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Publication Date
1963-08-14

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Contract No. W-7405-eng-48

ON THE LOW-TEMPERATURE THERMALLY-ACTIVATED MECHANISM

FOR PRISMATIC SLIP IN THE Ag-Al INTERMEDIATE HEXAGONAL PHASE

by

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August 14, 1963

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ABSTRACT

The effect of strain rate and temperature on the critical resolved shear stress for $(\bar{1}100)$ $[11\bar{2}0]$ prismatic slip was determined for the intermediate hexagonal phase containing about 67 at.% Ag and 33 at.% Al. Whereas the flow stress increased only slightly as the test temperature was first decreased below room temperature, a rapid increase in the flow stress was obtained with yet greater decreases in temperature from about $240^{\circ}K$ to $4^{\circ}K$. The effect of both temperature and strain rate on the flow stress over the low-temperature range could be completely rationalized in terms of the Peierls mechanism when the deformation is controlled by the rate of nucleation of pairs of kinks.

INTRODUCTION

A few years ago Mote, Tanaka and Dorn[1] observed that the critical resolved shear stress for prismatic slip of a 67 at. % Ag plus 33 at. % Al hexagonal intermediate phase by the $[1\bar{1}00]$ $(11\bar{2}0)$ mode decreased precipitously as the test temperature was increased from 4° to about $160^\circ K$. Their results for both basal and prismatic slip are given in Fig. 1. It is obvious that only the flow stress for prismatic slip is strongly temperature dependent, whereas the flow stress for basal slip is independent of temperature. If the temperature dependence of the flow stress were primarily due to interstital impurities, it might be expected that they would influence the flow stress for basal slip as well. Since the activation volume at $115^\circ K$ for prismatic slip was determined to be about $15b^3$, where b is the Burgers vector, this thermally activated deformation process was tentatively ascribed as being due to the Peierls mechanism. But the various analyses of the Peierls mechanism then available as formulated by Seeger[2] and also by Lothe and Hirth[3] did not agree well with the experimental data. Since that time a more realistic theory for the operation of the Peierls mechanism under conditions where the strain rate is determined by the rate of nucleation of pairs of kinks has been presented by Dorn and Rajnak.[4] The present investigation was therefore undertaken in order to provide the essential data for a careful check on the agreement between this theory and the low temperature deformation by prismatic slip of the above mentioned Ag_2Al intermediate phase.
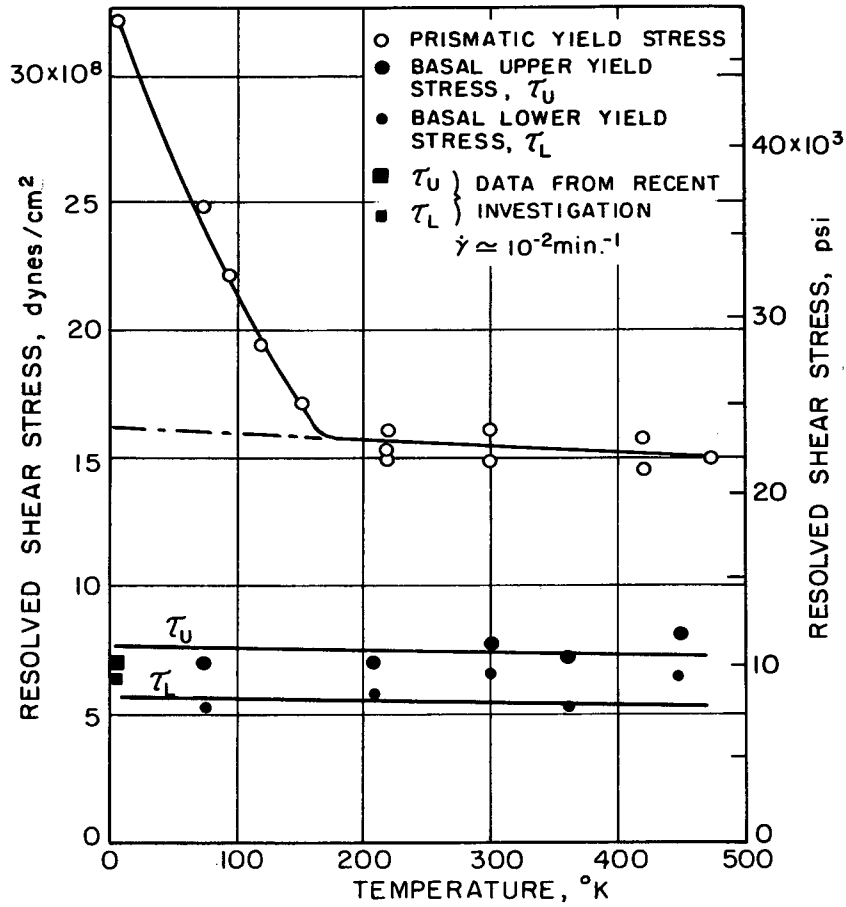
FIG. I EFFECT OF TEMPERATURE ON THE
CRITICAL RESOLVED SHEAR STRESS FOR
PRISMATIC AND BASAL SLIP.

MU-31512

EXPERIMENTAL TECHNIQUE

Single crystal specimens so oriented that the $\left[11\bar{2}0\right]$ direction and the normal to the $(1\bar{1}00)$ plane were at $45 \pm 2^{\circ}$ to the tensile axis were grown from the congruent melting composition of about Ag_2Al for the intermediate hexagonal phase by the technique previously used by Mote, Tanaka and Dorn.[1] A one inch long gage section 1/4 inch wide and 0.05 inch thick was carefully ground on each specimen which was then etched in a 40% nitric acid solution, annealed under argon at $923^{\circ}K$ for 15 minutes to remove the surface grinding effects and finally etched again in the nitric acid solution.

All tensile tests were conducted on an Instron Testing Machine. For the low temperature tests a specially designed Cryostat was used, the details of which will be described in a future paper. Axial stresses were determined to ± 100 psi and all recorded temperatures, except the $30^{\circ}K$ temperature where the inaccuracy was slightly larger, were controlled to within $\pm 0.5^{\circ}K$ of the recorded value.

In order to reduce the scatter in the data from crystal to crystal, each single crystal specimen was placed in a known state by prestraining at $273^{\circ}K$, which is the athermal region, at a shear strain rate of $\dot{\gamma} = 3.3 \times 10^{-4}$ per sec. following which it was then tested at various lower temperatures of $4^{\circ}, 30^{\circ}, 77^{\circ}, 104^{\circ}, 137^{\circ}, 162^{\circ}, 190^{\circ}, 197^{\circ}, 220^{\circ}$ and $250^{\circ}K$. One single specimen served for three different strain rate tests of $\dot{\gamma} = 8.3 \times 10^{-6}, 3.3 \times 10^{-4}$ and 1.67×10^{-2} per sec. at each temperature. Between two different strain rates the load was removed, low temperature was changed to $273^{\circ}K$ and again a prestraining experiment was conducted at $\dot{\gamma} = 3.3 \times 10^{-4}$ per sec. A typical set of data from one test is shown in Fig. 2.
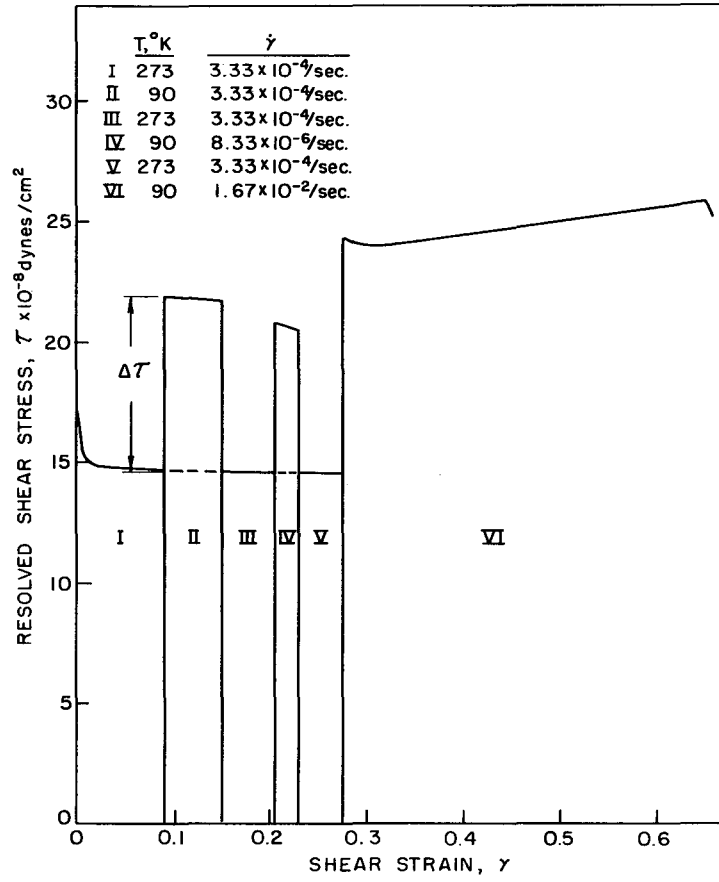
FIG. 2 RESOLVED SHEAR STRESS vs. TRUE STRAIN.

MU-31513

EXPERIMENTAL RESULTS

The stress, τ , that is required to cause plastic flow is usually the sum of two factors

$$\tau = \tau^* + \tau_A$$

(1)

where τ^* is the component of the stress that is needed to help dislocations to surmount barriers over which they move with the aid of thermal fluctuations and τ_A is the component of the stress that must be supplied to push the dislocations over such barriers that cannot be surmounted by thermal fluctuations. In general τ^* decreases rather rapidly with a decrease in temperature whereas τ_A decreases slowly with an increase in temperature usually in a manner that parallels the decrease in the shear modulus of elasticity, G, with temperature. Over the range of temperatures from about 175° to $273^\circ K$, τ decreased linearly with the temperature suggesting that τ^* was zero over this range. This concept is verified by the data recorded in Fig. 3 where the circles refer to the experimentally determined values of $G (1\bar{1}00) [11\bar{2}0]$ [5] and the squares are calculated from

$$G = \left(\frac{\tau_{273} + \Delta\tau_T}{\tau_{273}} \right) G_{273}$$

(2)

Over the yet lower ranges of test temperatures, where the flow stress decreases precipitously with an increase in temperature, the thermally activated component, τ^*, of the stress was deducted from the relationship
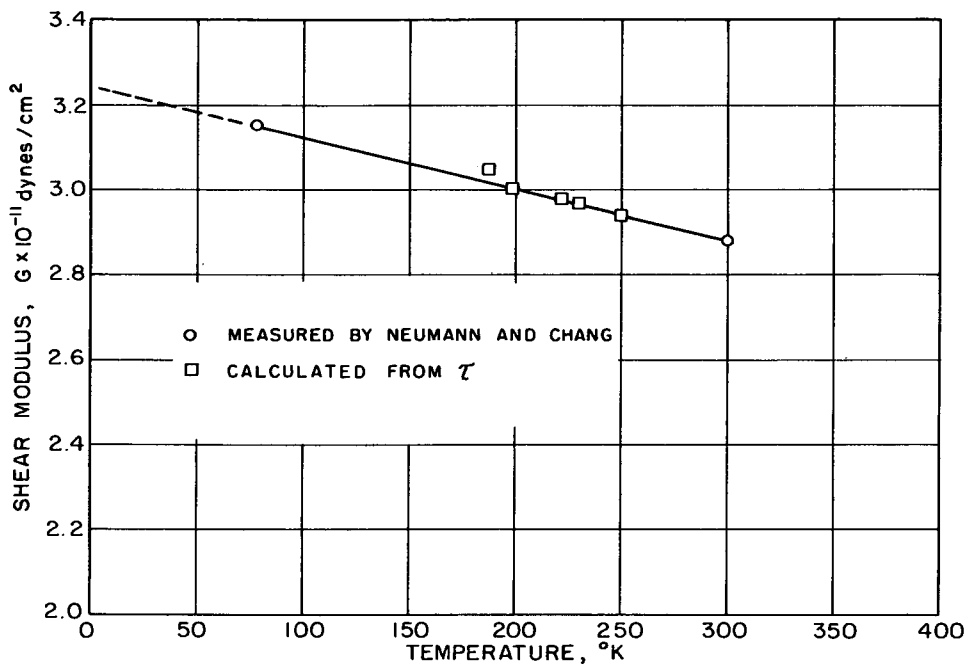
$$\tau^* = \tau_T - \tau_{273} \frac{G_T}{G_{273}}$$

(3)

FIG. 3 THE SHEAR MODULUS OF THE (Ī100) [I1Ī2O] SYSTEM vs. TEMPERATURE.

MU-31514

where τ_T is the total resolved shear stress for flow and G_T is the shear modulus of elasticity at temperature T. Values of τ^*, which are now corrected for specimen variation in τ_μ, are shown in Fig. 4 for three strain rates. The increasing flow stress with increasing strain rate as well as decreasing temperature attests to the fact that the operative deformation mechanism is thermally activated.

The shape of the τ^* versus T curves agree well with those that Dorn and Rajnak[4] have predicted when plastic flow arises from the nucleation of pairs of kinks by the Peierls mechanism. A significant feature of the nominal agreement between theory and experiment concerns the fact that both reveal that the τ^* versus T curves have a finite slope as τ^* approaches zero.
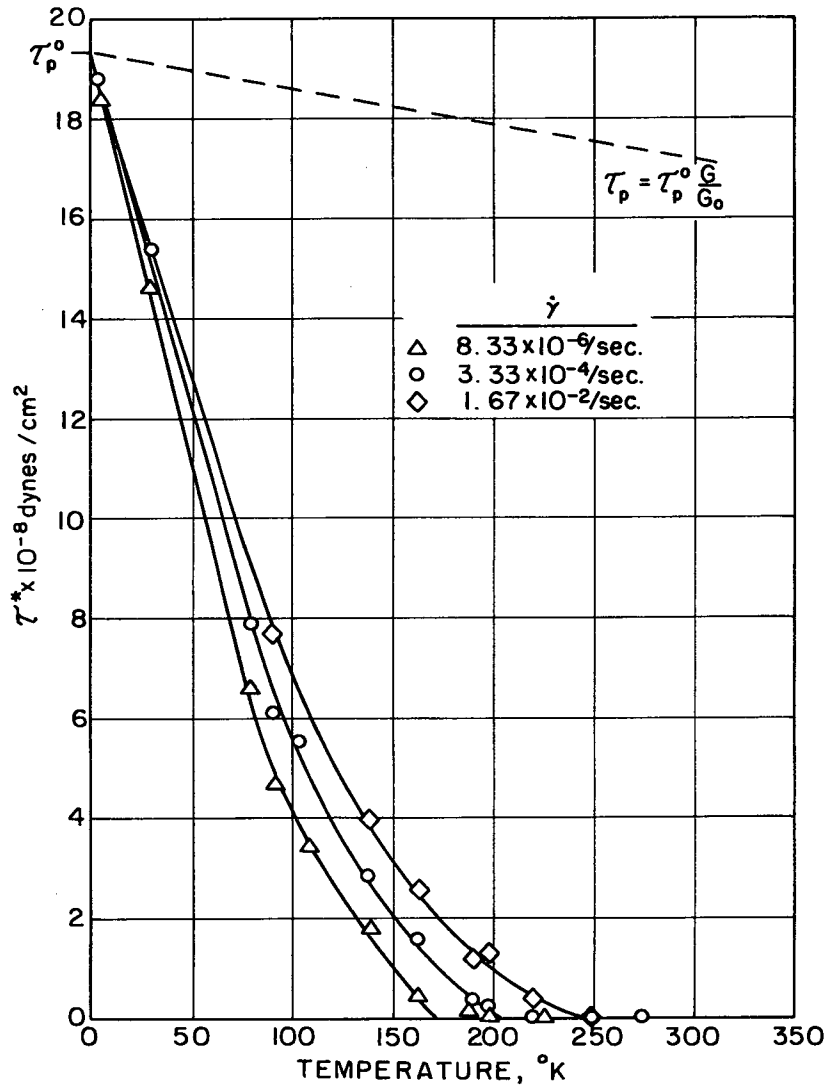
FIG. 4 THE THERMALLY ACTIVATED COMPONENT OF
THE FLOW STRESS vs. TEMPERATURE
FOR DIFFERENT STRAIN RATES. MU-31515

DISCUSSION

We will now compare quantitatively the experimental results with the theory for deformation controlled by the nucleation of pairs of kinks. For this purpose we recall that the plastic shear strain rate, for the simplest case where the deformation is controlled by the nucleation of pairs of kinks in the geometrically determined length L of dislocations, is given by

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

(4)

where ρ is the density of freely mobile dislocations, a is the distance between the Peierls valleys, b is the Burgers vector, γ is the Debye frequency, w is the width of a pair of kinks at the saddle-point free energy configuration, U_n is the saddle-point free energy for the nucleation of a pair of kinks, k is the Boltzmann constant and T is the absolute test temperature. The theory gives $U_n/2U_k$ as a function of τ^*/τ_p where U_k is the kink energy and τ_p is the Peierls stress, as shown by the curves of Fig. 5, for each of a series of values of α where α expresses the deviation of the shape of the Peierls hills from a sinusoidal periodic variation. The shape of the Peierls hill is defined in terms of α by

$$\Gamma(y) = \left(\frac{\Gamma_c + \Gamma_o}{2}\right) + \left(\frac{\Gamma_c + \Gamma_o}{2}\right)\cos 2\pi \frac{y}{a} + \frac{\alpha[\Gamma_c + \Gamma_o]}{4}\left(1 - \cos\frac{4\pi y}{a}\right)$$

where Γ_c is the line energy of a dislocation at the top of the Peierls hill where y = 0, Γ_o is the energy in the valley where $y = \pm a/2$ and $\Gamma(y)$ is the energy when the dislocation is displaced a distance y from the top of the hill. At $T = T_c$ where τ^* first becomes zero, the thermal energy that need be supplied is just $U_n = 2U_k$, and therefore, for this condition

$$\dot{\gamma} = \rho\, a\, b\, \gamma\, \frac{L}{w_c}\, e^{-\frac{2U_k(T_c)}{kT_c}}$$
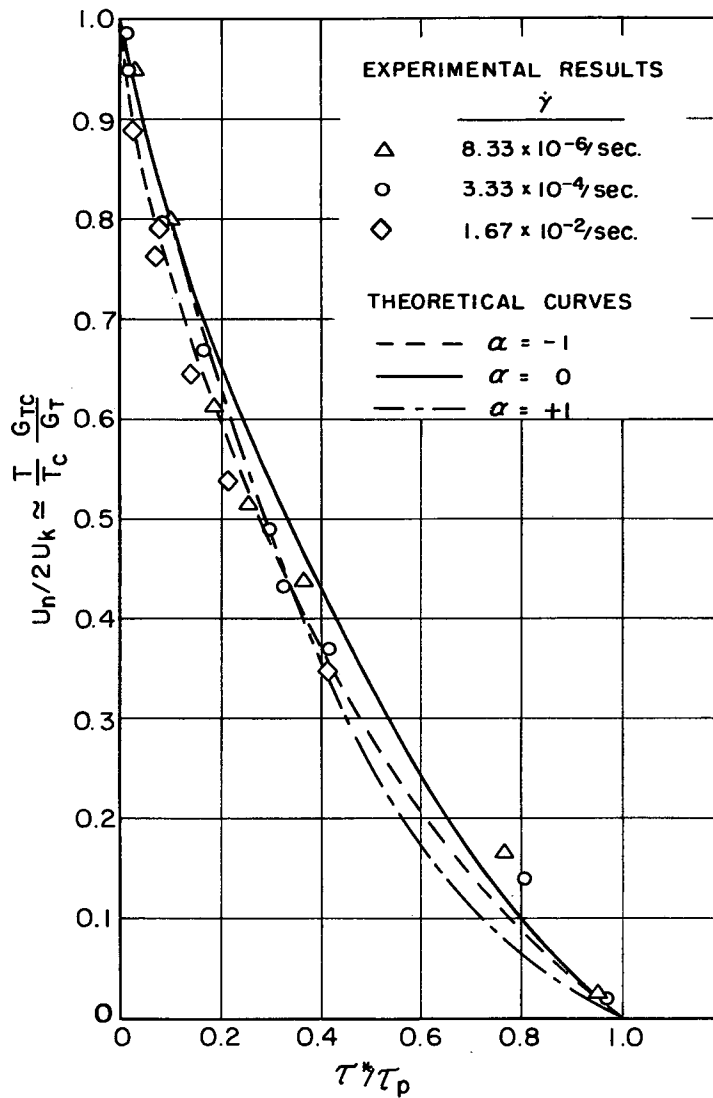
(5)

FIG. 5 THE THERMALLY ACTIVATED
COMPONENT OF THE FLOW STRESS vs.
TEMPERATURE IN DIMENSIONLESS UNITS.

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But, as shown by Dorn and Rajnak,[4] to a very good approximation, $w \simeq w_c$ and therefore, as shown by Eqns. 4 and 5,

$$\frac{U_n(T)}{2U_k(T)} = \frac{U_n(T)}{2U_k(T_c)\frac{G(T)}{G(T_c)}} \simeq \frac{T\,G(T_c)}{T_c\,G(T)}$$

(6)

Furthermore, taking as required by theory that the Peierls stress at the absolute zero is τ^* at the absolute zero, we obtain $\tau_p^\circ = 19.3 \times 10^8 \text{dynes/cm}^2$. Although Kuhlmann-Wilsdorf[6] suggested that the Peierls stress decreases quite rapidly with an increase in temperature as a result of a so-called "uncertainty" concept, the justification for such an assumption, as already pointed out by Friedel,[7] is weak. The present data suggest that the Peierls stress decreases only about linearly with an increase in temperature. We therefore assume that

$$\tau_p = \tau_p^\circ \frac{G(T)}{G(0)}$$

(7)

as shown by the broken line at the top of Fig. 4. The experimental data $U_n/2U_k$ as a function of $\frac{\tau^*}{\tau_p}$ as deduced with the aid of Eqns. 6 and 7 are shown by the points given in Fig. 5. The expected theoretical trends as shown by the solid curves in Fig. 5 are in excellent agreement with the experimental data and it appears to agree best with the curve representing $\alpha = -1$, excluding the 30°K data which might be somewhat in error. From the values of T_c for the two extreme strain rates recorded in Fig. 4, the value of the kink energy U_k is calculated by means of Eqn. 5 to be about 3.0×10^{-13} ergs or about 0.19 ev.

A most critical judgement on the validity of the Peierls mechanism is

obtained in terms of the activation volume which is defined as

$$
U^* = kT \frac{\partial \ln \dot{\gamma}}{\partial \tau^*} \simeq - \frac{\partial U_n}{\partial \tau^*} = - \frac{2 U_k}{\tau_p} \frac{\partial \left(\frac{U_n}{2 U_k} \right)}{\partial \left(\frac{\tau^*}{\tau_p} \right)}
$$

(8)

The activation volumes, deduced by applying the first equality of Eqn. 8 to

the data recorded in Fig. 4, are given as a function of the mean $\widetilde{U}^*$ in Fig. 6.

The datum points of $U^* \tau_p / 2 U_k$ as a function of $\widetilde{\tau}^* / \tau_p$ as deduced from

Fig. 6 and recorded in Fig. 7 should conform to the theoretical trend of

$\partial (U_n / 2 U_k) / \partial (\tau^* / \tau_p)$ as a function of $\widetilde{\tau}^* / \tau_p$ as deduced by Dorn and Rajnak[4]

and shown by the curves in Fig. 6. These data suggest that agreement is

excellent and although the correlation is insensitive to $\propto$ it is apparently

best for $\propto$ = -1.

Another check on the theory concerns the determination of the line

energy of a dislocation Γ_o from the experimental data. Using $R = \Gamma_c / \Gamma_o$

to be the ratio of the energy at the top and at the bottom of a Peierls hill,

theory demands that

$$
\frac{2 \pi U_k}{a \Gamma_o} = 4.44 \sqrt{R - 1}
$$

(9)

and

$$
\frac{\tau_p \, a b}{\pi \Gamma_o} = 1.3 (R - 1)
$$

(10)

for $\propto$ = -1. Considering the motion of edge dislocations, where a equals

the Burgers vector, Eqns. 9 and 10 give Γ_o = 5.73 x 10^{-4} ergs which is only

slightly greater than Gb^2 = 2.67 x 10^{-4} ergs while considering the motion of

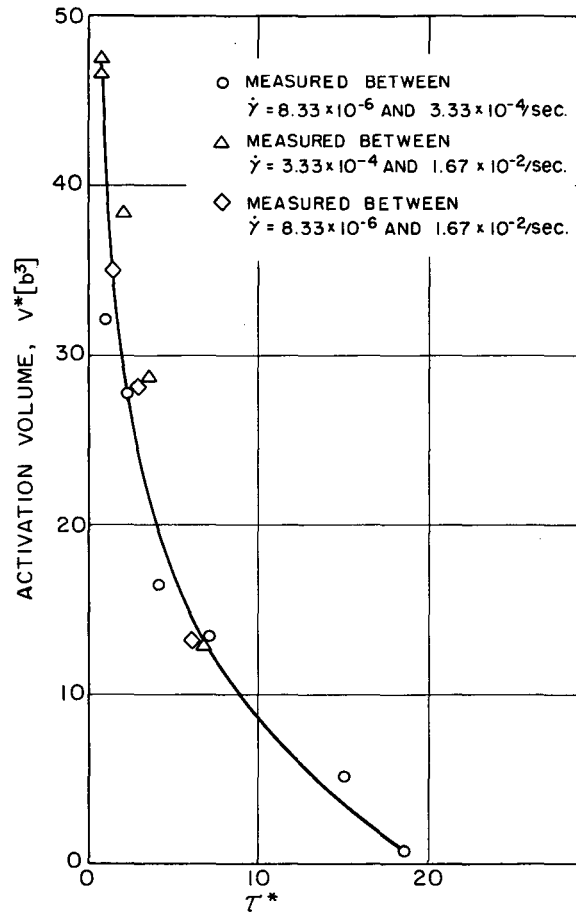screw dislocations where a equals 1.61b reveals Γ_o = 0.81 x 10^{-4} $\simeq \frac{Gb^2}{3}$,

FIG. 6 THE THERMALLY ACTIVATED
COMPONENT OF THE FLOW STRESS vs.
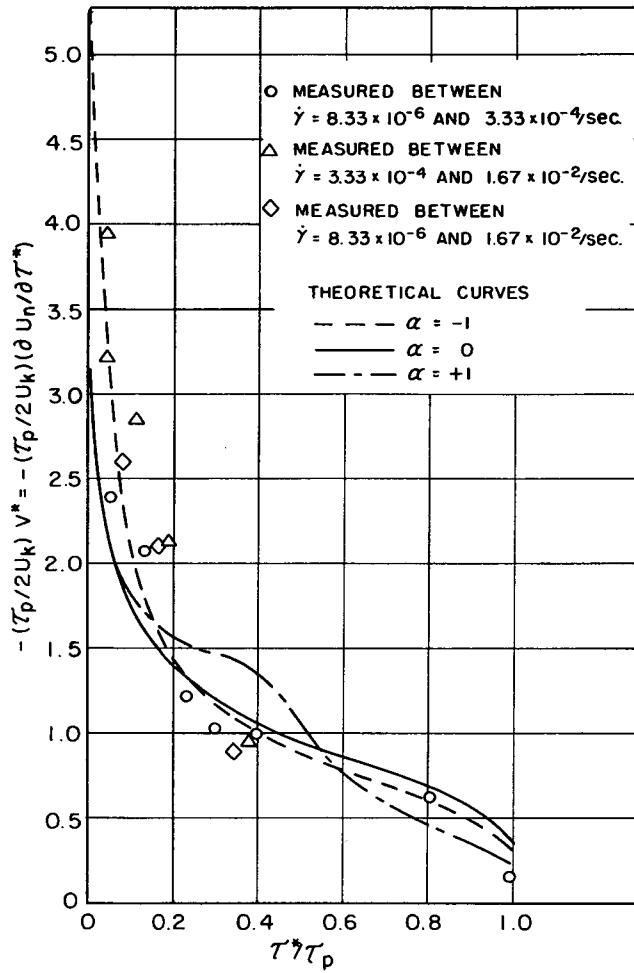THE ACTIVATION VOLUME IN UNITS OF b^3.

MU-31517

FIG. 7 THE THERMALLY ACTIVATED COMPONENT
OF THE FLOW STRESS vs. THE ACTIVATION
VOLUME IN DIMENSIONLESS UNITS.

MU-31518

thus agreeing well with theoretically estimated values of Γ_0. Furthermore,

estimating the value of γ to be 5.1×10^{12} from the Debye temperature,

and estimating $w_c \simeq 50b$ from Fig. 6, we obtain that $\rho\, L \simeq 300$, which is

a reasonable value.

CONCLUSION

The deformation of the hexagonal intermetallic alloy Ag + 33 at. % Al on the prismatic plane in the $[11\bar{2}0]$ direction is controlled by the nucleation of pairs of kinks in dislocations lying in Peierls potential valleys. This conclusion has been drawn since:

1. Both the change of the thermally activated component of the flow stress versus temperature and the activation volume against the thermally activated fraction of the flow stress fit the theory, which has been developed for the plastic deformation of materials by the Peierls mechanism.

2. The activation volume is less than $20\,b^3$, except for very small stresses. Some other mechanisms require activation volumes at least one order of magnitude higher.

3. The estimated values of τ_o and $\rho\,L$ are of the right order of magnitude.

ACKNOWLEDGMENTS

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