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A RATE THEORY OF DISLOCATION MOBILITY

by
A. S. Krausz

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A RATE THEORY OF DISLOCATION MOBILITY*

A. S. KRAUSZ†

The direct and indirect methods of dislocation velocity (v) measurements usually lead to the empirical expression

$$v \propto \tau^n$$

or

$$v \propto \exp(-c/\tau)$$

where τ is the stress and n, c are experimental constants. It is shown that the dislocation velocity can be described in terms of physical concepts by using the rate theory model of the asymmetrical energy barrier and assuming that the activation energy of the rate controlling process is linearly dependent on the stress. The equation obtained describes well the dislocation velocity in LiF, Ge, Si, InSb, GaSb, NaCl, Fe-Si, Ni, W, Zr, Pb, and in ice. An interpretation of the stress exponent n was also obtained in terms of the size and the shape of the energy barrier. This expression can be directly related to the yield drop and delay time phenomena.

THEORIE DE LA VITESSE DE DEPLACEMENT DES DISLOCATIONS

Les méthodes directes et indirectes de mesures de la vitesse des dislocations (v) conduisent habituellement à l'expression empirique

$$v \propto \tau^n$$

ou

$$v \propto \exp(-c/\tau)$$

où τ est la contrainte et n, c sont des constantes expérimentales. L'auteur montre que la vitesse de déplacement de la dislocation peut être décrite à l'aide de concepts physiques en utilisant le modèle de la barrière d'énergie asymétrique et en supposant que l'énergie d'activation du processus contrôlant la vitesse dépend linéairement de la contrainte. L'équation obtenue décrit bien la vitesse de déplacement des dislocations dans LiF, Ge, Si, InSb, GaSb, NaCl, FeSi, Ni, W, Zr, Pb, et dans la glace. L'auteur obtient également une interprétation de l'exposant n de la contrainte à l'aide de la taille et de la forme de la barrière d'énergie. Cette expression peut être reliée directement aux phénomènes du crochet de limite élastique et du temps de retard.

RATENTHEORIE DER VERSETZUNGSBEWEGLICHKEIT

Direkte oder indirekte Methoden zur Bestimmung der Versetzungsbeweglichkeit führen gewöhnlich zu dem empirischen Ausdruck

$$v \propto \tau^n$$

oder

$$v \propto \exp(-c/\tau),$$

wo τ die Spannung und n und c experimentelle Konstanten sind. Es wird gezeigt, dass die Versetzungsgeschwindigkeit physikalisch beschrieben werden kann mittels eines Modells aus der Ratentheorie für die asymmetrische Energiebarriere, unter der Annahme, dass die Aktivierungsenergie des geschwindigkeitsbestimmenden Prozesses linear von der Spannung abhängt. Die erhaltene Beziehung beschreibt gut die Versetzungsgeschwindigkeit in LiF, Ge, Si, InSb, GaSb, NaCl, Fe-Si, Ni, W, Zr, Pb und Eis. Der Spannungsexponent n wurde im Zusammenhang mit Grösse und Form der Energiebarriere interpretiert. Dieser Ausdruck kann direkt mit dem Abfall der Fließspannung und dem Verzögerungsphänomen verknüpft werden.

INTRODUCTION

The understanding of dislocation mobility has been hindered by the lack of a theoretical description expressed in terms of basic physical concepts. Little progress could be expected, however, in the development of the theory until sufficient experimental results had been accumulated from direct and indirect measurements of dislocation velocity. The experimental information obtained in the past few years encouraged the theoretical study of dislocation mobility and progress has been made already.

Gilman and Johnston⁽¹⁾ have shown by direct observation that the dislocation velocity v in LiF is a function of the stress and temperature and can be described by the empirical equations

$$v = C_1 \tau_a^n \exp(-C_2/T) \quad (1)$$

and, over a wider stress range, by

$$v = C_3 \exp(-C_4/\tau_a) \exp(-C_5/T) \quad (2)$$

where

τ_a is the applied stress

C_1 to C_5 are experimental constants

T is temperature, °K.

Experiments with many crystals, for example, NaCl,⁽²⁾ Fe-Si,⁽³⁾ W,⁽⁴⁾ Ge,⁽⁵⁾ Si,⁽⁶⁾ lead to similar

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conclusions. Utilizing these results significant progress has been made in the understanding of the delay time and yield drop phenomena.^(7,8)

Indirect, macroscopic measurements (constant strain rate tests, creep tests, etc.) have been used extensively to determine the dependence of the dislocation velocity on the applied stress and temperature. Using some of these tests a comparison could be made between the results of the direct, microscopic measurements obtained by etch pit or X-ray technique and the macroscopic behaviour. The correlation obtained has encouraged the use of indirect techniques of dislocation velocity measurements for crystals for which direct observation is not yet possible, among others Cu⁽⁹⁾ and Pb.⁽¹⁰⁾

To explain the experimental results it is desirable to derive the description of the dislocation velocity from basic principles and to express the behaviour represented by the empirical equations (1) and (2) in terms of physical concepts and quantities. Assuming specific mechanisms, several expressions⁽¹¹⁻¹³⁾ have been suggested to explain the microscopic dislocation velocity observations. The results of some of the indirect dislocation velocity measurements obtained in stress change experiments have been also represented by special forms of the rate theory.⁽¹⁴⁾

It is the purpose of this paper to report a more general description of dislocation mobility utilizing the rate theory. The proposed expression describes the dislocation velocity in terms of physical concepts and replaces the empirical equations (1) and (2). The model is not limited to a specific mechanism and is valid in the stress range over which the effects associated with very high velocities are negligible.

THE RATE THEORY MODEL

It has been suggested by Eyring⁽¹⁵⁾ that the number of activations, κ , contributed by each of the thermally activated processes to the total plastic deformation, can be described by the expression

$$\kappa \propto \frac{kT}{h} \exp \left(- \frac{\Delta H(\tau)}{kT} \right) \quad (3)$$

where

k is the Boltzmann constant,

T is the absolute temperature,

h is Planck's constant,

$\Delta H(\tau)$ is the apparent activation enthalpy.

Recently, Vineyard⁽¹⁶⁾ has derived from somewhat different assumptions an expression of the following form

$$\kappa \propto \nu^* \exp (-\Delta H(\tau)/kT) \quad (4)$$

where ν^* is a frequency defined in terms of the atomic frequencies associated with the dislocated region and with the activation process. It is necessary to point out that in this theory ν^* is not the Debye or the dislocation line frequency.

At present it is not possible to decide which of these two theories is preferable for the description of the dislocation velocity. For much of the following investigation it is satisfactory to represent both as

$$\kappa \propto A \exp (-\Delta H(\tau)/kT) \quad (5)$$

where A is defined by the physical quantities corresponding to either of the two theories.

Many of the rate-controlling mechanisms of plastic deformation have an apparent activation enthalpy $\Delta H(\tau)$ which depends linearly on the effective stress τ_{eff}

$$\Delta H(\tau) = \Delta H^* - V\tau_{\text{eff}} \quad (6)$$

where ΔH^* is the enthalpy of activation in the absence of stress and V is the apparent activation volume defined as

$$\left[\frac{d\Delta H}{d\tau_{\text{eff}}} \right]_{T, \text{ struct.}} = V$$

In the following model of the rate theory of dislocation velocity it is assumed that equation (6) is a good approximation to the apparent activation enthalpy.

Equation (5) describes a rate process controlled by a single mechanism. To obtain a rate expression which is valid over the whole stress range of this mechanism, a finite probability has to be allowed for the backward movement of the dislocations. It is then necessary to consider that the energy barrier may be asymmetrical and thus the distance l over which the dislocations travel from the initial to the activated state is in general different in the backward (l_b) direction from that in the forward (l_f) direction. Therefore both $V_f = V_b$ and $V_f \neq V_b$ have to be assumed. It is also necessary to consider the effect of a possible difference between the activation enthalpy in the forward direction ΔH_f^* and in the backward direction ΔH_b^* .

When described in terms of the two rate theories as represented by equations (5) and (6), the model leads to the following expression for the dislocation velocity

$$v = A_f \exp [(V_f \tau_{\text{eff}})/(kT)] - A_b \exp [-(V_b \tau_{\text{eff}})/(kT)] \quad (7)$$

where A_f and A_b are the products of the frequency term A of equation (5) and a factor λ associated

with the contribution of each activation to the dislocation movement as defined by the rate theory. Equation (7) is valid over the stress range where only one mechanism is rate controlling.

APPLICATION TO EXPERIMENTS

The dislocation velocity measurements obtained by etch pit technique in LiF,⁽¹⁾ NaCl,⁽²⁾ Fe-Si,⁽³⁾ W,⁽⁴⁾ Ni,⁽¹⁸⁾ Ge,^(5,17) Si,⁽⁶⁾ InSb,⁽⁵⁾ GaSb,⁽⁵⁾ and Mo,⁽¹¹⁾ were analyzed in terms of the rate theory using the proposed model. It was found that all of the investigated experimental results could be described well by equation (7) although no particular effort was made to obtain the best fit.

An example is shown in Fig. 1(a) in which the experimental results were originally⁽⁵⁾ represented by the empirical expression equation (1) with a low stress exponent n . In this figure $\log v$ is plotted against

FIG. 1(a). The stress dependence of the dislocation velocity in Ge according to Chaudhuri, Patel and Rubin.⁽⁵⁾ The symbols represent the average measured velocities. The curve was calculated from equation (7).

FIG. 1(b). The stress dependence of the dislocation velocity in LiF according to Gilman and Johnston.⁽¹¹⁾ The symbols represent the average measured velocities. The dotted curve corresponds to the empirical relationship $v \propto \exp(-c/\tau)$, the solid curve was calculated from equation (7).

TABLE I

	A_t	A_b/A_t	V_t/kT	V_b/kT
Fig. 1(a)	0.715×10^{-2}	1.13	0.2	0.1
Fig. 1(b)	1×10^{-11}	4.2×10^5	20.0	0.1
803°K	3.02×10^{-4}	1.114	0.2	0.1
735°K	4.65×10^{-5}	1.094	0.2	0.01
664°K	1.67×10^{-6}	1.139	0.2	0.01

$\log \tau_a$ for Ge. The equation obtained from the rate theory [equation (7)] was found to match the experimental points well when the constants listed in Table I were used. Another example, which represents the behaviour associated with a high stress exponent n , is shown in Fig. 1(b) in which $\log v$ is plotted against the reciprocal of the applied stress for LiF.⁽¹¹⁾ The figure shows again that the rate theory expression [equation (7)] is in good agreement with the measured values. Furthermore, while the empirical relations [equations (1) and (2)] are not valid at the very low stress range, a minimum stress (about 6.3×10^7 dyn/cm²) needed to move the dislocations is correctly predicted by the rate theory.

In a series of tests, Kabler⁽¹⁷⁾ measured a stress dependence of dislocation velocity in Ge (Fig. 2) which could not be represented by the usual empirical expressions [equations (1) and (2)]. It was found that equation (7) describes these observations well in both the high and medium stress range as shown in Fig. 2.

FIG. 2. The stress dependence of the dislocation velocity in Ge according to Kabler⁽¹⁷⁾ for 60° dislocations. The symbols represent the average measured dislocation velocities. The curves were calculated from equation (7). The diagram indicates that equation (7) describes the experimental results well even in the high stress range where the $v \propto \exp(-c/\tau)$ empirical relationship is not valid.

Rohde and Pitt⁽¹⁸⁾ obtained a logarithmic dependence between the dislocation velocity and the applied stress for Ni. Obviously this behaviour cannot be described by either of the two empirical expressions. When

$$V_b \tau_{\text{eff}} \gg kT,$$

equation (7) reduces to

$$v = A_f \exp [(V_f \tau_{\text{eff}})/(kT)],$$

in full agreement with the experimental results and with the interpretation given by Rohde and Pitt.

Equation (7) was also found to be in good agreement with the experimental results obtained in macroscopic tests when the dislocation geometry did not change. It is well known that these tests often show a symmetrical energy barrier behaviour represented by the relationship

$$v = 2A \sinh [(V \tau_{\text{eff}})/(kT)].$$

Obviously this is a special case of equation (7) with $A_f = A_b = A$ and $V_f = V_b = V$. An example of this behaviour and satisfying the requirements of equation (7) is the elastic after-effect in Zr at 77°K.⁽¹⁹⁾ When

$$V \tau_{\text{eff}} \gg kT$$

the dislocation velocity is

$$v = A \exp [(V \tau_{\text{eff}})/(kT)]. \quad (8)$$

Equation (8) describes the logarithmic behaviour observed at low temperature in constant stress creep or in variable stress creep including stress relaxation.⁽²⁰⁾

Wilson and Garofalo⁽⁹⁾ have shown that the stress relaxation of Pb can be described in the terms of Eyring's rate theory with an energy barrier $A_f = A_b$. In these experiments the stress relaxed completely within a few minutes indicating that the internal stress was probably very small. It was also assumed that the dislocation density did not change during the test. In this case equation (7) becomes

$$v = A \left[\exp \left(\frac{V_f \tau_{\text{eff}}}{kT} \right) - \exp \left(- \frac{V_b \tau_{\text{eff}}}{kT} \right) \right]. \quad (9)$$

A description essentially identical to this was suggested by Wilson and Garofalo. Substituting equation (9) into the well known relationship for strain rate

$$\dot{\gamma} = b \rho v$$

(where b is the Burger's vector and ρ is the mobile dislocation density) and observing that in this test ρ is constant and $\dot{\gamma}$ is proportional to the stress

change $\Delta \tau$, it follows that

$$\frac{d\Delta \tau}{dt} = CA \left[\exp \left(\frac{V_f \tau_{\text{eff}}}{kT} \right) - \exp \left(- \frac{V_b \tau_{\text{eff}}}{kT} \right) \right].$$

This equation describes the stress relaxation observed in Pb. It is of interest to note that although the experimental results are again well represented by the rate theory, the empirical equation

$$v = C \tau^n$$

cannot be matched satisfactorily to the experimental values. The symbol τ is used to emphasize that the internal stress τ_i is small and thus $\tau_{\text{eff}} \cong \tau_i$.

A typical example of the stress relaxation in ice⁽²¹⁾ is shown in Fig. 3. The experimental results were described by Readey and Kingery by the empirical expression:

$$\dot{\tau} \propto \tau^{2.49}.$$

Assuming as for Pb that the internal stress was small and that the dislocation geometry did not change during the test the rate theory leads to the equation:

$$\dot{\tau} = 0.67 \times 10^4 [\exp (0.472 \times 10^{-6} \tau) - 4 \exp (-0.472 \times 10^{-6} \tau)]. \quad (10)$$

The good agreement obtained between equation (10) and the observed behaviour is illustrated in Fig. 3. This indicates that the deformation process in ice involves asymmetrical energy barriers.

The foregoing discussion demonstrates that the results of the microscopic and macroscopic dislocation velocity measurements obtained in LiF, Ge, Si, InSb, GaSb, NaCl, Fe-Si, Ni, W, Zr, Pb and in ice

FIG. 3. The stress relaxation of ice single crystal.⁽²¹⁾ The cross-section of the specimen was taken as the unit of the area. The symbols represent the measured values and the curve was calculated from equation (10).

were well described by equation (7) in terms of physical quantities. In view of the fact that the shape of each curve is completely determined by only two parameters (the ratios A_f/A_b and V_f/V_b) and that these are subject to physical limitations, the agreement between the experimental and calculated values is considered as strong support of the proposed form of the rate theory.

THE INTERPRETATION OF EXPONENT n

It is also of interest to discuss the physical meaning of the stress exponent n . Using the empirical expression

$$\dot{\gamma} \propto \rho \tau^n$$

Gilman and Johnston^(7,8,22) have shown that the yield drop and delay time phenomena associated with the dislocation multiplication mechanism depend on n . It has been established that (subject to other conditions) the smaller the stress exponent n , the greater the yield drop in constant strain rate test and the longer the delay time in constant stress creep test (Fig. 4). The relationship between the dislocation structure and the stress exponent associated with these two phenomena has been discussed by Cottrell⁽²³⁾ and Hahn.⁽²⁴⁾ In consequence, a considerable amount of information is now available on the effect of n .

Using equation (7), an interpretation of the stress exponent n can be given in terms of physical quantities. It follows from the equation above that

$$n = \frac{d \ln \dot{\gamma}}{d \ln \tau}.$$

Substituting

$$\dot{\gamma} = b \rho v = b \rho \left[A_f \exp \left(\frac{V_f \tau}{kT} \right) - A_b \exp \left(\frac{V_b \tau}{kT} \right) \right]$$

the following expression is obtained:

$$n = \frac{d \ln v}{d \ln \tau} = \tau \frac{(V_f/kT) A_f \exp(V_f \tau/kT) + (V_b/kT) A_b \exp[-(V_b \tau)/(kT)]}{A_f \exp(V_f \tau/kT) - A_b \exp[-(V_b \tau)/(kT)]} \quad (11)$$

Fig. 4. The effect of the stress exponent n on the yield drop in constant strain rate test [according to Ref. (8)].

It is to be noted that while in this derivation the condition $\tau_{\text{eff}} \cong \tau_a$ is implied equations (7) and (11) are still valid when $\tau_{\text{eff}} \ll \tau_a$. To show this consider τ_{eff} expressed by $\tau_a - \tau_i$ in equation (6). Then equation (6) becomes

$$\begin{aligned} \Delta H(\tau) &= \Delta H^\ddagger - V \tau_{\text{eff}} \\ &= \Delta H^\ddagger - V(\tau_a - \tau_i) \\ &= (\Delta H^\ddagger + V \tau_i) - V \tau_a \end{aligned}$$

leading to equation (7) and thus to equation (11) as before but with τ_{eff} replaced by τ_a . The frequency terms A_f and A_b now include not only the Eyring or Vineyard rate theory terms, but also the $\exp(V \tau_i)/(kT)$ and $\exp(-V \tau_i)/(kT)$ factors.

Equation (11) defines the stress exponent n in terms of physical quantities over a wide range of conditions. For example, in the case of a symmetrical barrier when $A_f = A_b$ and $V_f = V_b = V$,

$$n = \frac{d \ln v}{d \ln \tau} = \frac{\tau V}{kT \tanh(V \tau)/(kT)}$$

A few other special cases are also of interest.

(a) When

$$A_b = 0$$

or

$$V_b \tau \gg kT$$

equation (14) reduces to

$$n = (d \ln v)/(d \ln \tau) = (V_f \tau)/(kT)$$

in agreement with the expression obtained by Hull and Noble⁽²⁵⁾ for logarithmic stress relaxation.

(b) When

$$V_b/kT = 0 \quad \text{and} \quad V_f \tau \ll kT$$

$$n = (d \ln v)/d \ln \tau$$

$$= \frac{[(V_f)/(kT)] \tau}{1 + [(V_f \tau)/(kT)] - A_b/A_f} \cong \frac{[(V_f)/(kT)] \tau}{1 - A_b/A_f}.$$

The stress exponent n depends on the asymmetry of the energy barrier. It is also clear that with this type of barrier, $A_b < A_f$ as n is always positive.

SUMMARY

It is suggested that the results of dislocation velocity measurements represented by the empirical equations

$$v \propto \tau^n \quad (1)$$

$$v \propto \exp(-c/\tau) \quad (2)$$

can be fully explained in terms of physical quantities using the rate theory. Two models were considered: the quantum statistical model of Eyring and the classical statistical theory of Vineyard. These models

describe the deformation rate by atomic or thermodynamic concepts. When it is assumed that one mechanism is rate controlling and the activation energy depends linearly on the stress, both theories lead to an expression which can be represented formally by the equation

$$v = A_f \exp \left(\frac{V_f \tau}{kT} \right) - A_b \exp \left(- \frac{V_b \tau_{\text{eff}}}{kT} \right) \quad (7)$$

This equation recognizes a finite probability for the backward movement of the dislocations and takes into consideration the possibility that in this direction the activation energy and the activation volume V may be different from that in the forward direction. The factors A_f and A_b are defined in terms of physical concepts (activation energy, temperature, stress) without introducing any empirical parameters.

The experimental results obtained by direct and indirect dislocation velocity measurements in LiF, NaCl, Ge, Si, InSb, GaSb, Fe-Si, W, Ni, Mo, Pb, Zr and in ice were investigated. The equation was found to describe well the dislocation mobility in all of these crystals. It was also shown that equation (7) correctly predicts a minimum stress needed to move the dislocations and explains the experimental results even for conditions when the empirical expressions are not valid.

The yield drop and delay time phenomena associated with the dislocation multiplication mechanism is controlled by the stress exponent n . The good agreement obtained between the dislocation velocity measurements and the rate theory expression [equation (7)] suggested that n could be expressed in physical terms as in equation (11). This equation relates the yield drop and delay time phenomena to the size and the shape of the energy barrier.

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