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Publisher's version / Version de l'éditeur:

Materials Science and Engineering, 6, pp. 260-264, 1972-05-01

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BY

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48038

REPRINTED FROM
MATERIALS SCIENCE AND ENGINEERING
VOL. 6, 1970
P. 260 - 264

RESEARCH PAPER NO. 521
OF THE
DIVISION OF BUILDING RESEARCH

OTTAWA

MAY 1972

PRICE 10 CENTS

NRCC 12626

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A Rate Theory Analysis of the Temperature Dependence of Dislocation Velocity

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(Received January 5, 1970; in revised form April 20, 1970)

SUMMARY

A previous study showed that when the apparent activation energy is a linear function of the stress the relation between the dislocation velocity, v , and the stress, τ , can be described well for many crystals on the basis of an asymmetrical potential energy barrier, account being taken of the forward and reverse processes. The present investigation was carried out to determine whether the temperature dependence of dislocation velocity could be described on the same basis, assuming that the activation parameters are independent of the temperature. It is shown that with these simple conditions the rate theory is in

good agreement with the experimental results obtained on the stress and temperature dependence of the dislocation velocity for Ge, Si and CaF_2 . A relationship was also derived from the absolute rate theory for the description of the stress sensitivity, $\partial \ln v / \partial \ln \tau$. The expression explains fully the experimental results obtained in Al, Cu and Ag in terms of physical quantities over the whole temperature range. It is concluded that the asymmetrical, triangular energy barrier shape is a useful approximation for the analysis of the thermally activated movement of dislocations.

ZUSAMMENFASSUNG

In einer früheren Arbeit wurde gezeigt, daß der Zusammenhang zwischen Versetzungsgeschwindigkeit v und Schubspannung τ für viele Kristalle gut mit der Vorstellung eines asymmetrischen Versetzungshindernisses beschrieben werden kann, wenn die scheinbare Aktivierungsenergie eine lineare Funktion der Spannung ist; dabei werden Vorwärts- und Rückwärtsprozesse berücksichtigt. Die vorliegende Untersuchung wurde durchgeführt um herauszufinden, ob die Temperaturabhängigkeit der Versetzungsgeschwindigkeit auf derselben Grundlage beschrieben werden kann wenn man annimmt, daß die Aktivierungsparameter nicht von der Temperatur abhängen. Es wird gezeigt, daß die Ratentheorie

unter diesen einfachen Annahmen in guter Übereinstimmung mit experimentellen Bestimmungen der Spannungs- und Temperaturabhängigkeit der Versetzungsgeschwindigkeit in Ge, Si und CaF_2 ist. Für die Spannungsempfindlichkeit $\partial \ln v / \partial \ln \tau$ wurde aus der absoluten Ratentheorie eine Beziehung abgeleitet. Diese Beziehung erklärt die experimentellen Ergebnisse an Al, Cu und Ag im gesamten Temperaturbereich allein mit physikalischen Größen. Es wird die Schlußfolgerung gezogen, daß die asymmetrische dreieckige Form der Energiebarriere eine nützliche Näherung für die Analyse der thermisch aktivierten Versetzungsbewegung ist.

RÉSUMÉ

Dans une étude antérieure le mouvement des dislocations a été décrit dans le cas de barrières d'énergie potentielle dissymétriques, la possibilité de sauts inverses des dislocations étant prise en considération. Lorsque l'énergie d'activation apparente est une fonction linéaire de la contrainte, ce modèle explique bien, dans le cas de beaucoup de cristaux, la variation de la vitesse v des dislocations avec la contrainte τ .

L'objet de la présente étude était de voir si la variation de la vitesse des dislocations en fonction de la température pouvait être décrite à l'aide du même modèle, les paramètres de l'activation thermique étant supposés indépendants de la température. On trouve qu'avec ces hypothèses simples, la théorie du

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glissement activé est en bon accord avec les résultats expérimentaux relatifs à la variation de la vitesse des dislocations en fonction de la contrainte et de la température dans Ge, Si et CaF₂. La théorie des vitesses absolues de réaction a également conduit à l'établissement d'une relation pour la sensibilité à la contrainte $\partial \ln v / \partial \ln \tau$. Cette relation explique entière-

ment et dans toute l'échelle des températures, à l'aide de grandeurs physiques, les résultats expérimentaux obtenus dans Al, Cu et Ag. On en conclut que la barrière d'énergie dissymétrique, de forme triangulaire, constitue une approximation permettant d'analyser utilement le mouvement thermoactivé des dislocations.

The establishment of the temperature and stress dependence of the activation rate is of central interest in the study of dislocation mobility. In a previous study¹, an investigation was carried out to determine whether the effect of the stress on the dislocation velocity, v , could be described by a linearly stress-dependent apparent activation energy ΔE . The linear stress dependence is mathematically advantageous and physically reasonable as there are several mechanisms for which

$$\Delta E = \Delta E^\ddagger - V\tau_{\text{eff}} \quad (1)$$

where $\Delta E^\ddagger$ is the activation energy, V is an activation volume and τ_{eff} is the effective stress acting on the dislocation. It was shown in this study that at the above condition the stress dependence of the dislocation velocity in Ge, Si, InSb, GaSb, NaCl, LiF, Fe-3% Si, W, Mo, Ni can be described well with the asymmetrical form of the rate equation

$$v = v_f \exp\left(-\frac{\Delta E_f^\ddagger - V_f \tau_{\text{eff}}}{kT}\right) - v_b \exp\left(-\frac{\Delta E_b^\ddagger + V_b \tau_{\text{eff}}}{kT}\right) \quad (2)$$

In eqn. (2) subscripts f and b indicate that the quantity is associated with the forward and the backward movements of the dislocation respectively. The other symbols have their usual meaning.

In terms of the absolute rate theory² eqn. (2) was expressed in explicit form for a quantum statistical system as

$$v = l_f \kappa_f \frac{kT}{h} \frac{Q_f^\ddagger}{Q_f^r} \exp\left(-\frac{\Delta E_f^\ddagger - V_f \tau_{\text{eff}}}{kT}\right) - l_b \kappa_b \frac{kT}{h} \frac{Q_b^\ddagger}{Q_b^r} \exp\left(-\frac{\Delta E_b^\ddagger + V_b \tau_{\text{eff}}}{kT}\right) \quad (3)$$

where $Q^\ddagger$ and Q^r are the partition functions for the activated state and the reactant state respectively, l is the average distance travelled by the dislocation after each activation, κ is the transmission coefficient; the other symbols have their usual meaning.

The analysis showed that eqn. (3) described well the stress dependence of the dislocation velocity for all of the investigated crystals. It is the purpose of the present paper to report the results of a study that was carried out to develop an understanding of the temperature dependence of the dislocation mobility.

DISCUSSION

The mathematically simplest temperature dependence can be expressed as:

$$\Delta E^\ddagger \neq f(T); V \neq f(T); l \neq f(T) \quad (4)$$

These conditions are well satisfied by several mechanisms for which the apparent activation energy is a linear function of the stress. In these cases the stress dependence represented by eqn. (2) is preserved and the investigation of the temperature dependence predicted by eqns. (2) and (3) can follow immediately when the restrictions of expression (4) are superimposed.

Analysis of the direct dislocation velocity measurements

It has been shown¹ that eqn. (3) represents well the stress dependence of the dislocation velocity in Ge^{3,4} and in Si⁵. The same experimental results and the measurements of Keig and Coble⁶ on CaF₂ were now analyzed with respect to the temperature dependence of the dislocation velocity using eqns. (3) and (4). Good matching was obtained within the experimental scatter over the whole temperature range for all of the investigated measurements. A typical example is shown in Fig. 1. It is concluded from these analyses that when the restrictions of expression (4) are superimposed eqn. (3) is a good approximation for the description of the thermally activated dislocation movement in Ge, Si and CaF₂.

Although it is more reliable to use the direct dislocation velocity measurements, it is difficult to obtain sufficient experimental data. This necessitates

Fig. 1. The stress and temperature dependence of the dislocation velocity in Si. The shading indicates the experimental scatter⁵. The curve was calculated from eqn. (3). The activation parameters are

$$l_f \kappa_f \frac{k}{h} \frac{Q_f^*}{Q_f} \approx l_b \kappa_b \frac{k}{h} \frac{Q_b^*}{Q_b} \approx 2 \times 10^5 \text{ cm sec}^{-1}$$

$$\Delta E_f^* = 2.235 \text{ eV}$$

$$\Delta E_b^* = 2.215 \text{ eV}$$

$$V_f = 71 \text{ Å}^3$$

$$V_b = 31.5 \text{ Å}^3$$

No particular effort was made to obtain the best fit.

using the observations obtained in indirect dislocation velocity measurements and analyzing the temperature dependence of the stress sensitivity.

Analysis of the indirect dislocation velocity measurements

It has often been observed that the slope of the $\ln v$ versus $\ln \tau$ relation is a function of the temperature⁷. For a triangular, asymmetrical energy barrier the rate theory of dislocation mobility [eqns. (2), (3), (4)] predicts that the stress sensitivity

$$\left(\frac{\partial \ln v}{\partial \ln \tau_{\text{eff}}} \right)_{T, \text{structure}} = n$$

depends on the temperature according to the following equation which has been derived from eqns. (2) and (4):

$$n = \left(\frac{\partial \ln v}{\partial \ln \tau_{\text{eff}}} \right)_{T, \text{structure}} = \frac{V_f \tau_{\text{eff}}}{kT} \frac{1 + \frac{v_b}{v_f} \frac{V_b}{V_f} \exp \frac{\Delta E_f^* - \Delta E_b^* - (V_f + V_b) \tau_{\text{eff}}}{kT}}{1 - \frac{v_b}{v_f} \exp \frac{\Delta E_f^* - \Delta E_b^* - (V_f + V_b) \tau_{\text{eff}}}{kT}} \quad (5)$$

In explicit form, according to eqns. (3) and (4), the temperature dependence of the stress sensitivity is

$$n = \left(\frac{\partial \ln v}{\partial \ln \tau_{\text{eff}}} \right)_{T, \text{structure}} = \frac{V_f \tau_{\text{eff}}}{kT} \frac{1 + \frac{V_b}{V_f} \frac{l_b \kappa_b}{l_f \kappa_f} \frac{Q_b^*}{Q_f^*} \frac{Q_f}{Q_b} \exp \frac{\Delta E_f^* - \Delta E_b^* - (V_f + V_b) \tau_{\text{eff}}}{kT}}{1 - \frac{l_b \kappa_b}{l_f \kappa_f} \frac{Q_b^*}{Q_f^*} \frac{Q_f}{Q_b} \exp \frac{\Delta E_f^* - \Delta E_b^* - (V_f + V_b) \tau_{\text{eff}}}{kT}} \quad (6)$$

Equation (5) describes the temperature dependence of the stress sensitivity when, as a first approximation, v_b/v_f is considered to be independent of the temperature. For a detailed expression of the temperature dependence, the explicit form given by eqn. (6) should be considered. In this equation the statistical mechanical terms can be transformed readily into the usual thermodynamic quantities.

In eqn. (5):

$$(\Delta E_f^* - \Delta E_b^*) < (V_f + V_b) \tau_{\text{eff}}.$$

From this condition it follows immediately that when T approaches zero:

$$nT \rightarrow \frac{V_f \tau_{\text{eff}}}{k}$$

If the temperature-independent part ($v_b V_b/v_f V_f$ and v_b/v_f) of the pre-exponential factor in the numerator of eqn. (5) is denoted by α and in the denominator by β , two cases have to be considered:

(1) $\beta = 1$

As the temperature increases, nT increases indefinitely and the slope of the nT versus T relation may approach

$$\left(\frac{\partial nT}{\partial T} \right)_{\tau_{\text{eff}}, \text{structure}} = \frac{(V_f + V_b) \tau_{\text{eff}}}{\Delta E_b^* - \Delta E_f^* + (V_b + V_f) \tau_{\text{eff}}} \quad (7)$$

A schematic representation of the nT versus T relation is shown in Fig. 2 for $\beta = 1$. When the temperature dependence of v_b/v_f is significant, eqn. (7) has to be modified according to eqn. (6).

Fig. 2. Schematic representation of the nT vs. T relation for $\beta = 1$.(2) $\beta < 1$

As the temperature increases, nT increases asymptotically

$$nT \rightarrow \frac{V_f \tau_{\text{eff}}}{k} \frac{1 + \alpha}{1 - \beta}.$$

An inflection occurs at the temperature T_i at which

$$\begin{aligned} \tanh \frac{1}{2} \ln \beta \exp \frac{-\Delta E_b^\ddagger + \Delta E_f^\ddagger - (V_b + V_f) \tau_{\text{eff}}}{k T_i} \\ = \frac{-\Delta E_b^\ddagger + \Delta E_f^\ddagger - (V_b + V_f) \tau_{\text{eff}}}{2k T_i}. \end{aligned} \quad (8)$$

A schematic representation of the nT versus T relation for $\beta < 1$ is shown in Fig. 3. The possible temperature dependence of the pre-exponential factor v_b/v_f in eqn. (8) can also be considered as before.

These conclusions have now to be compared with the information available in the literature on the temperature and stress dependence of n .

Fig. 3. Schematic representation of the nT vs. T relation for $\beta < 1$.

Li^{8,9} showed from a thermodynamic argument that as the temperature approaches 0°K the stress sensitivity

$$nT \rightarrow \frac{V_f \tau_{\text{eff}}}{k}$$

and

$$\left(\frac{\partial nT}{\partial T} \right)_{\tau_{\text{eff}}, \text{structure}} = 0.$$

This is in full agreement with the conclusions derived from the rate theory given by eqn. (6). Li's theory does not explain the temperature dependence of the stress sensitivity above absolute zero; eqns. (5) and (6), however, describe the n versus T relation over the whole temperature range.

The nT versus T measurements of Basinski¹⁰ carried out on Al, Cu and Ag single crystals were analyzed using eqn. (5). Figure 4 shows that the rate theory describes well the observed behaviour*.

Fig. 4. The $(1/nT)$ vs. T relation measured at constant strain rate level in Al single crystals¹¹. The curve was calculated from eqn. (6) using the form

$$\frac{1}{nT} =$$

$$\frac{V_f \tau_{\text{eff}}}{k} v_f \exp \left(- \frac{\Delta E_f^\ddagger - V_f \tau_{\text{eff}}}{kT} \right) - \frac{V_b \tau_{\text{eff}}}{k} v_b \exp \left(- \frac{\Delta E_b^\ddagger + V_b \tau_{\text{eff}}}{kT} \right)$$

and

$$\Delta E_f^\ddagger = 0.585 \text{ eV}$$

$$\Delta E_b^\ddagger = 0.0216 \text{ eV}$$

$$V_f = 1400 \text{ Å}^3$$

$$V_b = 28 \text{ Å}^3$$

$$\alpha l_f \kappa_f \frac{k}{h} \frac{Q_s^\ddagger}{Q_f^\ddagger} \approx \alpha l_b \kappa_b \frac{k}{h} \frac{Q_b^\ddagger}{Q_s^\ddagger} \approx 3 \times 10^{-5} \text{ sec}^{-1} \text{ deg}^{-1}$$

where α is the usual geometrical factor.

* In an isolated study, using an expression similar in form, Schmid¹¹ analyzed the stress sensitivity of Cu. His analysis, however, was incorrect and led to erroneous results.

These results are considered as good evidence in support of the investigated form of the rate theory and it is concluded that the linear approximation represented by eqns. (5) and (6) describes fully the previously unexplained behaviour of the stress sensitivity in terms of physical quantities over the whole temperature range.

CONCLUSIONS AND SUMMARY

It has already been shown that for a linearly stress-dependent apparent activation energy the stress dependence of the dislocation velocity can be described well with the absolute rate theory if the energy barrier is asymmetrical. As a continuation of this study an investigation was carried out to determine whether the same rate equation could describe the temperature dependence of the dislocation velocity when the activation parameters are independent of the temperature. The investigation led to the following conclusions:

(1) When the energy barrier is approximated with an asymmetrical triangle the absolute rate theory predicts well the experimental results obtained for both the stress and temperature dependence of the dislocation velocity in Ge, Si and CaF_2 .

(2) The analysis indicates that the predicted temperature dependence of the stress sensitivity is also in good agreement with the experimental results obtained with Al, Cu and Ag. The thermodynamic argument of Li on the value and slope of the nT

versus T relation at absolute zero is supported by the rate theory. The previously unexplained relation between the stress sensitivity and temperature is fully described by the rate theory in terms of physical quantities over the whole temperature range.

ACKNOWLEDGEMENTS

The author is much in debt to K. J. Laidler for the many discussions which contributed materially to this paper. For the kind comments the author expresses his gratitude to H. Eyring. This paper is a contribution from the Division of Building Research, National Research Council of Canada, and is published with the approval of the Director of the Division.

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