as seen from Eqn. 18. Therefore Eqn. 19 with $\lambda = \lambda_c$ gives a solution of Euler's

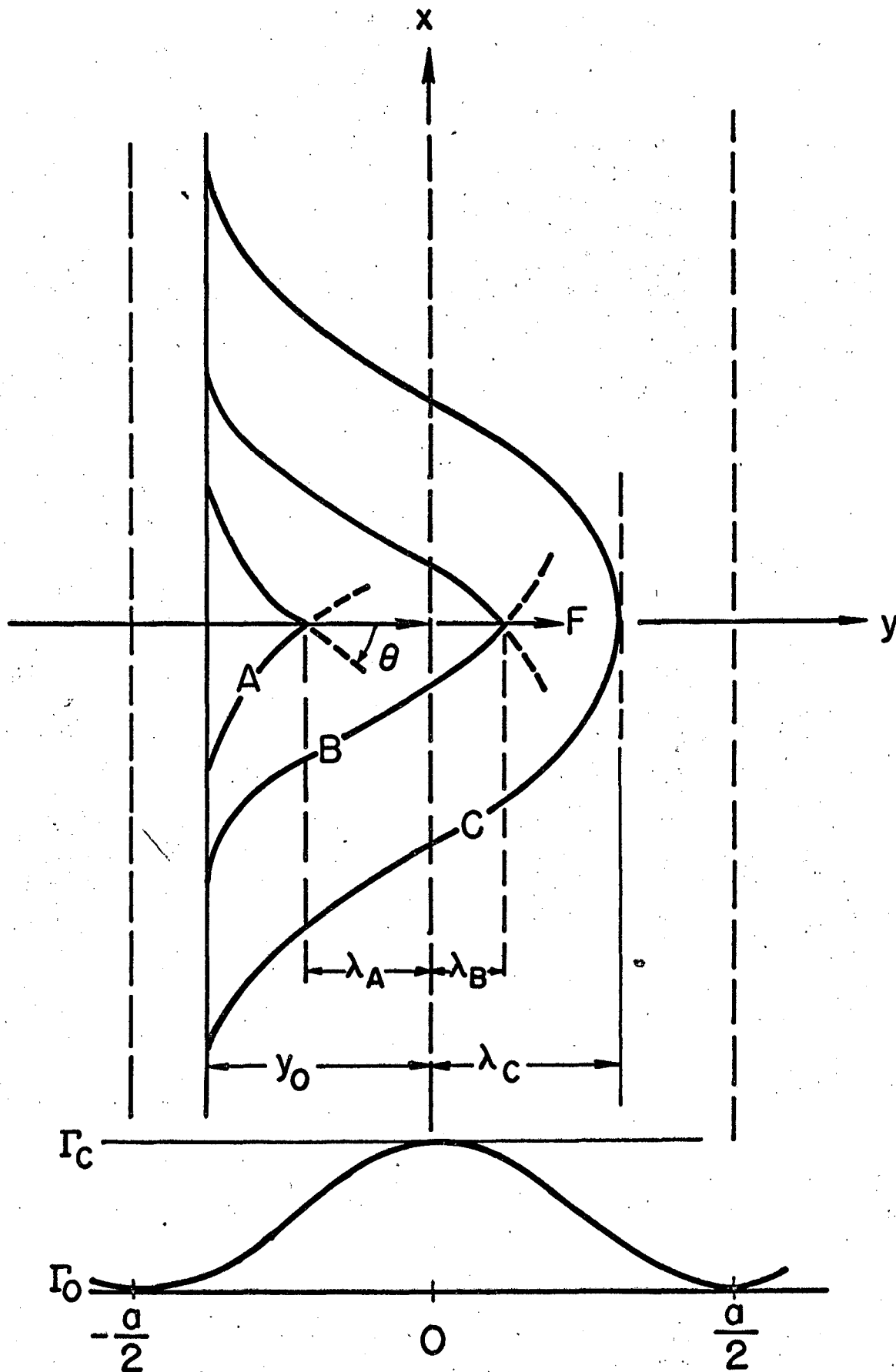


Fig. 5 Model for Nucleation of a Pair of Kinks.

equation. If $\lambda > \lambda_c$ the slope $\frac{dy}{dx}$ becomes imaginary showing that there are no solutions for $\lambda > \lambda_c$. This physical meaning of this situation is clear. If you require that a dislocation pass through a point $x = 0$, $y = \lambda > \lambda_c$ it will disassociate into a pair of kinks traveling to $\pm \infty$ under the action of the applied stress. To see that the "critical" solution passing through λ_c gives the minimum energy for the formation of a kink pair it is only necessary to note that any loop which eventually forms a kink pair must at some time pass through the point $y = \lambda_c$, $x = 0$. Its energy at this time must be higher than that of the critical solutions since the critical solution was the solution of Euler's equation passing through λ_c which minimized the energy.

Introducing Eqns. 18 and 20 into Eqn. 15 gives the energy for nucleation of a pair of kinks, U_n , as

$$U_n = U(\lambda_c) = \int_{-\infty}^{+\infty} \left[\frac{(\Gamma\{y\})^2}{\tau^*b(y-y_0) + \Gamma\{y_0\}} - \Gamma\{y_0\} - \tau^*b(y-y_0) \right] dx \quad (22)$$

and changing the variable of integration gives

$$U_n = 2 \int_{\lambda_0}^{\lambda_c} \sqrt{(\Gamma\{y\})^2 - (\tau^*b(y-y_0) + \Gamma\{y_0\})^2} dy \quad (23)$$

The results of the numerical integration of Eqn. 23 are given in the appendix. $U_n/2U_k$ is insensitive to the physically acceptable ranges in R . Consequently, the curves shown in Fig. 6 were plotted only for the value of $R = 1.00$. Furthermore, the shape of the Peierls' hills has only a small effect on $U_n/2U_k$.

It is most significant that the $U_n/2U_k$ vs. τ^*/τ_p curves are universal relationships that depend exclusively on well-defined physical quantities arising from the atomic bonding in the crystal. This shows that the energy to nucleate a pair of kinks is independent of the details of the statistical distribution of

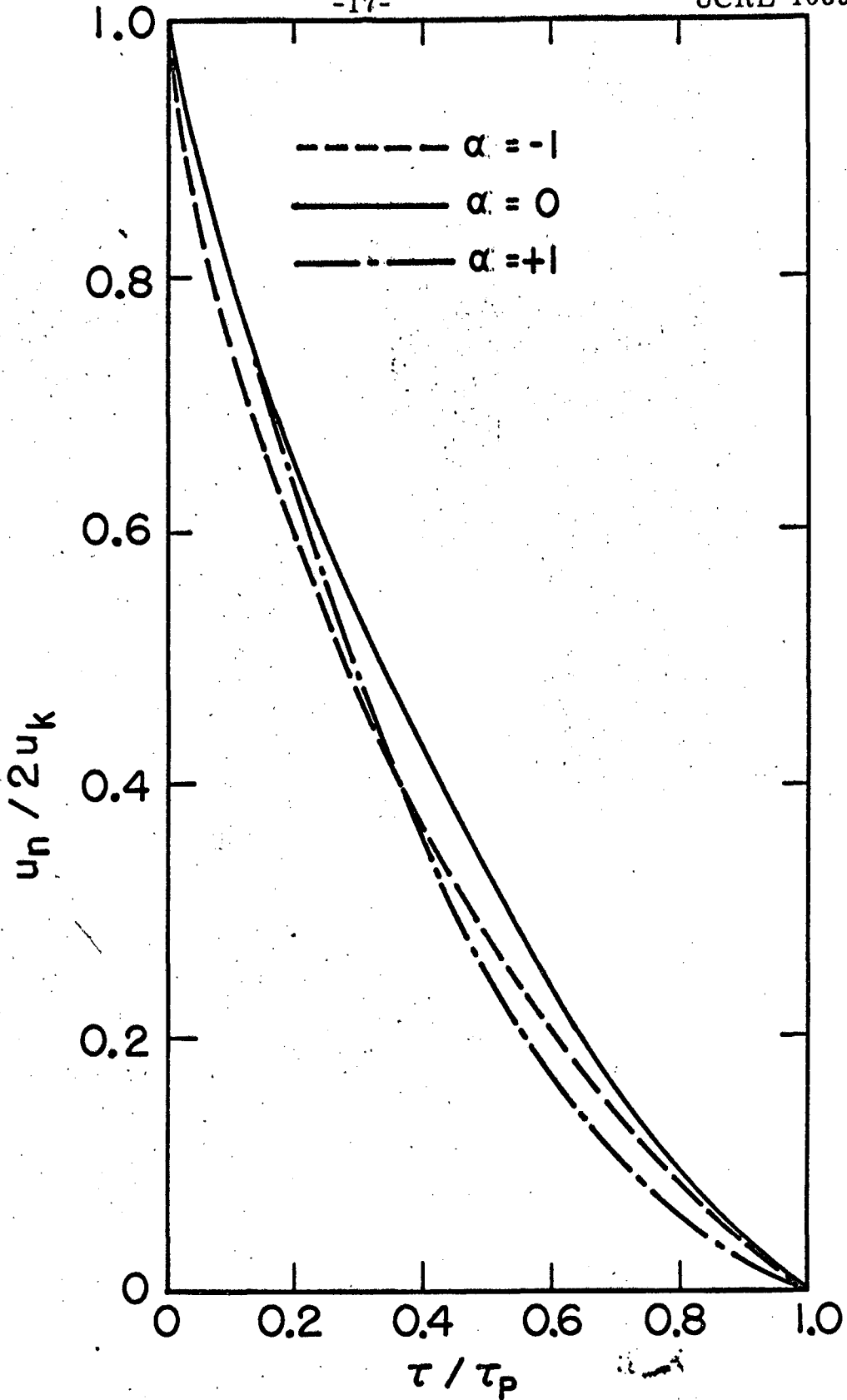


Fig. 6 Energy to Nucleate a Pair of Kinks.

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dislocations. When the stress is zero, the energy to nucleate a pair of kinks is, as expected, just $2U_k$ (i. e. twice the kink energy) and when the stress equals the Peierls' stress, $U_n = 0$, since no additional thermal energy is needed to nucleate kink pairs, the stress itself being capable of doing this without aid from thermal fluctuations.

We will define the quantity $\partial U_n / \partial \tau^*$ as the activation volume, v^* ; it represents the Burgers' vector times the area swept out during the nucleation of the critical loop. Whereas the activation volume so defined is quite large for intersection and other dislocation mechanisms, it has quite small values ranging from about 5 to $50b^3$ for the Peierls' process. It is therefore a rather critical quantity that serves to distinguish the Peierls' process from many other dislocation mechanisms which might on many occasions have almost the same activation energies as the energies required to nucleate a pair of kinks. The values of

$$\frac{\partial \left(\frac{U_n}{2U_k} \right)}{\partial \left(\frac{\tau^*}{\tau_p} \right)} = \frac{\tau_p}{2U_k} \frac{\partial U_n}{\partial \tau^*} = \frac{\tau_p}{2U_k} v^* \quad (24)$$

as a function of τ^* / τ_p and α are shown in the appendix. Since these are insensitive to the physical acceptable variations in R , only the values for $R = 1.001$ are plotted in Fig. 7.

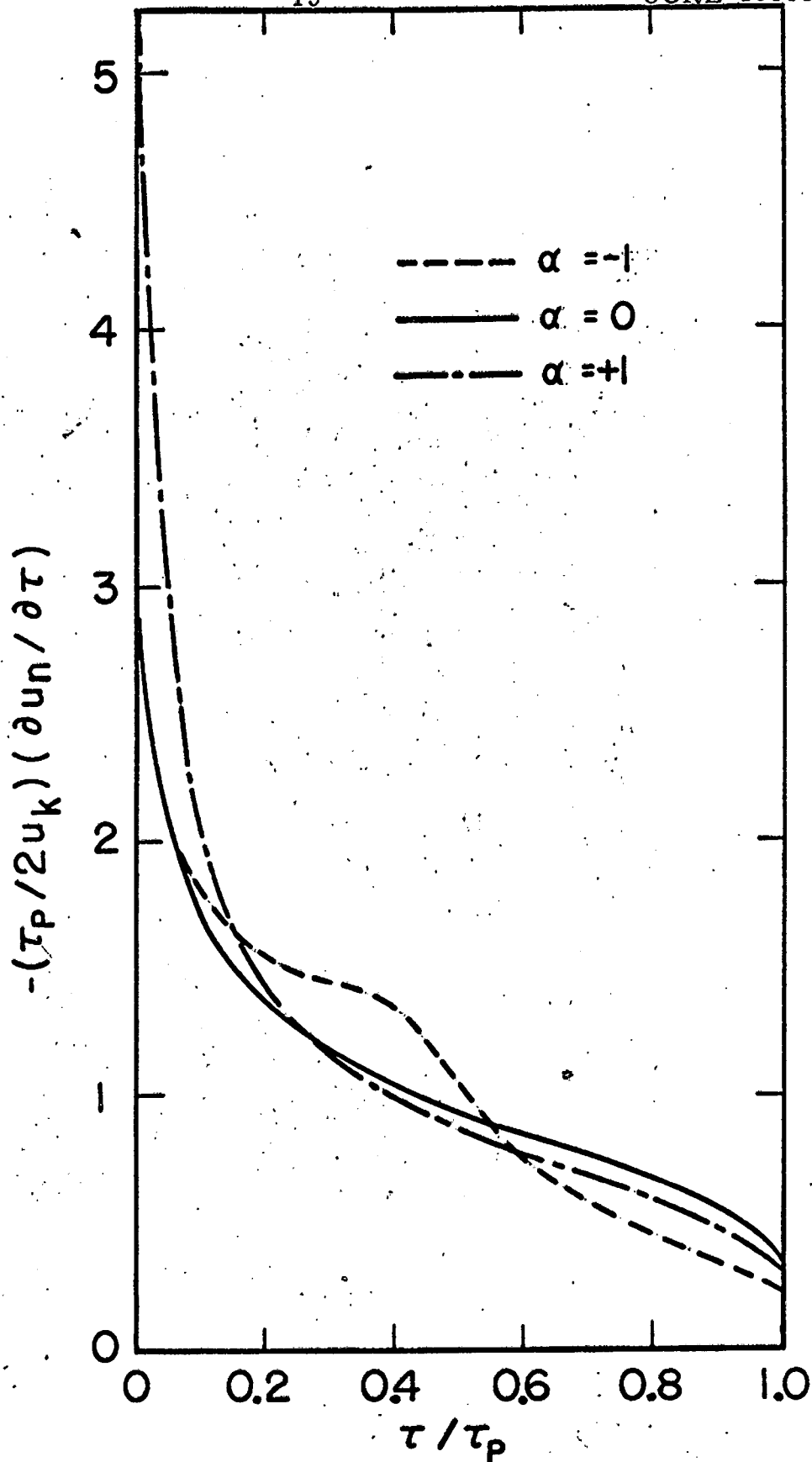


Fig. 7 Activation Volume.

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IV. KINETIC EQUATIONS
FOR DEFORMATION BY THE PEIERLS' MECHANISM

In this section we will estimate the effects of stress and temperature on the macroscopic plastic strain rate when the deformation is controlled by the Peierls' mechanism in terms of the energy required to nucleate a pair of kinks. Although we will later consider more complex situations we will assume here that L is the mean, geometrically limited, length swept out by a pair of kinks once nucleation occurs in that length. First we will assume that the time required for the migration of the kinks over this length is small relative to the time required for the nucleation of a kink. It is immediately apparent that the frequency of nucleation of a pair of kinks in any length L should be directly proportional to L , neglecting, of course, end conditions. Suppose we conceive the fluctuation in thermal energy to occur at a point as depicted for the various stages of nucleation shown in Fig. 5. The frequency of a vibration would be about $\nu = \frac{c}{2b}$, i.e. the Debye frequency, and where c = the speed of sound. Consequently the embryonic kinks would collapse in about b/c seconds. In this time, therefore, a shock would have traveled out only a distance b along the x direction of the dislocation and the critical size pair of kinks would not have formed even though sufficient energy were available. The issue is that the energy must be spread over the length of the embryonic pair of kinks, w . Since the activation volume is a measure of the Burgers' vector times the area swept out when the dislocation configuration becomes critical,

$$w \approx \frac{-4}{b(\lambda_c - y_0)} \frac{\partial U_n}{\partial \tau^*} = \frac{-8U_k}{\tau_p b(\lambda_c - y_0)} \frac{\partial (U_n/2U_k)}{\partial (\tau^*/\tau_p)} \quad (26)$$

and can never be less than $2b$. In general the variation in w with τ^* has only a negligible effect on the results and we will neglect this in the following. Therefore, using the Boltzmann approach, the frequency for nucleation, ν_n , of a pair of kinks in length L is approximately

$$\nu_n = \nu \frac{L}{w} e^{-\frac{U_n}{kT}}, \quad (25)$$

where ν is the Debye frequency, w is the width of the critical size loop forming the embryonic kinks and kT is the Boltzmann's constant times the absolute temperature. In this formulation the reverse reaction of having a kink pair nucleated in the opposite direction to the applied stress is neglected because, under even a small stress, it occurs so infrequently.

If it is assumed that the kink velocity is large compared to the rate of nucleation, the forward velocity, v , of the dislocation obeying the Peierls' process is

$$v = a\nu_n = \nu \frac{La}{w} e^{-\frac{U_n}{kT}}, \quad (27)$$

or

$$\frac{kT}{2U_k} \ln v - \frac{kT}{2U_k} \ln \frac{vLa}{w} = -\frac{U_n}{2U_k} \quad (27a)$$

Fig. 8 is a plot of $-\frac{U_n}{2U_k}$ versus $\frac{\tau^*}{\tau_p}$, illustrating at high stresses the type of linear relationship between $\ln v$ and $\ln \tau^*$ observed in Li F by Johnston and Gilman⁸ and in silicon iron by Stein and Low⁹ and Erickson.¹⁰ Of course the velocity of dislocations obeying the Peierls' mechanism does

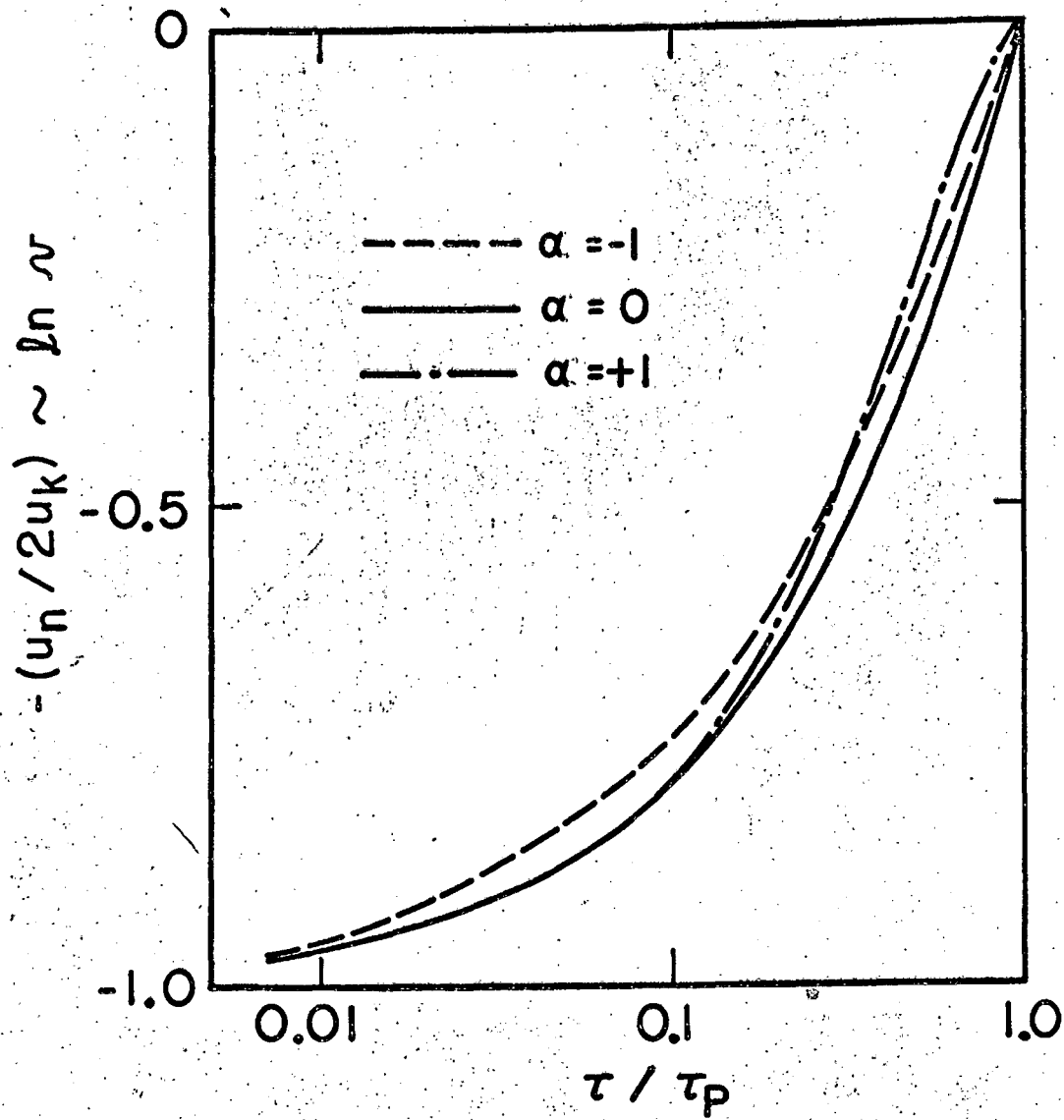


Fig. 8 Effect of Stress on Dislocation Velocities.

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not depend only on τ^* but is also influenced to some extent by L and the other parameters of Eqn. 27a. Furthermore this relationship is no longer valid above $\tau^* = \tau_p$, where an alternate mechanism becomes controlling.

Since, in general, the plastic strain rate, $\dot{\gamma}$, is given by $\dot{\gamma} = \rho b v$, where ρ is the total length of thermally activatable dislocations per cm^3 ,

$$\dot{\gamma} = \rho a b \frac{L}{w} v e^{-\frac{U_n}{kT}} \quad (28)$$

over the region where the Peierls' mechanism controls the deformation rate. At high temperatures, thermal fluctuations with energy $2U_k$ are so frequent that plastic deformation takes place even as τ^* approaches zero. The temperature, T_{cp} , at which this occurs for a given $\dot{\gamma}$ is defined by

$$\dot{\gamma} = \rho a b \frac{L}{w} v e^{-\frac{2U_k}{kT_{cp}}} \quad (29)$$

Therefore, for tests done at the same strain rate where $\rho a b L v$ is a constant, and neglecting the minor effect of τ^* on w ,

$$\frac{U_n}{2U_k} \approx \frac{T}{T_{cp}} \quad (30)$$

as seen from Eqns. 28 and 29. Substituting in the relationship of Eqn. 23, gives the variation of τ^*/τ_p versus T/T_{cp} shown in Fig. 6. Although T_{cp} varies with ρL as well as the remaining physical variables, the τ^*/τ_p versus T/T_{cp} curves are universally appropriate to all crystals undertaking the Peierls' mechanism. Whereas the preliminary judgment on the operations of the Peierls' mechanism can most readily be made by plotting data as shown in Fig. 6, the critical judgment yet rests on agreement with the activation volumes shown in Fig. 7.

We have assumed in the preceding discussion that only one pair of kinks moves in each geometrically determined length L at any one time. The length L is at most the distance between nodes on the dislocations but could also be as small as the distance between superjogs and even single jogs themselves. Nevertheless, it appears to be desirable to ascertain what conditions must apply when Eqn. 28 is valid and what alternate formulations are useful when more than a single pair of kinks appear over segment L at one time. The frequency of formation of a pair of kinks in length L is given by Eqn. 25. The average frequency, \bar{v}_a , with which a pair of kinks formed in a length L and moved out of L and were thus annihilated is

$$\bar{v}_a = \frac{2v_k}{L} \quad (31)$$

where v_k is the velocity of a kink. Therefore, Eqn. 28 is valid so long as

$$\bar{v}_a \gg \bar{v}_n \quad \text{or}$$

$$L^2 \ll \frac{2Wv_k}{\gamma} e^{+\frac{U_n}{kT}} \quad (32)$$

When formulated in terms of the strain rate by introduction of Eqn. 28, this inequality reduces to

$$v_k \gg \frac{L\dot{\gamma}}{2\rho ab} \quad (33)$$

Considering therefore a moderately fast strain-rate test of 10^{-3} per sec. and introducing the reasonable values of $\rho = 10^8$ per cm^2 , $a \approx b \approx 3 \times 10^{-8}$ cm., and letting $L = 10^{-4}$ cm, we obtain that Eqn. 28 will be valid when $v_k \gg \frac{1}{2}$ cm/sec.

At present we suggest three possible limiting velocities for kinks, namely:

Frank's relativistic velocity $v_k = c$, (34a)

Liebfried's phonon interaction velocity $v_k = \frac{10}{3} \frac{U^* b^3 c}{kT}$, (34b)

Thermally activated $v_k = 4c e^{-\frac{U_m}{kT}} \sinh \frac{U^* b^3}{kT}$, (34c)

where c is the velocity of sound and U_m is the activation energy for the motion of a kink. Both 34a and 34b give extremely high kink velocities under usual conditions amounting from about 3×10^5 to 3×10^6 cm/sec. Furthermore, since U_m must be quite small, the kink velocity for the thermally activated mechanism can also be expected to satisfy Eqn. 33.

Whereas Eqn. 33 is satisfied and Eqn. 28 is therefore valid for the usual testing conditions, it is possible that it no longer applies for high strain-rate tests or in materials that have extremely low densities of mobile dislocations. In this event several kinks may be moving along length L at one time. In order to estimate the plastic strain rate under these conditions we assume that under steady-state conditions each pair of kinks sweeps over a length l , in which the positive and negative kinks of each pair are annihilated upon collision with kinks of the opposite sign. Thus, the frequency of nucleation of a pair of kinks in l equals the frequency with which they are annihilated and

$$\dot{\gamma}_n = \frac{v l}{w} e^{-\frac{U_n}{kT}} = \dot{\gamma}_a = \frac{2 v_k}{l} \quad (34)$$

or

$$l^2 = \frac{2 w v_k}{v} e^{+\frac{U_n}{kT}} \quad (35)$$

The strain rate is given by

$$\dot{\gamma} = \rho a b \frac{l}{w} v e^{-\frac{U_n}{kT}} = \rho a b \sqrt{\frac{2 v_k v}{w}} e^{-\frac{U_n}{kT}} \quad (36)$$

V. CORRELATION BETWEEN THEORY AND EXPERIMENT

In this section the validity of the theory will be established by comparing the theoretical predictions with various experimental data on the plastic deformation of some BCC metals and prismatic slip in two HCP metals. In these comparisons it will soon become apparent that, although the experimental data scatter rather uniformly to either side of the predictions and thus strongly confirm the validity of the theory, the experimental data currently available are simply not good enough to permit use of the full details of the theory. For this reason in making the comparisons we will neglect the effect of temperature on the shear modulus of elasticity and on the values of $2U_k$ and U_n ; we will make comparisons only with the theory for sinusoidal Peierls' hills for which $\lambda = 0$; we will use only the simple formulation of the theory as given by Eqn. 28, where only single kinks are formed in length L at one time; we will neglect the effect of T and τ^* on the preexponential terms in Eqn. 28; and, in contrast to the thoughts expressed by Kuhlmann-Wilsdorf in the discussion of Friedel's paper,⁷ we will assume that the Peierls' stress does not change much with temperature, a concept that is in agreement with Friedel's⁷ evaluation of this issue.

Figure 9 is a schematic representation of an experimentally determined yield stress versus temperature diagram of a material that deforms by the Peierls' process. The applied shear stress (or about 1/2 of the tensile stress for polycrystalline metals) is given by

$$\tau = \tau^* + \tau_A \quad , \quad (37)$$

where τ^* is the stress required to aid the thermal activation of the Peierls' process and therefore decreases precipitously as T increases and τ_A is the stress necessary to overcome such athermal mechanisms as long-range back

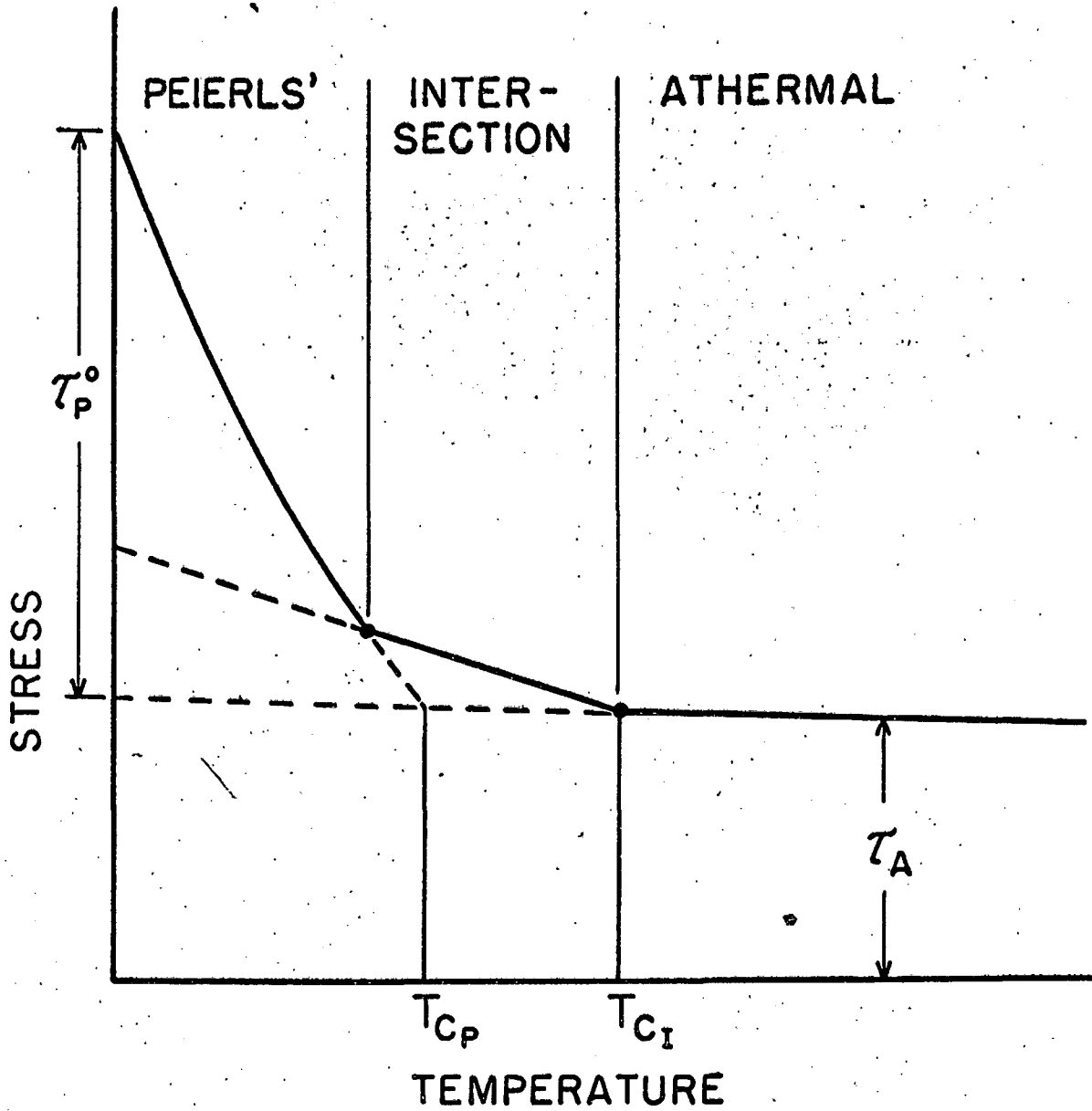


Fig. 9 - T Relation for a Material Undergoing a Peierls' Mechanism and Intersection.

stresses, short-range order stresses, etc. and therefore decreases only modestly as the temperature increases, usually parallel to the shear modulus of elasticity. The shear stress at yielding versus the temperature when the deformation is controlled by the intersection process is also shown. When

τ_p^0 is extremely small, as it must be in FCC metals, the deformation will be exclusively controlled by intersection. For higher values of the Peierls' stress, the low temperature deformation will be controlled by the Peierls' process and the higher temperature deformation will, as shown in Fig. 9, be controlled by intersection when $T_{cp} < T_{c_I}$ where T_{cp} is the critical temperature defined in Eqn. 29 and T_{c_I} is the critical temperature for the intersection mechanism defined in an analogous manner. More frequently, however, $T_{cp} > T_{c_I}$ and the Peierls' process controls over the entire low temperature range. Immediately above the highest critical temperature, the deformation is athermal and at yet higher temperatures (not shown in Fig. 8), it again becomes thermally activated as a result of "dynamic" recovery.

As seen in Fig. 9, the values of τ_p^0 and T_{cp} may be determined directly from the experimental data. Then plotting τ^*/τ_p^0 versus T/T_{cp} for the low temperature range should result in good agreement with the theoretical predictions given in Fig. 6, when the Peierls' mechanism is operative. Conversely, using the experimentally determined values of τ_p^0 and T_{cp} , it is possible to introduce (by application of Fig. 6) the theoretically predicted τ^*-T curve on the experimental data. Typical examples of the second procedure for the case of prismatic slip in single crystals of Be¹¹ and Ag plus 33 at. % Al¹² are shown in Fig. 10. With the exception of the lowest temperature data for Be, which must be discounted because of the initiation of twinning, the agreement is excellent. Thus we see that the low temperature prismatic slip in Be is handicapped by an extremely high Peierls' stress. A more critical confirmation that Ag₂Al obeys the Peierls'

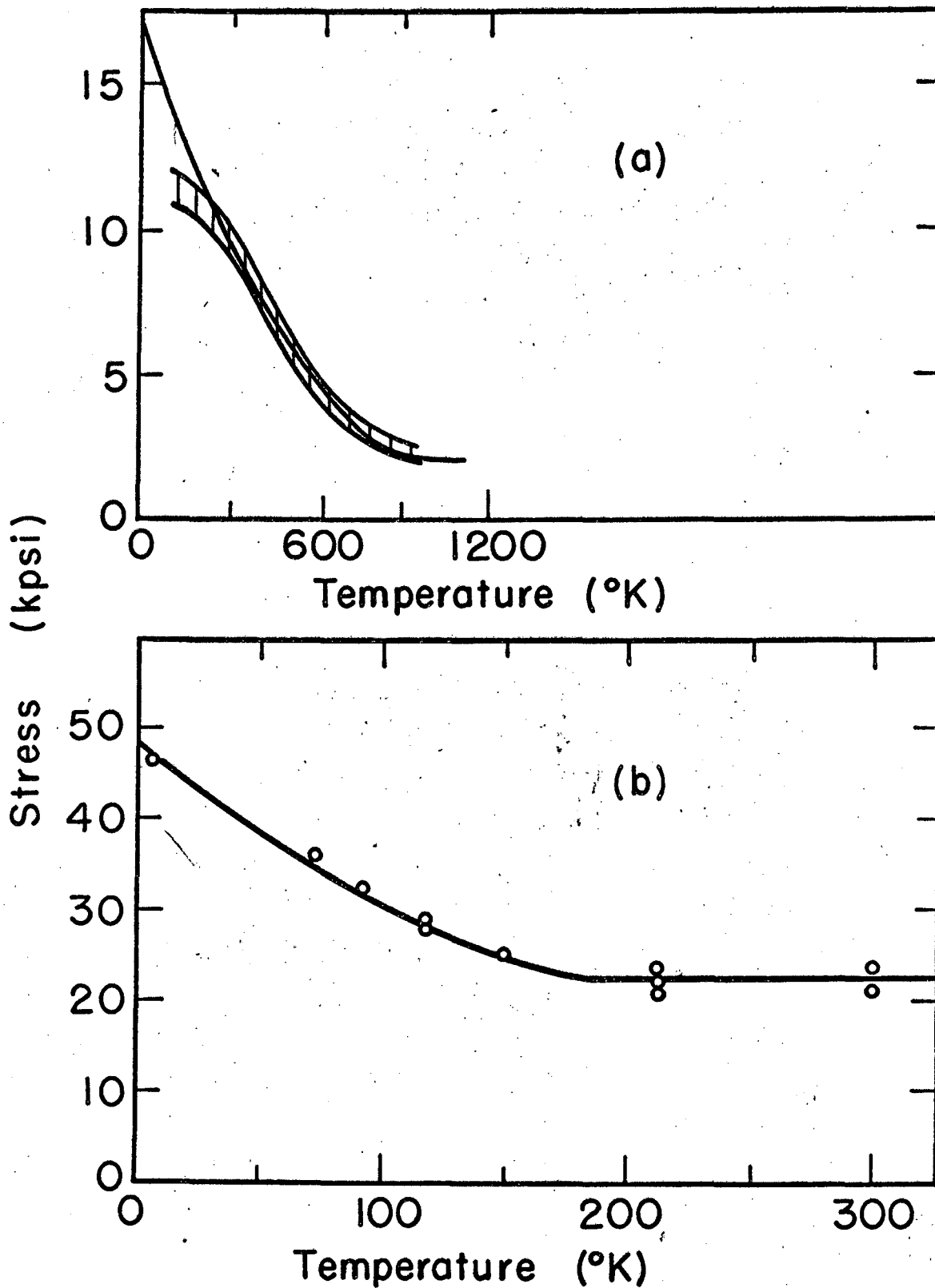


Fig.10 Resolved Shear Stress vs. Temperature for Single Crystals of Two Hexagonal Materials . a) Be b) Ag₂Al

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mechanism results from the auxiliary data that have been obtained on activation volumes. The data of Mote, et. al.¹² gives an activation volume at 115°K of about $16b^3$, which is certainly a strong indication of the Peierls' mechanism.

The validity of the Peierls' theory presented in the previous sections of this report is best illustrated by comparing the theoretical predictions with the detailed correlations of experimental data recently summarized so excellently by Conrad.¹³⁻¹⁴ Since Conrad neglected the possible effects of interstitials on the thermally activated portion of the low temperature deformation of the BCC metals, we will also assume that such interstitials did not slow down the velocity of the kink enough to disqualify the use of the simple theory as formulated in Eqn. 28. In the following we will use Conrad's data as he plotted them; since, however, we have the advantage of the guidance given by a good theory, we will select more appropriate values of T_{c_p} than was possible by merely viewing the experimental data. We have plotted the experimental datum points for each metal separately, as shown in Figs. 11-13, and in terms of T_{c_p} and superimposed the theoretical curve for $\alpha = 0$ on the same graph. Thus the solid lines in Figs. 11-13, give the theoretically predicted trends. Within the scatter of the experimental data, the agreement between theory and experiment is excellent. The lower value of T_{c_p} for single, as contrasted with polycrystalline W, as shown by Eqn. 29, can be attributed to higher values of $\frac{\rho L}{\delta}$ in the single crystal tests. The Peierls' stresses obtained from these data are given in Table II. Furthermore, letting $\tau_0 = 5Gb^2$, where δ , in this context, will be assumed to be 1/2,

$$R-1 = \tau_p / G \pi \delta,$$

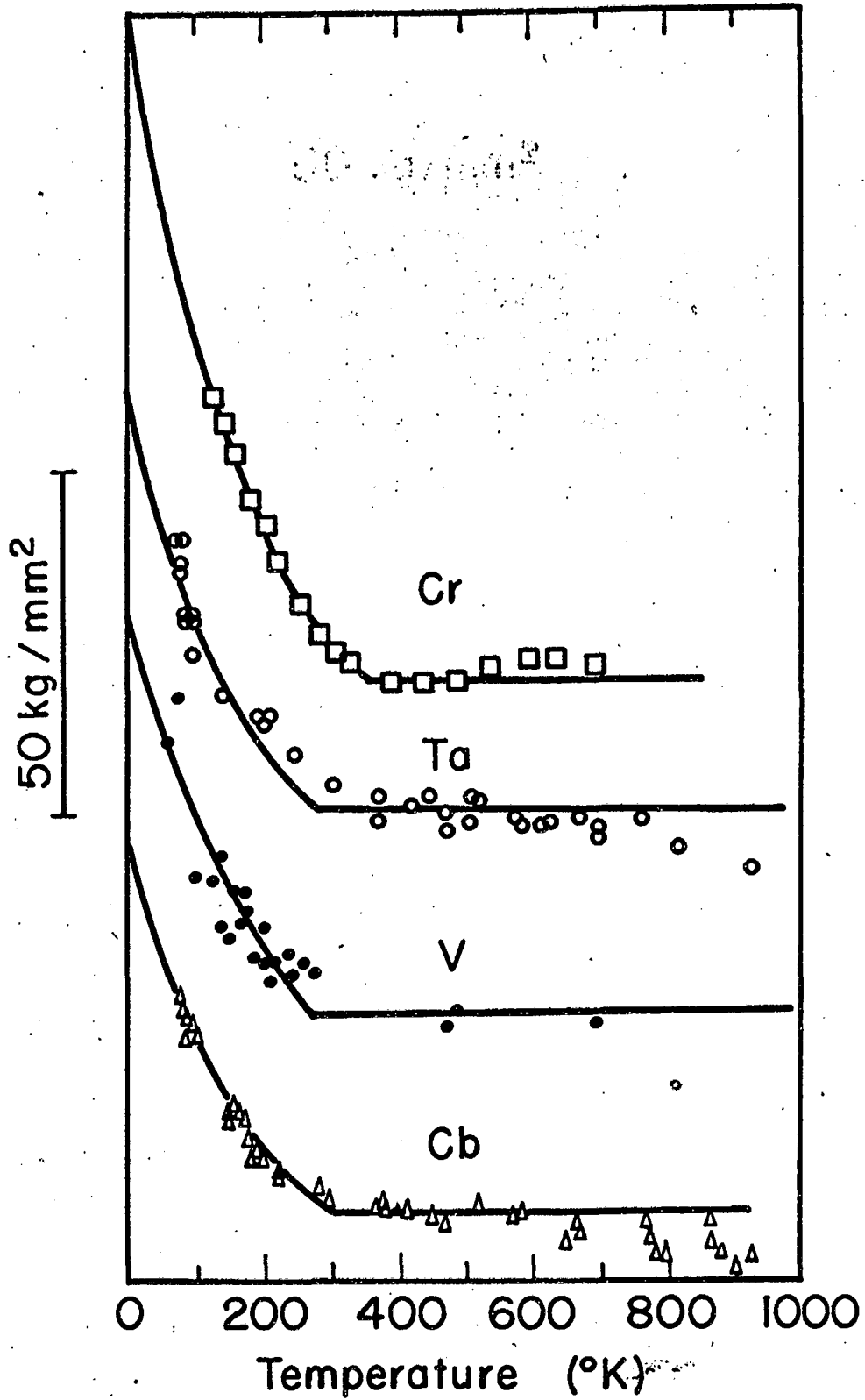


Fig. 11: Resolved Shear Stress vs. Temperature for BCC Metals.

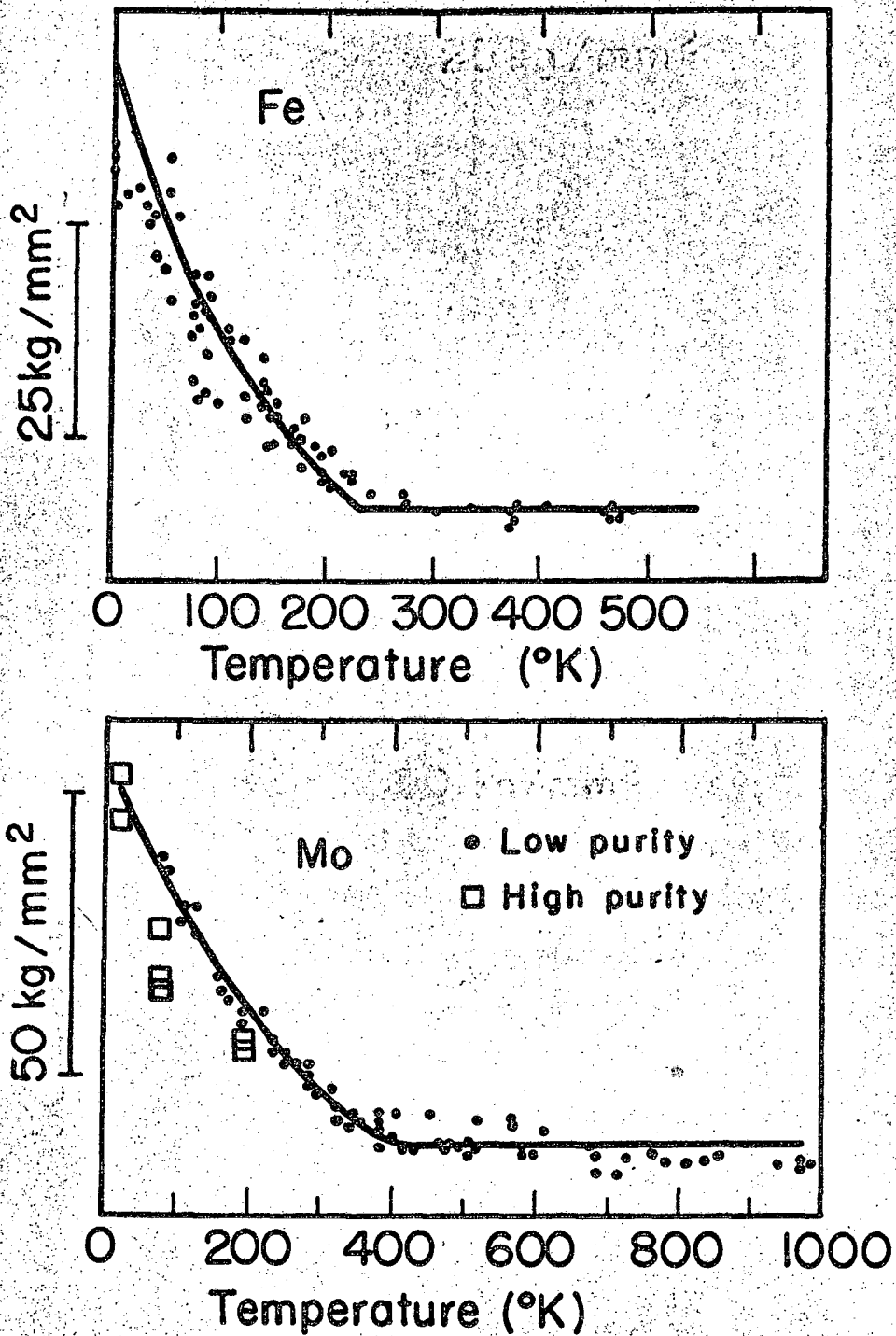


Fig.12 Resolved Shear Stress vs. Temperature for BCC Metals.

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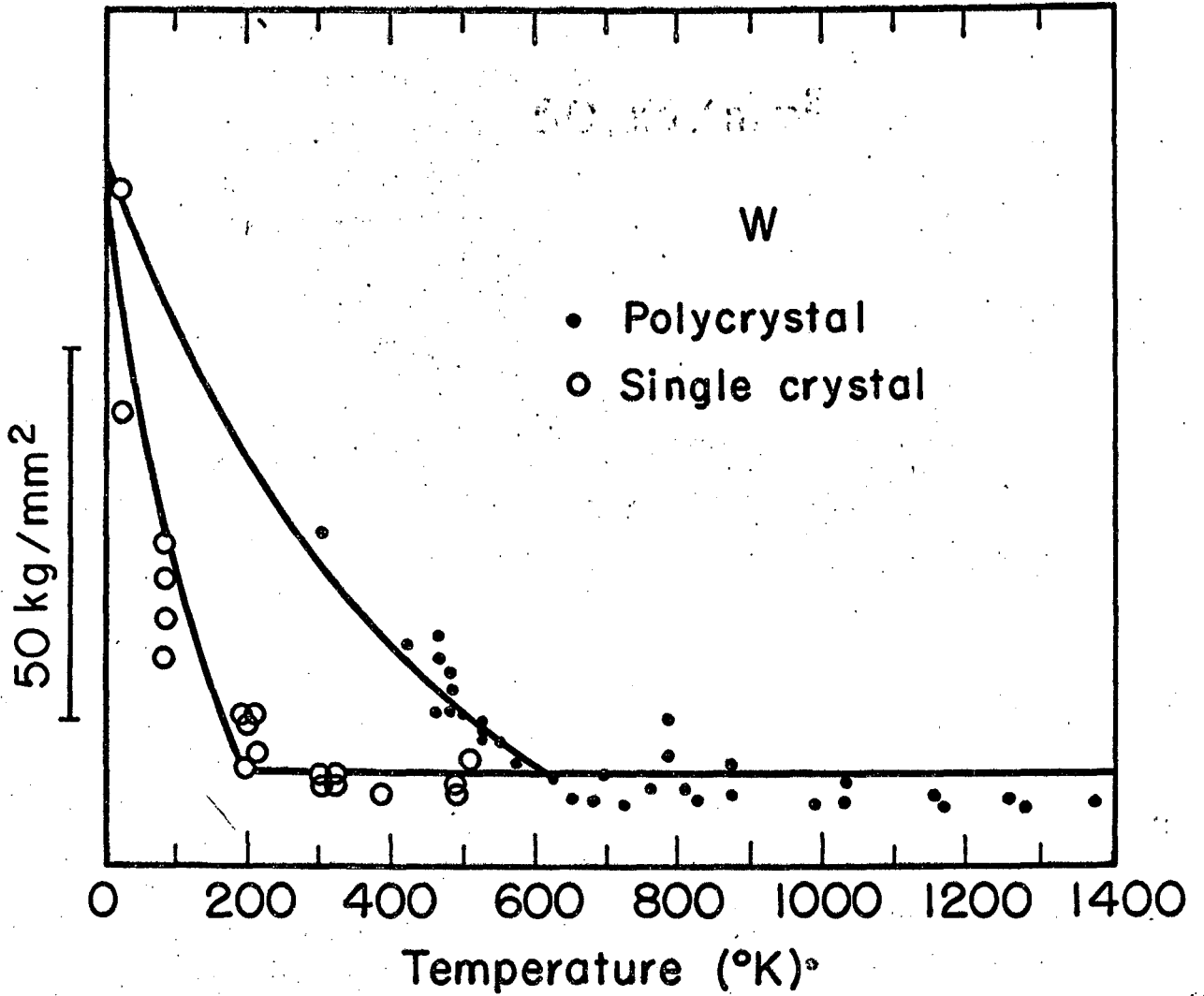


Fig. 13 Resolved Shear Stress vs. Temperature for BCC Metals.

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as can be deduced from Eqn. 2 for τ_p in terms of $R - 1$ when $\alpha = 0$ and $a = b$.

Table II

Deduced Values of the Peierls' Stress

At. No.	Metal	G dynes/cm ²	τ_p dynes/cm ²	R	2U _k e. v.
23	V	5.2 x 10 ⁸	58 x 10 ⁵	1.00029	0.55
24	Cr	11.4 x 10 ⁸	97 x 10 ⁵	1.00042	0.70
26	Fe	7.4 x 10 ⁸	55 x 10 ⁵	1.00023	0.55
41	Cb	4.0 x 10 ⁸	56 x 10 ⁵	1.00046	0.50
42	Mo	12.7 x 10 ⁸	70 x 10 ⁵	1.00025	0.70
73	Ta	7.0 x 10 ⁸	60 x 10 ⁵	1.00026	0.72
74	W	15.7 x 10 ⁸	85 x 10 ⁵	1.00034	0.80

Conrad also summarized the known data on the experimentally determined activation energies as a function of the stress for several BCC metals. These activation energies were generally obtained from the usual technique of the effect of changes in temperature on strain rate or the equivalent thereof. As shown in Fig. 6, however, unique universally valid curves should be obtained when τ^*/τ_p is plotted as a function of $U_n/2U_k$; furthermore, such curves should agree well with those of τ^*/τ_p versus T/T_{c_p} . This is indeed the case. Thus we have plotted Conrad's data on this universal basis, dividing his experimentally determined activation energies U_n , by the activation energy $2U_k$, shown in Table II, obtained by extrapolation of the experimentally determined values of U_n as τ^*

approaches zero. The experimental datum points shown in Figs.14-17 agree remarkably well with the solid theoretical curve. In the vicinity of $\tau^* = 0$, the experimentally determined values of U_n increase rapidly because athermal mechanisms begin to become operative here.

The most reliable verification of the Peierls' process concerns agreement between the theoretical and experimentally deduced activation volumes. The experimental activation volumes are usually obtained by the effect of small changes in strain rate on the flow stress. According to Eqn. 28 we define β as

$$\beta = \frac{\partial \ln \dot{\gamma}}{\partial \tau^*} = \frac{\partial \ln \rho}{\partial \tau^*} - \frac{\partial \ln w}{\partial \tau^*} - \frac{1}{kT} \frac{\partial U_n}{\partial \tau^*} \quad (39)$$

We take βkT as the apparent activation volume, v_a , where

$$v_a = \beta kT = kT \frac{\partial \ln \rho}{\partial \tau^*} - \frac{\partial \ln w}{\partial \tau^*} - \frac{\partial U_n}{\partial \tau^*} \quad (40)$$

and the negative or last term of Eqn. 40 is the theoretical activation volume, v^* , defined theoretically by Eqn. 24 and shown in Fig. 7. Whereas the term containing w is always negligible small, v_a can on occasions be slightly larger than v^* as a result of the possible increase in dislocation density, ρ , as the stress is increased. In Figs.18 and 19 we have plotted the data reported by Conrad for the experimentally determined values of v_a/b^3 as a function of τ^*/τ_p ; using the previously determined value of $2U_k$ we have drawn the curves for theoretical activation volumes v^*/b^3 . Again the agreement is very good and leaves no doubt that the BCC metals discussed here deform by the Peierls' mechanism.

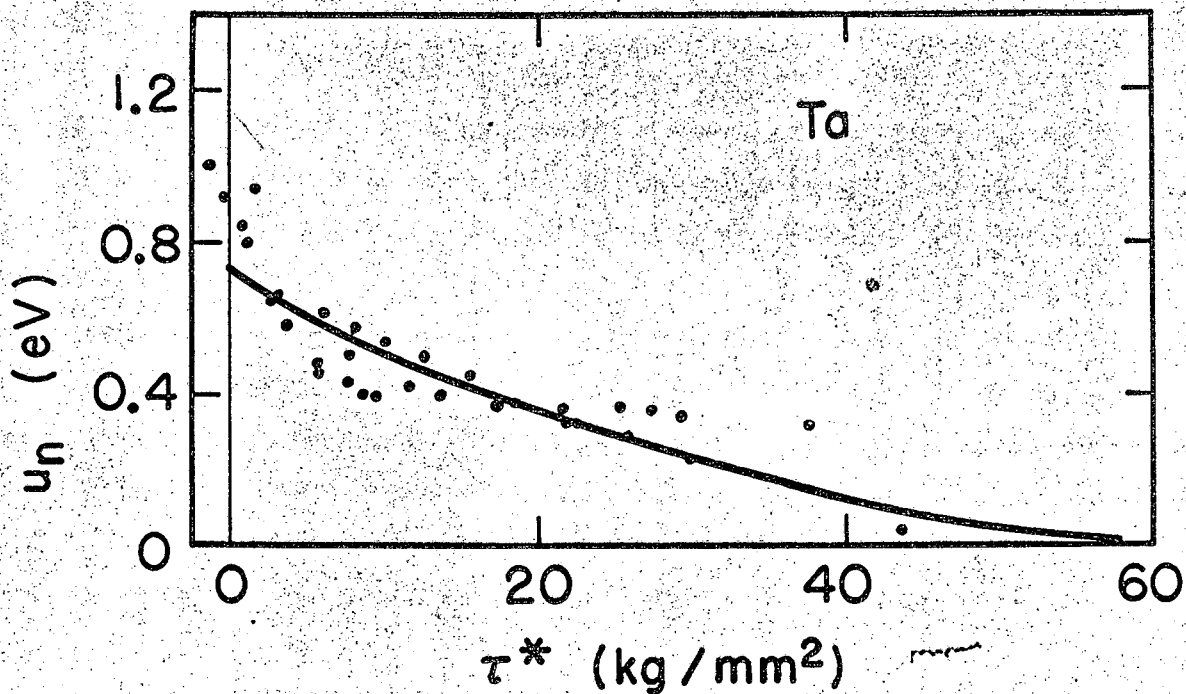
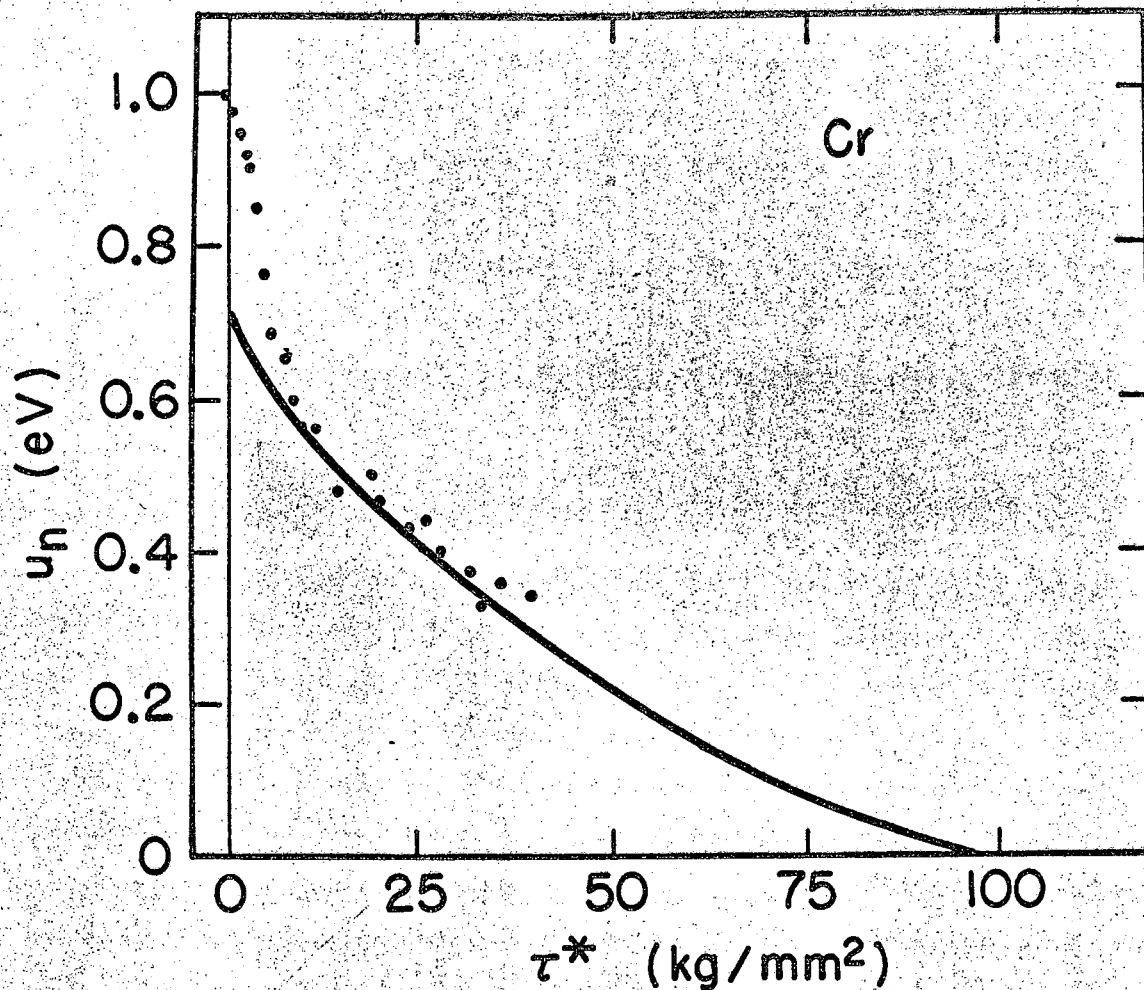


Fig. 14 Activation Energy vs. Stress for BCC Metals.

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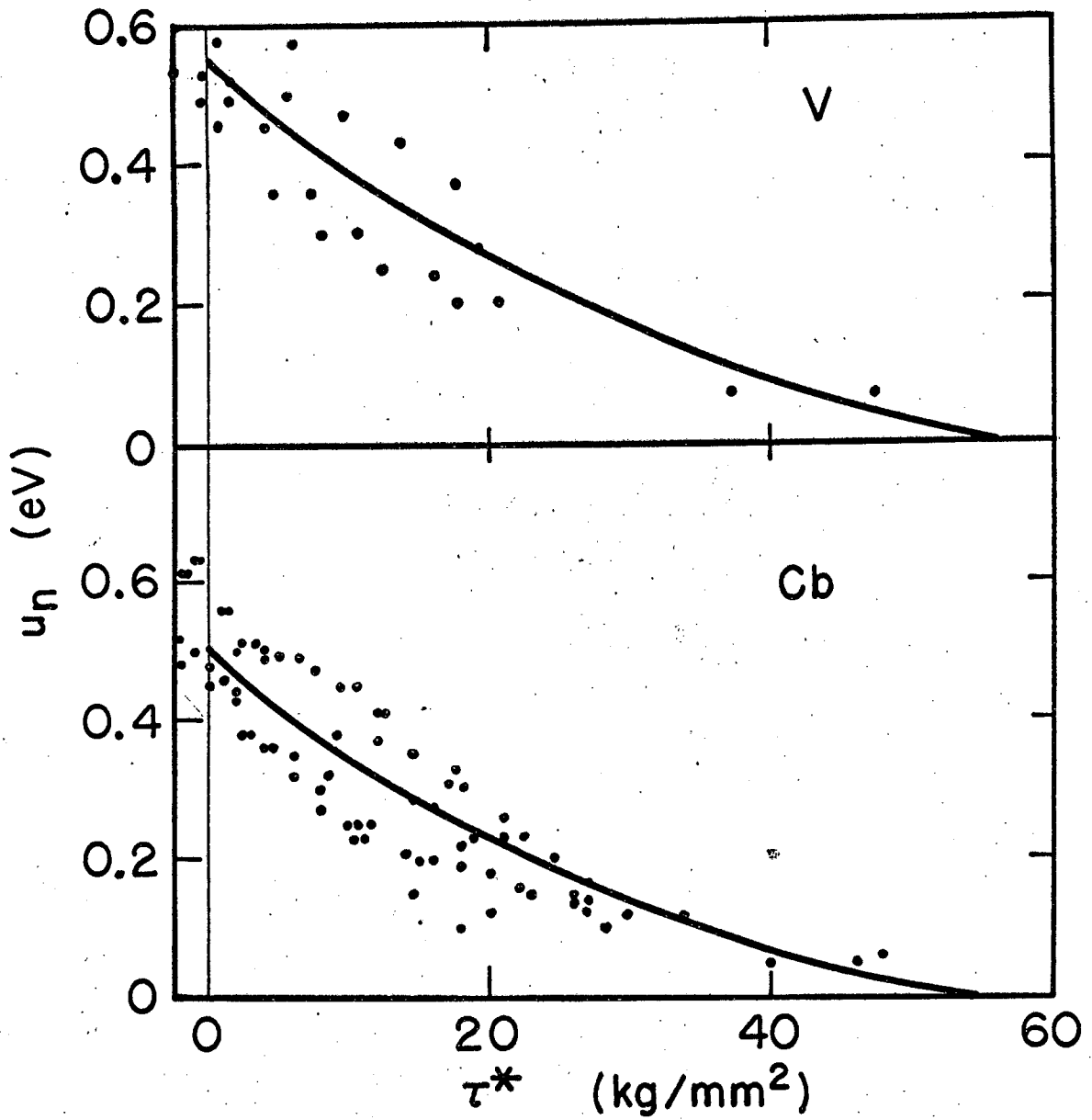


Fig. 15 Activation Energy vs. Stress for BCC Metals.

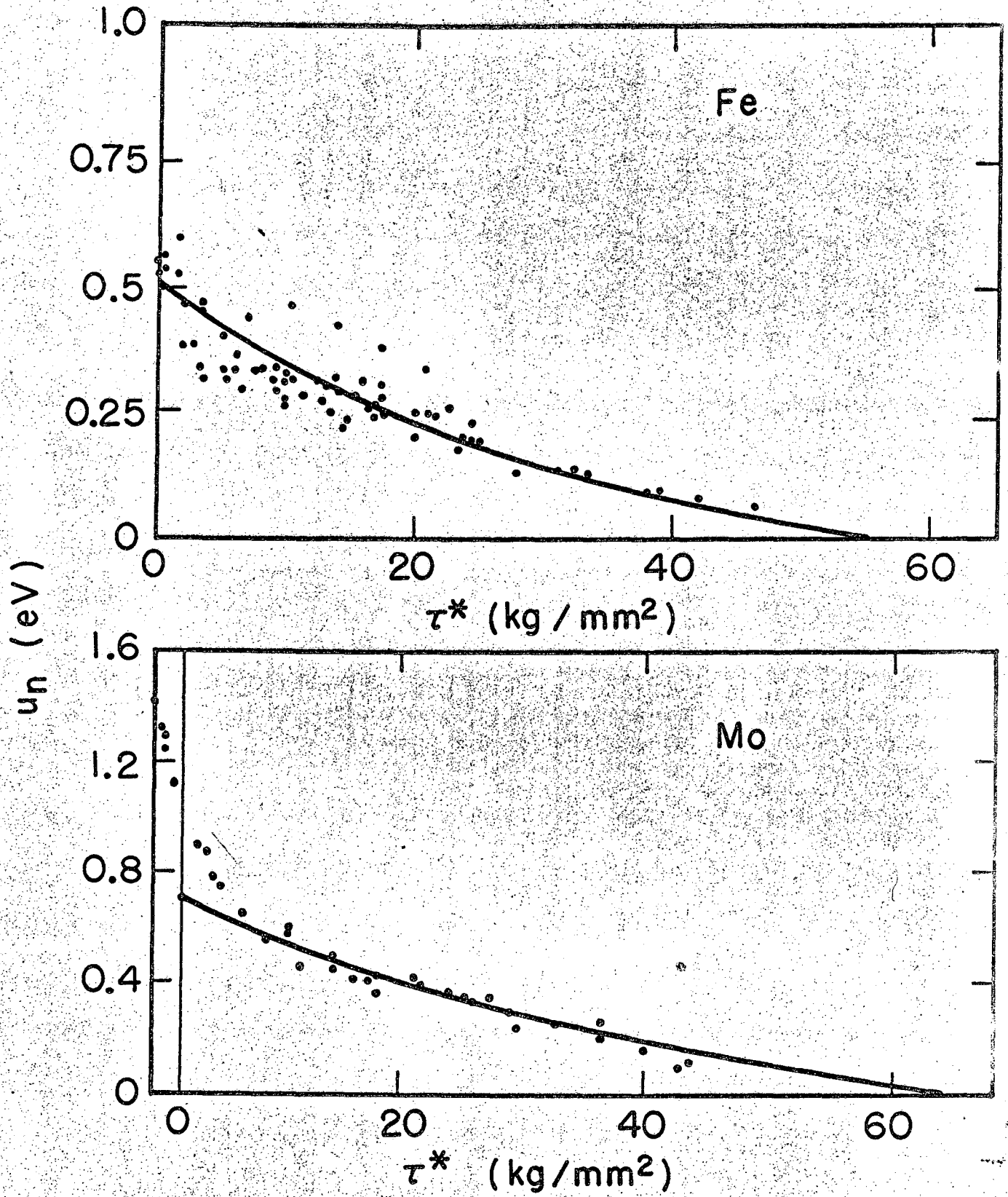


Fig. 16 Activation Energy vs. Stress for BCC Metals.

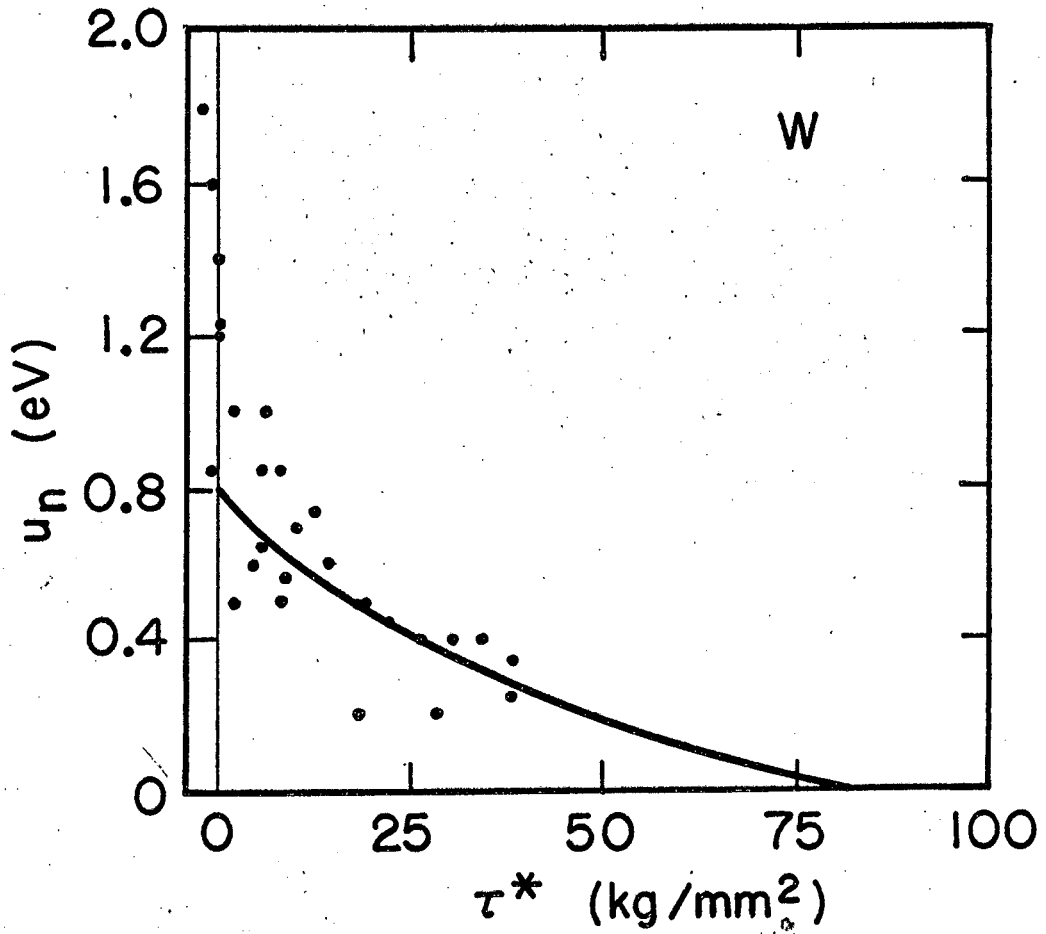


Fig.17 Activation Energy vs. Stress for BCC Metals.

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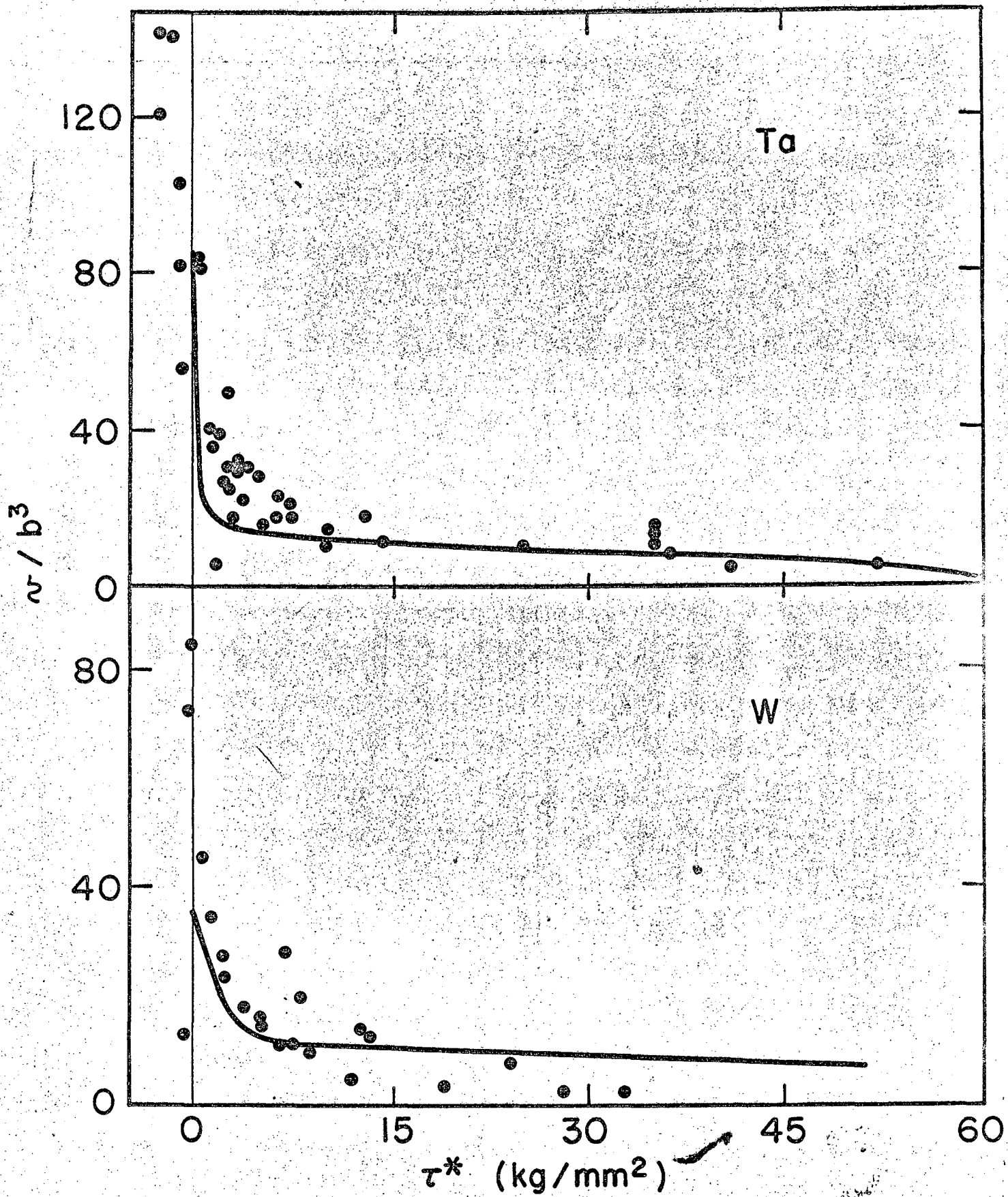


Fig. 18 Activation Volume vs. Stress for BCC Metals.

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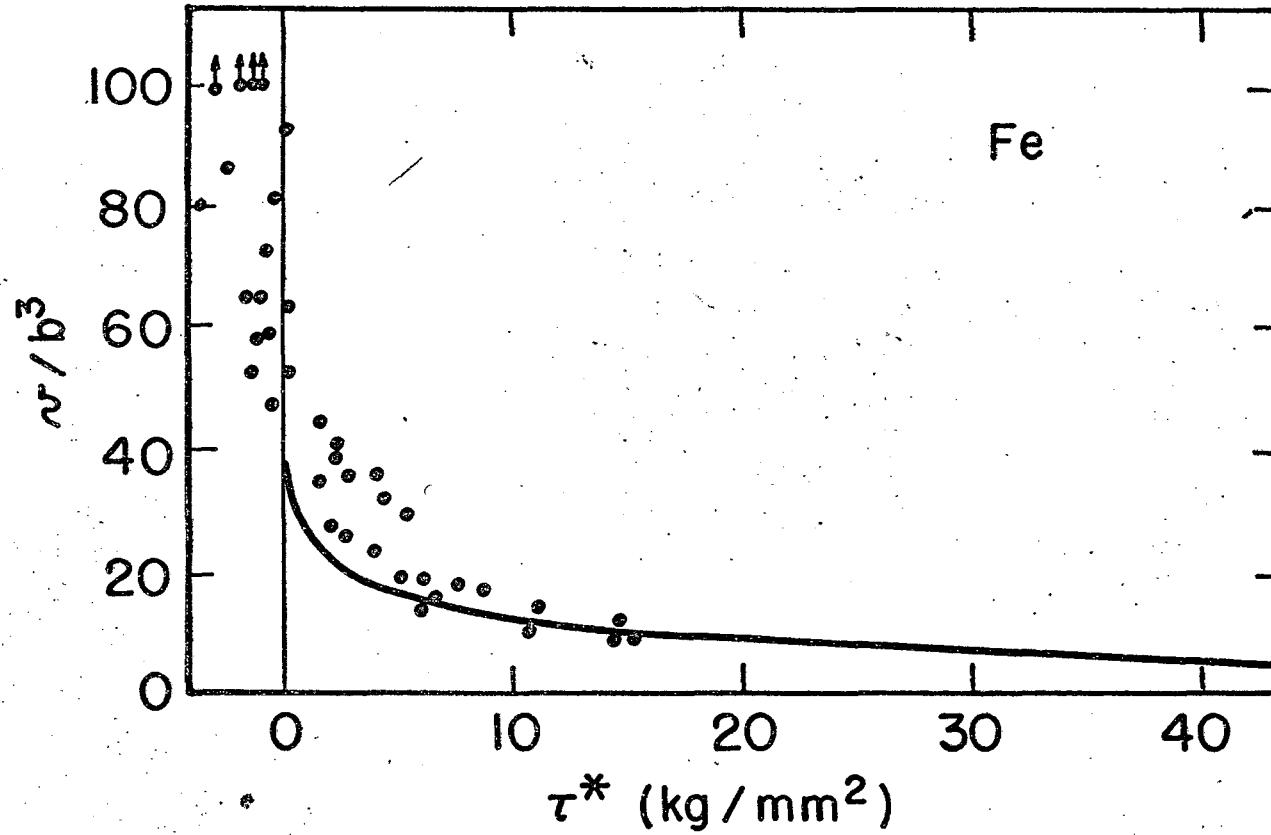


Fig. 19 Activation Volume vs. Stress for BCC Metals.

VI. CONCLUSIONS

1. An accurate theory has been developed for describing the plastic deformation of materials by the thermally activated Peierl's mechanism.

2. The theory agrees very well with many experimental data on the prismatic slip of some hexagonal CP metals and the deformation of BCC metals.

3. Additional advances in this area are now contingent on more accurate experimental data.

VIII. ACKNOWLEDGMENTS

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APPENDIX

Tabulated here is the computer output for the evaluation of U_n . The notation is as follows:

$$R = \frac{\Gamma_c}{\Gamma_o}$$

$$\text{Alpha} = \alpha$$

$$K = \frac{\tau_{ba}}{\pi(\Gamma_c - \Gamma_o)}$$

$$E1 = \frac{\pi \Gamma_o}{2a} (2U_k)$$

$$Z_o = \frac{2\pi y_o}{a}$$

$$Z_c = \frac{2\pi \lambda_c}{a}$$

$$E = U_n / 2U_k$$

$$\text{Difference} = \frac{\partial \left(\frac{U_n}{2U_k} \right)}{\partial K} = \frac{\partial U_n}{\partial C} \cdot \frac{\pi(\Gamma_c - \Gamma_o)}{2U_k a b}$$

R= 1.0001 ALPHA= 0.0010 E1= 0.56567E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31316E 01	0.27727E 01	0.97146E 00	-0.28545E 01
0.08030	-0.30613E 01	0.21831E 01	0.83611E 00	-0.19252E 01
0.15060	-0.29906E 01	0.18294E 01	0.72861E 00	-0.15292E 01
0.22090	-0.29191E 01	0.15512E 01	0.63431E 00	-0.13415E 01
0.29120	-0.28464E 01	0.13128E 01	0.54910E 00	-0.12120E 01
0.36150	-0.27721E 01	0.10814E 01	0.47079E-00	-0.11139E 01
0.43180	-0.26955E 01	0.87581E 00	0.39860E-00	-0.10270E 01
0.50210	-0.26161E 01	0.66439E 00	0.33151E-00	-0.95436E 00
0.57240	-0.25327E 01	0.45833E-00	0.26926E-00	-0.88543E 00
0.64270	-0.24442E 01	0.24857E-00	0.21158E-00	-0.82053E 00
0.71300	-0.23485E 01	0.35526E-01	0.15845E-00	-0.75581E 00
0.78329	-0.22424E 01	-0.20028E-00	0.10988E-00	-0.69085E 00
0.85359	-0.21196E 01	-0.45894E-00	0.66383E-01	-0.61872E 00
0.92389	-0.19644E 01	-0.78090E 00	0.28915E-01	-0.53297E 00
0.99419	-0.16796E 01	-0.13562E 01	0.11449E-02	-0.39503E-00

R= 1.0001 ALPHA= -0.2500 E1= 0.54100E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31283E 01	0.27226E 01	0.96840E 00	-0.31596E 01
0.08243	-0.30317E 01	0.20595E 01	0.82128E 00	-0.20312E 01
0.15486	-0.29351E 01	0.17108E 01	0.70916E 00	-0.15481E 01
0.22729	-0.28385E 01	0.14353E 01	0.61271E 00	-0.13316E 01
0.29972	-0.27416E 01	0.12090E 01	0.52696E 00	-0.11839E 01
0.37215	-0.26444E 01	0.10020E 01	0.44930E-00	-0.10722E 01
0.44458	-0.25464E 01	0.80880E 00	0.37834E-00	-0.97967E 00
0.51701	-0.24472E 01	0.61802E 00	0.31315E-00	-0.90012E 00
0.58944	-0.23458E 01	0.43857E-00	0.25329E-00	-0.82639E 00
0.66187	-0.22412E 01	0.26062E-00	0.19831E-00	-0.75905E 00
0.73430	-0.21315E 01	0.69065E-01	0.14796E-00	-0.69525E 00
0.80673	-0.20137E 01	-0.13026E-00	0.10232E-00	-0.63007E 00
0.87916	-0.18819E 01	-0.35605E-00	0.61621E-01	-0.56192E 00
0.95159	-0.17214E 01	-0.63739E 00	0.26704E-01	-0.48208E-00
1.02402	-0.14379E 01	-0.11604E 01	0.89620E-03	-0.35632E-00

R= 1.0100 ALPHA= 0.0010 E1= 0.56672E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31316E 01	0.27727E 01	0.97137E 00	-0.28626E 01
0.08030	-0.30613E 01	0.21831E 01	0.83633E 00	-0.19210E 01
0.15060	-0.29906E 01	0.18294E 01	0.72901E 00	-0.15267E 01
0.22090	-0.29191E 01	0.15512E 01	0.63480E 00	-0.13401E 01
0.29120	-0.28464E 01	0.13128E 01	0.54964E 00	-0.12114E 01
0.36150	-0.27721E 01	0.10814E 01	0.47134E-00	-0.11138E 01
0.43180	-0.26955E 01	0.87581E 00	0.39912E-00	-0.10273E 01
0.50210	-0.26161E 01	0.66439E 00	0.33198E-00	-0.95506E 00
0.57240	-0.25327E 01	0.45833E-00	0.26967E-00	-0.88636E 00
0.64270	-0.24442E 01	0.24857E-00	0.21191E-00	-0.82160E 00
0.71300	-0.23485E 01	0.35526E-01	0.15869E-00	-0.75695E 00
0.78329	-0.22424E 01	-0.20028E-00	0.11005E-00	-0.69198E 00
0.85359	-0.21196E 01	-0.45894E-00	0.66480E-01	-0.61976E 00
0.92389	-0.19644E 01	-0.78090E 00	0.28953E-01	-0.53382E 00
0.99419	-0.16796E 01	-0.13562E 01	0.11459E-02	-0.39555E-00

R= 1.0100 ALPHA= -0.2500 EI= 0.54201E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31283E 01	0.27226E 01	0.96826E 00	-0.31738E 01
0.08243	-0.30317E 01	0.20595E 01	0.82146E 00	-0.20268E 01
0.15486	-0.29351E 01	0.17108E 01	0.70951E 00	-0.15456E 01
0.22729	-0.28385E 01	0.14353E 01	0.61317E 00	-0.13302E 01
0.29972	-0.27416E 01	0.12090E 01	0.52747E 00	-0.11832E 01
0.37215	-0.26444E 01	0.10020E 01	0.44982E-00	-0.10721E 01
0.44458	-0.25464E 01	0.80880E 00	0.37884E-00	-0.97998E 00
0.51701	-0.24472E 01	0.61802E 00	0.31360E-00	-0.90074E 00
0.58944	-0.23458E 01	0.43857E-00	0.25368E-00	-0.82722E 00
0.66187	-0.22412E 01	0.26062E-00	0.19863E-00	-0.76002E 00
0.73430	-0.21315E 01	0.69065E-01	0.14820E-00	-0.69629E 00
0.80673	-0.20137E 01	-0.13026E-00	0.10249E-00	-0.63111E 00
0.87916	-0.18819E 01	-0.35605E-00	0.61721E-01	-0.56289E 00
0.95159	-0.17214E 01	-0.63739E 00	0.26744E-01	-0.48290E-00
1.02402	-0.14379E 01	-0.11604E 01	0.89717E-03	-0.35685E-00

R= 1.0001 ALPHA= 0.2500 EI= 0.58835E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31336E 01	0.28075E 01	0.97387E 00	-0.26131E 01
0.08243	-0.30756E 01	0.22330E 01	0.84250E 00	-0.18137E 01
0.15486	-0.30172E 01	0.19099E 01	0.73613E 00	-0.14686E 01
0.22729	-0.29581E 01	0.16247E 01	0.64082E 00	-0.13159E 01
0.29972	-0.28980E 01	0.13597E 01	0.55339E 00	-0.12071E 01
0.37215	-0.28364E 01	0.11138E 01	0.47257E-00	-0.11158E 01
0.44458	-0.27728E 01	0.87852E 00	0.39757E-00	-0.10354E 01
0.51701	-0.27065E 01	0.64045E 00	0.32788E-00	-0.96220E 00
0.58944	-0.26368E 01	0.39081E-00	0.26340E-00	-0.89014E 00
0.66187	-0.25624E 01	0.14279E-00	0.20432E-00	-0.81579E 00
0.73430	-0.24815E 01	-0.11861E-00	0.15066E-00	-0.74079E 00
0.80673	-0.23911E 01	-0.38935E-00	0.10272E-00	-0.66195E 00
0.87916	-0.22853E 01	-0.68189E 00	0.60828E-01	-0.57833E 00
0.95159	-0.21496E 01	-0.10288E 01	0.25807E-01	-0.48351E-00
1.02402	-0.18896E 01	-0.16097E 01	0.83444E-03	-0.34478E-00

R= 1.0100 ALPHA= 0.2500 EI= 0.58946E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31336E 01	0.28075E 01	0.97381E 00	-0.26189E 01
0.08243	-0.30756E 01	0.22330E 01	0.84275E 00	-0.18096E 01
0.15486	-0.30172E 01	0.19099E 01	0.73655E 00	-0.14661E 01
0.22729	-0.29581E 01	0.16247E 01	0.64134E 00	-0.13146E 01
0.29972	-0.28980E 01	0.13597E 01	0.55394E 00	-0.12066E 01
0.37215	-0.28364E 01	0.11138E 01	0.47312E-00	-0.11159E 01
0.44458	-0.27728E 01	0.87852E 00	0.39809E-00	-0.10359E 01
0.51701	-0.27065E 01	0.64045E 00	0.32834E-00	-0.96303E 00
0.58944	-0.26368E 01	0.39081E-00	0.26379E-00	-0.89119E 00
0.66187	-0.25624E 01	0.14279E-00	0.20462E-00	-0.81692E 00
0.73430	-0.24815E 01	-0.11861E-00	0.15088E-00	-0.74193E 00
0.80673	-0.23911E 01	-0.38935E-00	0.10286E-00	-0.66301E 00
0.87916	-0.22853E 01	-0.68189E 00	0.60904E-01	-0.57923E 00
0.95159	-0.21496E 01	-0.10288E 01	0.25834E-01	-0.48419E-00
1.02402	-0.18896E 01	-0.16097E 01	0.83490E-03	-0.34514E-00

R= 1.0001 ALPHA= -0.5000 E1= 0.51403E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31216E 01	0.26459E 01	0.96436E 00	-0.35645E 01
0.08753	-0.29683E 01	0.19112E 01	0.80128E 00	-0.21034E 01
0.16506	-0.28220E 01	0.15599E 01	0.68316E 00	-0.15236E 01
0.24259	-0.26857E 01	0.13029E 01	0.58453E 00	-0.12721E 01
0.32012	-0.25596E 01	0.10954E 01	0.49878E-00	-0.11061E 01
0.39765	-0.24419E 01	0.90541E 00	0.42246E-00	-0.98433E 00
0.47518	-0.23308E 01	0.72922E 00	0.35380E-00	-0.88556E 00
0.55271	-0.22242E 01	0.55617E 00	0.29148E-00	-0.80382E 00
0.63024	-0.21201E 01	0.39413E-00	0.23485E-00	-0.73047E 00
0.70777	-0.20166E 01	0.23404E-00	0.18327E-00	-0.66527E 00
0.78529	-0.19112E 01	0.62260E-01	0.13634E-00	-0.60535E 00
0.86282	-0.18006E 01	-0.11602E-00	0.94058E-01	-0.54538E 00
0.94035	-0.16792E 01	-0.31752E-00	0.56524E-01	-0.48412E-00
1.01788	-0.15336E 01	-0.56810E 00	0.24448E-01	-0.41372E-00
1.09541	-0.12796E 01	-0.10329E 01	0.81869E-03	-0.30478E-00

R= 1.0100 ALPHA= -0.5000 E1= 0.51496E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31216E 01	0.26459E 01	0.96425E 00	-0.35750E 01
0.08753	-0.29683E 01	0.19112E 01	0.80151E 00	-0.20991E 01
0.16506	-0.28220E 01	0.15599E 01	0.68356E 00	-0.15213E 01
0.24259	-0.26857E 01	0.13029E 01	0.58503E 00	-0.12709E 01
0.32012	-0.25596E 01	0.10954E 01	0.49932E-00	-0.11056E 01
0.39765	-0.24419E 01	0.90541E 00	0.42301E-00	-0.98419E 00
0.47518	-0.23308E 01	0.72922E 00	0.35431E-00	-0.88610E 00
0.55271	-0.22242E 01	0.55617E 00	0.29194E-00	-0.80447E 00
0.63024	-0.21201E 01	0.39413E-00	0.23525E-00	-0.73129E 00
0.70777	-0.20166E 01	0.23404E-00	0.18359E-00	-0.66621E 00
0.78529	-0.19112E 01	0.62260E-01	0.13659E-00	-0.60634E 00
0.86282	-0.18006E 01	-0.11602E-00	0.94227E-01	-0.54635E 00
0.94035	-0.16792E 01	-0.31752E-00	0.56623E-01	-0.48502E-00
1.01788	-0.15336E 01	-0.56810E 00	0.24488E-01	-0.41449E-00
1.09541	-0.12796E 01	-0.10329E 01	0.81972E-03	-0.30528E-00

R= 1.0001 ALPHA= 0.5000 E1= 0.60973E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31349E 01	0.28339E 01	0.97582E 00	-0.24177E 01
0.08753	-0.30832E 01	0.22907E 01	0.84441E 00	-0.16950E 01
0.16506	-0.30311E 01	0.19607E 01	0.73560E 00	-0.14034E 01
0.24259	-0.29784E 01	0.16616E 01	0.63681E 00	-0.12743E 01
0.32012	-0.29248E 01	0.13929E 01	0.54532E 00	-0.11800E 01
0.39765	-0.28699E 01	0.11098E 01	0.45966E-00	-0.11049E 01
0.47518	-0.28132E 01	0.81866E 00	0.37987E-00	-0.10291E 01
0.55271	-0.27542E 01	0.52557E 00	0.30667E-00	-0.94417E 00
0.63024	-0.26921E 01	0.22706E-00	0.24072E-00	-0.85065E 00
0.70777	-0.26258E 01	-0.73825E-01	0.18252E-00	-0.75073E 00
0.78529	-0.25538E 01	-0.36202E-00	0.13200E-00	-0.65163E 00
0.86282	-0.24733E 01	-0.64655E 00	0.88579E-01	-0.56005E 00
0.94035	-0.23792E 01	-0.93420E 00	0.51826E-01	-0.47405E-00
1.01788	-0.22586E 01	-0.12537E 01	0.21801E-01	-0.38727E-00
1.09541	-0.20275E 01	-0.17780E 01	0.69969E-03	-0.27218E-00

R= 1.0100 ALPHA= 0.5000 E1= 0.61090E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31349E 01	0.28339E 01	0.97581E 00	-0.24194E 01
0.08753	-0.30832E 01	0.22907E 01	0.84470E 00	-0.16910E 01
0.16506	-0.30311E 01	0.19607E 01	0.73607E 00	-0.14011E 01
0.24259	-0.29784E 01	0.16616E 01	0.63737E 00	-0.12731E 01
0.32012	-0.29248E 01	0.13929E 01	0.54591E 00	-0.11797E 01
0.39765	-0.28699E 01	0.11098E 01	0.46023E-00	-0.11052E 01
0.47518	-0.28132E 01	0.81866E 00	0.38039E-00	-0.10298E 01
0.55271	-0.27542E 01	0.52557E 00	0.30710E-00	-0.94521E 00
0.63024	-0.26921E 01	0.22706E-00	0.24107E-00	-0.85180E 00
0.70777	-0.26258E 01	-0.73825E-01	0.18277E-00	-0.75185E 00
0.78529	-0.25538E 01	-0.36202E-00	0.13218E-00	-0.65264E 00
0.86282	-0.24733E 01	-0.64655E 00	0.88689E-01	-0.56091E 00
0.94035	-0.23792E 01	-0.93420E 00	0.51883E-01	-0.47474E-00
1.01788	-0.22586E 01	-0.12537E 01	0.21821E-01	-0.38775E-00
1.09541	-0.20275E 01	-0.17780E 01	0.69998E-03	-0.27242E-00

R= 1.0001 ALPHA= -0.7500 E1= 0.48333E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31017E 01	0.25131E 01	0.95925E 00	-0.40752E 01
0.09418	-0.28114E 01	0.17650E 01	0.78259E 00	-0.20987E 01
0.17835	-0.26117E 01	0.14316E 01	0.66300E 00	-0.14207E 01
0.26253	-0.24609E 01	0.11960E 01	0.56588E 00	-0.11538E 01
0.34670	-0.23358E 01	0.10037E 01	0.48243E-00	-0.99137E 00
0.43088	-0.22256E 01	0.82866E 00	0.40861E-00	-0.87700E 00
0.51505	-0.21246E 01	0.66787E 00	0.34232E-00	-0.78755E 00
0.59923	-0.20291E 01	0.50985E 00	0.28218E-00	-0.71440E 00
0.68340	-0.19365E 01	0.36173E-00	0.22749E-00	-0.64971E 00
0.76758	-0.18445E 01	0.21091E-00	0.17759E-00	-0.59280E 00
0.85175	-0.17508E 01	0.53822E-01	0.13219E-00	-0.53938E 00
0.93593	-0.16522E 01	-0.11278E-00	0.91213E-01	-0.48681E-00
1.02011	-0.15435E 01	-0.29721E-00	0.54833E-01	-0.43220E-00
1.10428	-0.14124E 01	-0.53027E 00	0.23708E-01	-0.36976E-00
1.18846	-0.11820E 01	-0.95636E 00	0.79244E-03	-0.27224E-00

R= 1.0100 ALPHA= -0.7500 E1= 0.48416E-00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31017E 01	0.25131E 01	0.95921E 00	-0.40790E 01
0.09418	-0.28114E 01	0.17650E 01	0.78289E 00	-0.20946E 01
0.17835	-0.26117E 01	0.14316E 01	0.66347E 00	-0.14188E 01
0.26253	-0.24609E 01	0.11960E 01	0.56643E 00	-0.11528E 01
0.34670	-0.23358E 01	0.10037E 01	0.48301E-00	-0.99105E 00
0.43088	-0.22256E 01	0.82866E 00	0.40918E-00	-0.87713E 00
0.51505	-0.21246E 01	0.66787E 00	0.34285E-00	-0.78799E 00
0.59923	-0.20291E 01	0.50985E 00	0.28266E-00	-0.71507E 00
0.68340	-0.19365E 01	0.36173E-00	0.22790E-00	-0.65052E 00
0.76758	-0.18445E 01	0.21091E-00	0.17792E-00	-0.59370E 00
0.85175	-0.17508E 01	0.53822E-01	0.13244E-00	-0.54031E 00
0.93593	-0.16522E 01	-0.11278E-00	0.91386E-01	-0.48773E-00
1.02011	-0.15435E 01	-0.29721E-00	0.54934E-01	-0.43305E-00
1.10428	-0.14124E 01	-0.53027E 00	0.23749E-01	-0.37048E-00
1.18846	-0.11820E 01	-0.95636E 00	0.79350E-03	-0.27271E-00

R= 1.0001 ALPHA= 0.7500 E1= 0.62992E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31359E 01	0.28546E 01	0.97754E 00	-0.22457E 01
0.09418	-0.30877E 01	0.23207E 01	0.84366E 00	-0.15905E 01
0.17835	-0.30393E 01	0.19883E 01	0.73130E 00	-0.13349E 01
0.26253	-0.29903E 01	0.16869E 01	0.62801E 00	-0.12271E 01
0.34670	-0.29404E 01	0.13796E 01	0.53070E 00	-0.11561E 01
0.43088	-0.28893E 01	0.10628E 01	0.43896E-00	-0.10899E 01
0.51505	-0.28366E 01	0.71242E 00	0.35365E-00	-0.10134E 01
0.59923	-0.27818E 01	0.34389E-00	0.27772E-00	-0.90206E 00
0.68340	-0.27241E 01	-0.14147E-01	0.21344E-00	-0.76367E 00
0.76758	-0.26627E 01	-0.33486E-00	0.15998E-00	-0.63515E 00
0.85175	-0.25959E 01	-0.60424E 00	0.11525E-00	-0.53137E 00
0.93593	-0.25214E 01	-0.86261E 00	0.77312E-01	-0.45068E-00
1.02011	-0.24344E 01	-0.11189E 01	0.45310E-01	-0.38017E-00
1.10428	-0.23231E 01	-0.14082E 01	0.19105E-01	-0.31132E-00
1.18846	-0.21107E 01	-0.18836E 01	0.61494E-03	-0.21966E-00

R= 1.0100 ALPHA= 0.7500 E1= 0.63121E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31359E 01	0.28546E 01	0.97747E 00	-0.22533E 01
0.09418	-0.30877E 01	0.23207E 01	0.84392E 00	-0.15865E 01
0.17835	-0.30393E 01	0.19883E 01	0.73175E 00	-0.13326E 01
0.26253	-0.29903E 01	0.16869E 01	0.62856E 00	-0.12259E 01
0.34670	-0.29404E 01	0.13796E 01	0.53127E 00	-0.11558E 01
0.43088	-0.28893E 01	0.10628E 01	0.43949E-00	-0.10904E 01
0.51505	-0.28366E 01	0.71242E 00	0.35411E-00	-0.10143E 01
0.59923	-0.27818E 01	0.34389E-00	0.27808E-00	-0.90315E 00
0.68340	-0.27241E 01	-0.14147E-01	0.21371E-00	-0.76471E 00
0.76758	-0.26627E 01	-0.33486E-00	0.16018E-00	-0.63604E 00
0.85175	-0.25959E 01	-0.60424E 00	0.11538E-00	-0.53212E 00
0.93593	-0.25214E 01	-0.86261E 00	0.77396E-01	-0.45130E-00
1.02011	-0.24344E 01	-0.11189E 01	0.45354E-01	-0.38066E-00
1.10428	-0.23231E 01	-0.14082E 01	0.19119E-01	-0.31166E-00
1.18846	-0.21107E 01	-0.18836E 01	0.61511E-03	-0.21983E-00

R= 1.0001 ALPHA= -1.0000 E1= 0.44409E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.28685E 01	0.22929E 01	0.95956E 00	-0.40436E 01
0.10161	-0.25352E 01	0.16328E 01	0.78806E 00	-0.18720E 01
0.19322	-0.23762E 01	0.13353E 01	0.67159E 00	-0.12714E 01
0.28483	-0.22554E 01	0.11179E 01	0.57558E 00	-0.10480E 01
0.37644	-0.21525E 01	0.93263E 00	0.49212E-00	-0.91108E 00
0.46805	-0.20599E 01	0.77483E 00	0.41791E-00	-0.81001E 00
0.55966	-0.19733E 01	0.62521E 00	0.35082E-00	-0.73238E 00
0.65127	-0.18902E 01	0.47782E-00	0.28969E-00	-0.66729E 00
0.74288	-0.18086E 01	0.33715E-00	0.23385E-00	-0.60951E 00
0.83449	-0.17267E 01	0.19607E-00	0.18278E-00	-0.55749E 00
0.92610	-0.16424E 01	0.48848E-01	0.13620E-00	-0.50852E 00
1.01771	-0.15529E 01	-0.11070E-00	0.94037E-01	-0.46020E-00
1.10932	-0.14535E 01	-0.28642E-00	0.56555E-01	-0.40915E-00
1.20093	-0.13328E 01	-0.50510E 00	0.24461E-01	-0.35033E-00
1.29254	-0.11184E 01	-0.90701E 00	0.81610E-03	-0.25810E-00

R= 1.0100 ALPHA= -1.0000 E1= 0.44498E-00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.28685E 01	0.22929E 01	0.95926E 00	-0.40736E 01
0.10161	-0.25352E 01	0.16328E 01	0.78815E 00	-0.18678E 01
0.19322	-0.23762E 01	0.13353E 01	0.67187E 00	-0.12693E 01
0.28483	-0.22554E 01	0.11179E 01	0.57597E 00	-0.10468E 01
0.37644	-0.21525E 01	0.93263E 00	0.49256E-00	-0.91052E 00
0.46805	-0.20599E 01	0.77483E 00	0.41837E-00	-0.80989E 00
0.55966	-0.19733E 01	0.62521E 00	0.35126E-00	-0.73257E 00
0.65127	-0.18902E 01	0.47782E-00	0.29009E-00	-0.66771E 00
0.74288	-0.18086E 01	0.33715E-00	0.23420E-00	-0.61009E 00
0.83449	-0.17267E 01	0.19607E-00	0.18306E-00	-0.55817E 00
0.92610	-0.16424E 01	0.48848E-01	0.13641E-00	-0.50925E 00
1.01771	-0.15529E 01	-0.11070E-00	0.94185E-01	-0.46093E-00
1.10932	-0.14535E 01	-0.28642E-00	0.56641E-01	-0.40983E-00
1.20093	-0.13328E 01	-0.50510E 00	0.24495E-01	-0.35090E-00
1.29254	-0.11184E 01	-0.90701E 00	0.81691E-03	-0.25847E-00

R= 1.0001 ALPHA= 1.0000 E1= 0.64923E-01

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31366E 01	0.28709E 01	0.97888E 00	-0.21117E 01
0.10161	-0.30907E 01	0.23353E 01	0.84164E 00	-0.14982E 01
0.19322	-0.30446E 01	0.20043E 01	0.72531E 00	-0.12698E 01
0.28483	-0.29979E 01	0.17014E 01	0.61707E 00	-0.11816E 01
0.37644	-0.29505E 01	0.13834E 01	0.51368E 00	-0.11286E 01
0.46805	-0.29019E 01	0.99840E 00	0.41444E-00	-0.10833E 01
0.55966	-0.28518E 01	0.55097E 00	0.32341E-00	-0.99362E 00
0.65127	-0.27996E 01	0.92883E-01	0.24864E-00	-0.81614E 00
0.74288	-0.27448E 01	-0.25906E-00	0.19054E-00	-0.63430E 00
0.83449	-0.26864E 01	-0.54114E 00	0.14342E-00	-0.51436E 00
0.92610	-0.26230E 01	-0.78410E 00	0.10380E-00	-0.43243E-00
1.01771	-0.25524E 01	-0.10155E 01	0.69967E-01	-0.36932E-00
1.10932	-0.24700E 01	-0.12484E 01	0.41180E-01	-0.31424E-00
1.20093	-0.23648E 01	-0.15123E 01	0.17436E-01	-0.25919E-00
1.29254	-0.21647E 01	-0.19516E 01	0.56376E-03	-0.18417E-00

R= 1.0100 ALPHA= 1.0000 E1= 0.65056E 00

K	Z0	ZC	E	DIFFERENCE
0.01000	-0.31366E 01	0.28709E 01	0.97887E 00	-0.21131E 01
0.10161	-0.30907E 01	0.23353E 01	0.84197E 00	-0.14944E 01
0.19322	-0.30446E 01	0.20043E 01	0.72584E 00	-0.12677E 01
0.28483	-0.29979E 01	0.17014E 01	0.61768E 00	-0.11806E 01
0.37644	-0.29505E 01	0.13834E 01	0.51429E 00	-0.11286E 01
0.46805	-0.29019E 01	0.99840E 00	0.41498E-00	-0.10841E 01
0.55966	-0.28518E 01	0.55097E 00	0.32384E-00	-0.99481E 00
0.65127	-0.27996E 01	0.92883E-01	0.24897E-00	-0.81726E 00
0.74288	-0.27448E 01	-0.25906E-00	0.19078E-00	-0.63518E 00
0.83449	-0.26864E 01	-0.54114E 00	0.14360E-00	-0.51508E 00
0.92610	-0.26230E 01	-0.78410E 00	0.10393E-00	-0.43303E-00
1.01771	-0.25524E 01	-0.10155E 01	0.70046E-01	-0.36983E-00
1.10932	-0.24700E 01	-0.12484E 01	0.41221E-01	-0.31465E-00
1.20093	-0.23648E 01	-0.15123E 01	0.17450E-01	-0.25948E-00
1.29254	-0.21647E 01	-0.19516E 01	0.56395E-03	-0.18432E-00

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