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The Solute Atmosphere Round a Moving Dislocation and its Dragging Stress

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ABSTRACT

Setting an imaginary tetragonal lattice round a dislocation, the concentration change at each lattice point was calculated in a very short time interval from the jump frequencies of solute atoms between the nearest lattice points, considering the interaction between a solute atom and the dislocation. Repeating this calculation with a high-speed computer, the forming process of a solute atmosphere round a moving dislocation and the stress effected on the dislocation by this atmosphere were obtained. This method is for a non-steady state, from which, if required, a steady state can be obtained as the limiting case.

§ 1. INTRODUCTION

A solute atmosphere will be formed round a moving dislocation at high temperatures, at which the diffusion rate of solute atoms is sufficiently high. The dragging stress effected on the dislocation by this atmosphere may be important for the high-temperature mechanical properties of alloys.

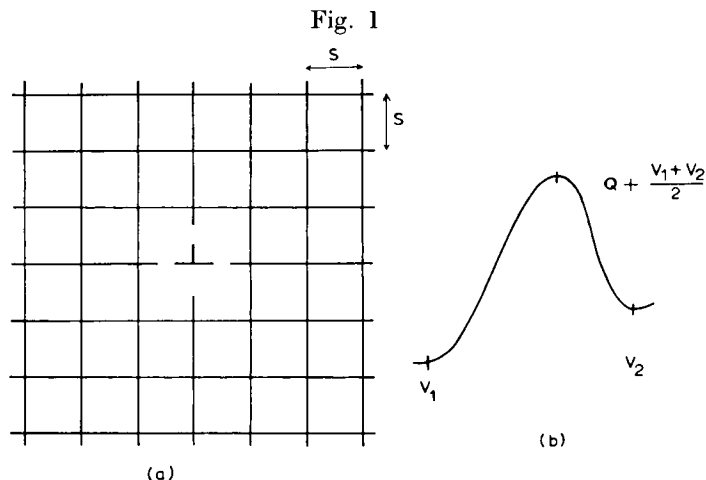
Cottrell and Jaswon (1949) analysed the steady-state atmosphere and its dragging stress, and showed that the stress increases almost proportionally to the dislocation velocity when the velocity is low enough relative to the diffusion rate of solute atoms. Since their investigation, this dragging mechanism has been applied to the high-temperature plasticity in solid-solution alloys with many successes (Weertman 1957, Weertman and Weertman 1965, Horiuchi, Yoshinaga and Hama 1965, Horiuchi and Yoshinaga 1965, Asada, Horiuchi, Yoshinaga and Nakamoto 1967, and Asano, Izumi and Tanaka 1968). However, in the temperature and strain-rate range where the diffusion rate of solute atoms is comparable with the dislocation velocity, the atmosphere which can follow the dislocation motion will be reduced in size and concentration with increasing velocity of the dislocation, and then the dragging stress will decrease also (Cottrell 1953). Yoshinaga and Morozumi (1971) concluded that the dynamical instability in plasticity expected from the mechanism just mentioned may have close relations with the Portevin-Le Chatelier effect observed in considerably solution-hardened alloys when deformed at elevated temperatures. Their theory was confirmed experimentally by Yoshinaga, Toma, Abe and Morozumi (1971) to be well applicable to the

serrations observed in vanadium containing interstitial impurities. As to the atmosphere and its dragging stress under the conditions where the P-L effect is observed, however, calculated values comparable with experimental results have not yet been shown. A computer calculation on this problem will be presented in the present paper.

§ 2. CALCULATION METHOD

2.1. Calculation Method with Known Interaction Energy between a Solute Atom and a Dislocation

For the calculation, the method used as a first approximation will be described in the following. At first, an imaginary tetragonal lattice is constructed round a dislocation as shown in fig. 1 (a) and the lattice constant is taken as the jump distance of solute atoms, s . Then concentrations are considered to change due to jumps of solute atoms between these lattice points.



(a) The imaginary tetragonal lattice round a dislocation used. (b) Schematic representation of the potential barrier for the solute atom diffusion interacting with a dislocation.

When the interaction energy between a solute atom and a dislocation is given as a function of the solute atom position, a solute atom at a lattice point is assumed to jump to one of the nearest lattice points through a potential barrier as shown in fig. 1 (b). The activation energy may be $Q + (V_2 - V_1)/2$ for the jump from site 1 to site 2 and $Q + (V_1 - V_2)/2$ for the reverse jump, where Q is the activation energy for the solute atom diffusion when the dislocation is not present, and V_1 and V_2 are the interaction energies in sites 1 and 2 respectively.

Next, any solute atom flow is not considered between the dislocation centre and its nearest lattice points, because the centre is a singular point, i.e. a hole is made at the centre.

When the dislocation lies along the z axis, each flow of solute atoms will be confined in an xy plane and the concentration is independent of the z coordinate.

When the dislocation is at rest, the rate of concentration change at a given lattice point due to the solute flow between this and its right nearest lattice point may be given under the assumptions used as

$$\frac{\partial c(x, y)}{\partial t} = p\nu c(x+s, y) \{1 - c(x, y)\} \exp \left[-\frac{1}{kT} \left\{ Q + \frac{V(x, y) - V(x+s, y)}{2} \right\} \right] \\ - p\nu c(x, y) \{1 - c(x+s, y)\} \exp \left[-\frac{1}{kT} \left\{ Q + \frac{V(x+s, y) - V(x, y)}{2} \right\} \right], \quad (1)$$

where p is the geometrical factor, ν is the vibration frequency of the solute atom including the entropy term. This expression comes from the thoughts that the changing rate is determined by the difference in the rates of solute atoms jumping into, from, and out to, the right nearest lattice point. The rate of solute atoms coming into the lattice point concerned from its right nearest lattice point may be proportional to the concentration at the right nearest, $c(x+s, y)$, to the probability that the site concerned is vacant, $1 - c(x, y)$, and to the exponential factor which represents the probability of the solute atom having enough vibrational energy to overcome the potential barrier (the first term in the right-hand side of eqn. (1)). The rate of solute atoms jumping out to the nearest lattice point may be expressed as the second term in the same manner.

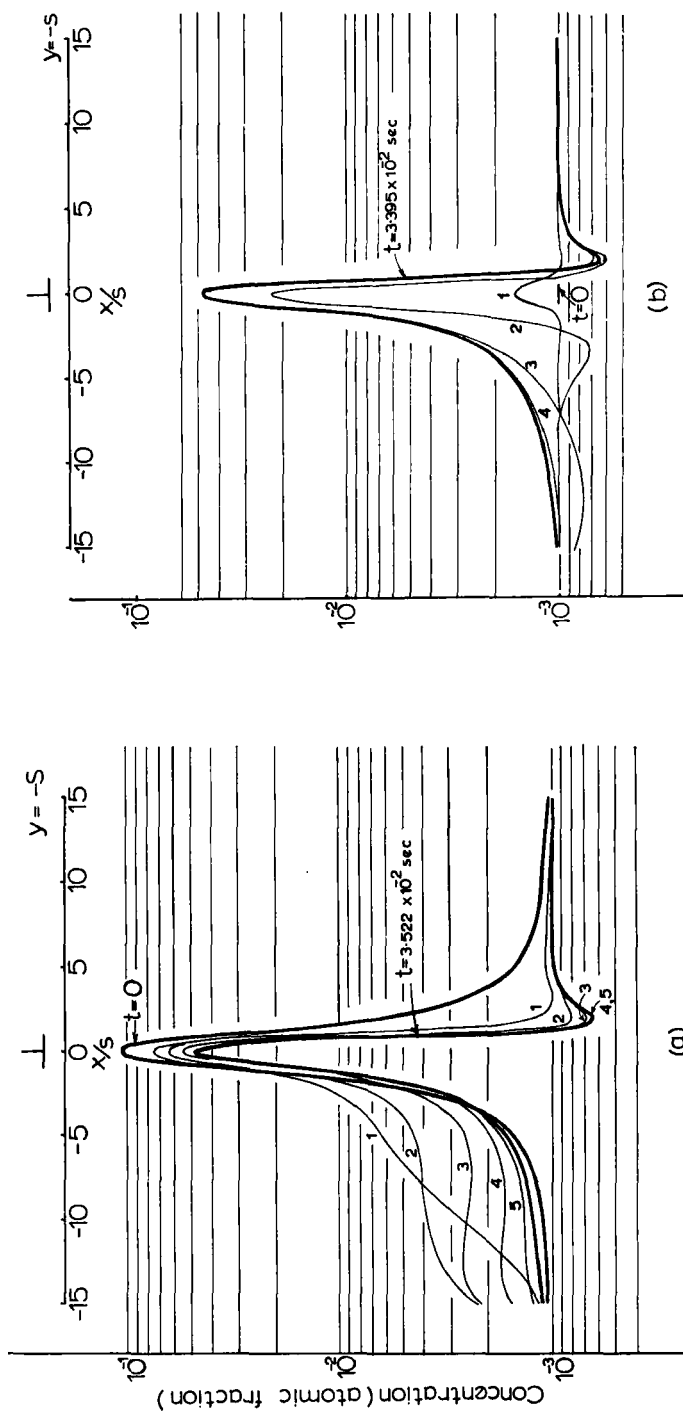
The concentration changes due to the solute flows between the site concerned and its other three nearest sites, left, above and below, may be given in the same manner as eqn. (1), and the total sum of these four contributions will be the rate of concentration change at the lattice point concerned.

When the dislocation moves in the x direction with a velocity of v , for the fixed coordinates to the moving dislocation, the concentration in the right nearest site comes into, and the concentration in the site noted goes out to, the left nearest site with the corresponding rate to the velocity v . The changing rate of concentration due to this process may be expressed as $v \{c(x+s, y) - c(x, y)\}/s$.

Considering the common factor through the eight terms derived from the four nearest sites, $p\nu \exp(-Q/kT) = D/s^2$, where D is the diffusion coefficient of the solute, we obtain finally

$$\frac{\partial c(x, y)}{\partial t} = \frac{D}{s^2} \left[c(x+s, y) \{1 - c(x, y)\} \exp \left\{ \frac{V(x+s, y) - V(x, y)}{2kT} \right\} \right. \\ \left. - c(x, y) \{1 - c(x+s, y)\} \exp \left\{ \frac{V(x, y) - V(x+s, y)}{2kT} \right\} + \dots \right] \\ + v \{c(x+s, y) - c(x, y)\}/s. \quad (2)$$

Fig. 2



Changes of the concentration distribution round a dislocation as the dislocation moves. Bold curves show the initial and near to the steady-state concentration distributions at 300°C and for a dislocation velocity of $2 \times 10^3 \text{ Å/sec}$. (a) The case where the initial atmosphere is the one in thermal equilibrium round a stationary dislocation. The curves numbered 1, 2, 3, 4 and 5 show the concentration distributions after 3.807×10^{-3} , 7.894×10^{-3} , 1.434×10^{-2} , 2.031×10^{-2} and $2.677 \times 10^{-2} \text{ sec}$ respectively. (b) The case where the dislocation has no atmosphere initially. The curves numbered 1, 2, 3 and 4 show the concentration distributions after 1.479×10^{-5} , 1.748×10^{-3} , 1.163×10^{-2} and $2.077 \times 10^{-2} \text{ sec}$ respectively.

The right-hand side of eqn. (2) can be calculated easily in any sites when the concentrations and the interaction energies are known at every lattice point. Representing the right-hand side as $F(x, y)$, the concentration change in a very small time interval, Δt , is obtained from the equation

$$\Delta c(x, y) = F(x, y)\Delta t. \quad . \quad . \quad . \quad . \quad . \quad . \quad (3)$$

In other words, if the concentration distribution is known at a time t , the distribution after an elapsed time Δt is obtainable.

Giving the concentration distribution in thermal equilibrium round a stationary dislocation as the initial atmosphere, as an example, the changing process of the concentration distribution is obtainable when the stationary dislocation is forced to move with a velocity v (fig. 2 (a)).

2.2. Concentration Dependence of the Interaction Energy

A solute atmosphere being formed, the stress field round a dislocation will be relaxed (Cottrell and Bilby 1949). Therefore, the interaction energy between a solute atom and a dislocation must depend on the concentration in the position of the solute atom. In the following, this concentration dependence will be discussed for a solute atom interacting with an edge dislocation hydrostatically.

The rate of volume expansion round an edge dislocation lying along the z axis and with Burgers vector in the x direction is given at the position (x, y) from the dislocation as

$$\Delta_d = - \frac{1-2\nu}{2\pi(1-\nu)} b \frac{y}{x^2+y^2}, \quad . \quad . \quad . \quad . \quad . \quad (4)$$

where ν is Poisson's ratio and b is the strength of the dislocation.

If the rate of volume expansion due to solute atoms of concentration c is Δ_c , the rate increase produced by introducing the dislocation will be $(\Delta_d - \Delta_c)$. Then the hydrostatic pressure due to the dislocation will decrease there in the ratio $(\Delta_d - \Delta_c)/\Delta_d$ from that for uniform distribution of solute atoms. Taking the volume of a solute atom as Ω and the volume expansion produced by introducing a solute atom in a site as $\Delta v = \Delta_1 \Omega$, the interaction energy between a solute atom in a position of concentration c and a dislocation may be given by

$$V = -p(1 - \Delta_c/\Delta_d)\Delta v, \quad . \quad . \quad . \quad . \quad . \quad (5)$$

where p is the hydrostatic pressure produced by the dislocation when the solute distribution is uniform and is given in this case by

$$p = - \frac{1+\nu}{3\pi(1-\nu)} \mu b \frac{y}{x^2+y^2}. \quad . \quad . \quad . \quad . \quad . \quad (6)$$

Here μ is the shear modulus.

2.2.1. *For substitutional solid solutions*

Taking the radii of the solute and solvent atoms in a solid solution as R and R_0 respectively, a misfit parameter ϵ is defined as

$$R = R_0(1 + \epsilon). \quad (7)$$

Another misfit parameter ϵ_0 derived from the concentration dependence of the lattice constant, a , is defined as

$$\epsilon_0 = \frac{1}{a} \frac{da}{dc}. \quad (8)$$

When the mean solute concentration is c_0 , we may have for a dilute solution

$$\Delta_c = 3\epsilon_0(c - c_0). \quad (9)$$

This volume expansion corresponds to the lattice parameter change as if the size of the solvent atom increased there on the average to

$$R_0' = R_0(1 + \epsilon_0 c). \quad (10)$$

If an effective misfit parameter, ϵ_{eff} , is defined as

$$R = R_0'(1 + \epsilon_{\text{eff}}), \quad (11)$$

we obtain from eqns. (7), (10) and (11)

$$\epsilon_{\text{eff}} = \epsilon - \epsilon_0 c. \quad (12)$$

The rate of volume expansion due to inserting one solute atom in the region of concentration c may be given by

$$\Delta_1 = 3\epsilon_{\text{eff}}. \quad (13)$$

Then, taking

$$\Omega \approx \frac{4}{3}\pi R_0^3, \quad (14)$$

we may have

$$\Delta v = 4\pi\epsilon R_0^3(1 - c\epsilon_0/\epsilon). \quad (15)$$

If the change in lattice constant by alloying occurs mainly due to the atomic size difference and the overall change in the crystal other than that due to this localized change is small, we have $\epsilon \approx \epsilon_0$, and then from eqns. (4), (5), (6), (9) and (15) the interaction energy may be given by

$$V = A \left\{ \frac{y}{x^2 + y^2} + \frac{6\pi(1-\nu)}{1-2\nu} \frac{\epsilon(c-c_0)}{b} \right\} (1-c), \quad (16)$$

where

$$A = \frac{4}{3} \frac{1+\nu}{1-\nu} \mu b \epsilon R_0^3. \quad (17)$$

2.2.2. *For interstitial solutes situated in octahedral sites in b.c.c. lattice*

There is a tetragonality in the strain round an interstitial solute atom situated in an octahedral site in a b.c.c. lattice. Taking the strain produced in the c direction as ϵ_1 and in the a directions as ϵ_2 when a solute atom is inserted in a unit cell, the mean strain ϵ_u of the unit cell may be defined as

$$3\epsilon_u = \epsilon_1 + 2\epsilon_2 \quad . \quad . \quad . \quad . \quad . \quad . \quad (18)$$

for the hydrostatic interaction considered here. This mean strain may be related to the concentration dependence of the lattice parameter as

$$\epsilon_u = \frac{1}{a} \frac{da}{dc_u}, \quad . \quad . \quad . \quad . \quad . \quad . \quad (19)$$

where c_u is the solute atom fraction per unit cell. When the fractions of solute atoms to the matrix atoms and to the interstitial sites are taken as c and c_1 respectively, these three fractions are related each other as

$$c_u = 2c = 6c_1. \quad . \quad . \quad . \quad . \quad . \quad . \quad (20)$$

Using ϵ_u and c_1 as the strain and the concentration of the solute atom respectively,

$$\begin{aligned} \Delta_c &= 3 \left(\frac{1}{a} \cdot \frac{da}{dc} \right) (c - c_0) \\ &= 18\epsilon_u(c_1 - c_{10}). \quad . \quad . \quad . \quad . \quad . \quad . \quad (21) \end{aligned}$$

The volume expansion produced by inserting a solute atom in the region of concentration c_1 may be given similarly as § 2.2.1 by

$$\Delta v = 4\pi \left(\frac{a}{2} \right)^3 \epsilon_u(1 - c_1). \quad . \quad . \quad . \quad . \quad . \quad . \quad (22)$$

Then the interaction energy may be given from eqns. (4), (5), (6), (21) and (22) by

$$V = A \left\{ \frac{y}{x^2 + y^2} + \frac{36\pi(1 - \nu)}{1 - 2\nu} \frac{\epsilon_u(c_1 - c_{10})}{b} \right\} (1 - c_1), \quad . \quad . \quad (23)$$

where

$$A = \frac{4}{3} \frac{1 + \nu}{1 - \nu} \mu \epsilon_u b \left(\frac{a}{2} \right)^3 \quad . \quad . \quad . \quad . \quad . \quad . \quad (24)$$

On deriving eqns. (16) and (23) for the interaction energy, the localized strains produced by the solute atoms were averaged and taken as uniform change of the lattice parameter and further the interaction between solute atoms was not considered. Then the results obtained are approximate.

Further, the concentration in eqn. (2) should be also the fraction of solute atoms to the interstitial sites for the interstitial alloys discussed here.

§ 3. CALCULATED RESULTS

Consider the case of vanadium containing 0.1 at. % carbon in solution as an example, and take the required parameters as $s = a/2 = 1.516 \text{ \AA}$, $b = 2.726 \text{ \AA}$, $\nu = 0.36$, $\mu = 5 \times 10^3 \text{ kg/mm}^2$, $\epsilon_u = 0.11$, and $D = D_0 \exp(-Q/RT)$, where $D_0 = 0.0045 \text{ cm}^2/\text{sec}$ and $Q = 27.3 \text{ kcal/mole}$, then we obtain from eqn. (24) $A = 1.4 \times 10^{-12} \text{ erg \AA}$, and from eqn. (23) 0.57 eV for the interaction energy at the imaginary lattice point $(0, -s)$ directly below the dislocation.

Since the mean velocity of dislocations is given by $\dot{\epsilon}_p/\rho b$ when the moving dislocation density is ρ and the shear strain rate is $\dot{\epsilon}_p$, the velocity may lie in the range from 10 to 10^6 \AA/sec under usual conditions, considering $\dot{\epsilon}_p = 10^{-5} \sim 10^{-2}/\text{sec}$ and $\rho = 10^7 \sim 10^9/\text{cm}^2$.

According to Yoshinaga and Morozumi (1971), the critical velocity for the solute atmosphere formation round a moving dislocation is given by

$$v_{\text{CL}} \simeq AD/kTb^2. \quad . \quad . \quad . \quad . \quad . \quad . \quad (25)$$

When $v_{\text{CL}} = 10 \text{ \AA/sec}$, the lower limiting temperature to form the solute atmosphere round the dislocation is estimated from eqn. (25) to be about 200°C . Then the calculations described below will be confined to the temperature range above 200°C .

Cottrell (1953) approximated the size of the atmosphere in thermal equilibrium round a stationary dislocation to a cylinder along the dislocation with a radius of

$$l = A/kT \quad . \quad . \quad . \quad . \quad . \quad . \quad (26)$$

in his calculations as to the dragging stress in steady state. In the alloy considered here $l = 21.4 \text{ \AA}$ at 200°C . Then a dimension of 33×33 imaginary lattice points is used for the present computer calculations, provided that the mean concentration is given at the lattice points in the periphery of this dimension.

3.1. *Changes of the Atmosphere as the Dislocation Moves*

Figure 2 (a) shows how the concentration distribution changes as the dislocation moves when a stationary dislocation having the atmosphere in thermal equilibrium is forced to move suddenly with a velocity of $2 \times 10^3 \text{ \AA/sec}$ at 300°C , illustrating the distribution only in the imaginary lattice plane directly below the dislocation in order to eliminate the complexity of the figure.

Under the conditions described, the concentration in the vicinity of the dislocation decreases as the dislocation moves and settles down almost to the steady state (indicated in the figure as a bold solid curve) after about 0.035 sec .

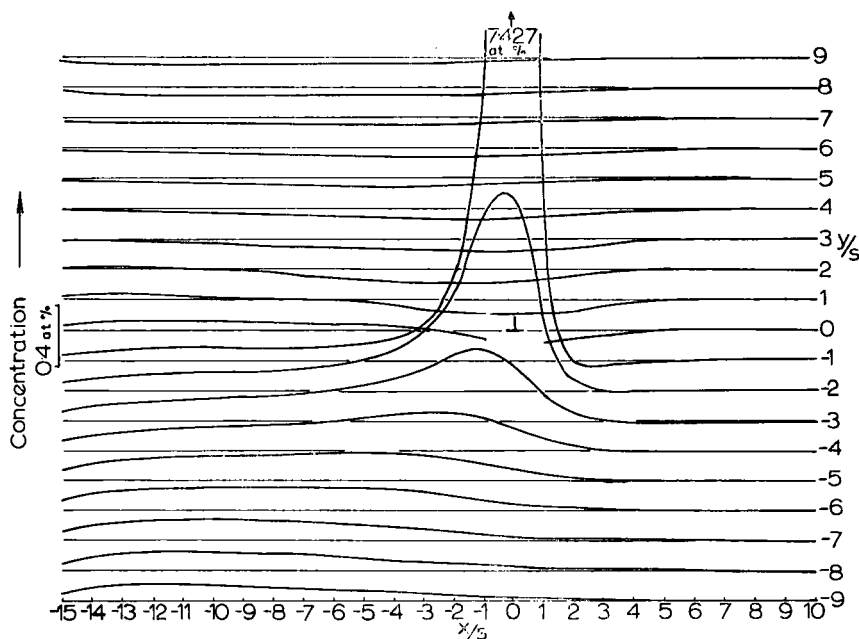
Figure 2 (b) shows the forming process of the solute atmosphere as the dislocation moves which has initially no atmosphere, at the same temperature and velocity as in fig. 2 (a). In this case, the atmosphere nearly in

steady state is seen to be formed after about 0.034 sec. As a matter of fact, the steady state atmosphere achieved is independent of the initial conditions used, as is seen by comparing figs. 2 (a) and (b).

An example for the whole concentration distribution nearly in the steady state is shown in fig. 3, where the concentration distribution on each imaginary lattice plane of $y = ns$ (n is an integer) is shown, the level of the lattice plane (indicated as a fine line) being the mean concentration.

It is seen in this figure that the position of the concentration maximum on a lattice plane in the lower half region or of the minimum on a lattice plane in the upper half region migrates backward as the lattice plane goes away from the slip plane.

Fig. 3



The concentration distribution nearly in the steady state at 300°C and for a dislocation velocity of 10^3 Å/sec.

3.2. Changes of the Dragging Stress as the Dislocation Moves

Each imaginary lattice point in the plane of fig. 1 occupies an area of s^2 perpendicular to the dislocation line, that is, a volume of s^2 for the dislocation of a unit length. If a volume Ω' is occupied by a site for the solute atom, there are s^2/Ω' sites for the solute atom in the volume of s^2 . Then, the lattice point has cs^2/Ω' solute atoms per unit dislocation length, where c is the fraction of the solute atoms to the sites.

For substitutional solid solutions, $\Omega' = \Omega_u/m$, if m atoms belong to a unit cell of volume Ω_u (then $\Omega' = a^3/4$ for f.c.c. and $a^3/2$ for b.c.c.), and the atomic fraction should be used for the concentration. On the other hand,

for the interstitial solid solutions concerned, we have $\Omega' = a^3/6$, when the concentration is expressed as the fraction to the interstitial sites as described previously.

Since the resisting force of a solute atom to the slipping motion of the dislocation is $\partial V/\partial x$ (Cottrell and Jaswon 1949), the resolved shear stress τ necessary to move the dislocation with a solute atmosphere may be given by

$$\tau b = \sum (cs^2/\Omega') \frac{\partial V}{\partial x}, \quad . \quad . \quad . \quad . \quad . \quad . \quad (27)$$

where the summation should be taken over all the lattice points considered.

When eqn. (27) is applied to vanadium containing 0.1 at. % carbon, we obtain the dragging stress as shown in fig. 4.

Figure 4 (a) shows the changing processes of the dragging stress when a stationary dislocation with the atmosphere in thermal equilibrium at 300°C is forced to move suddenly with the various velocities indicated.

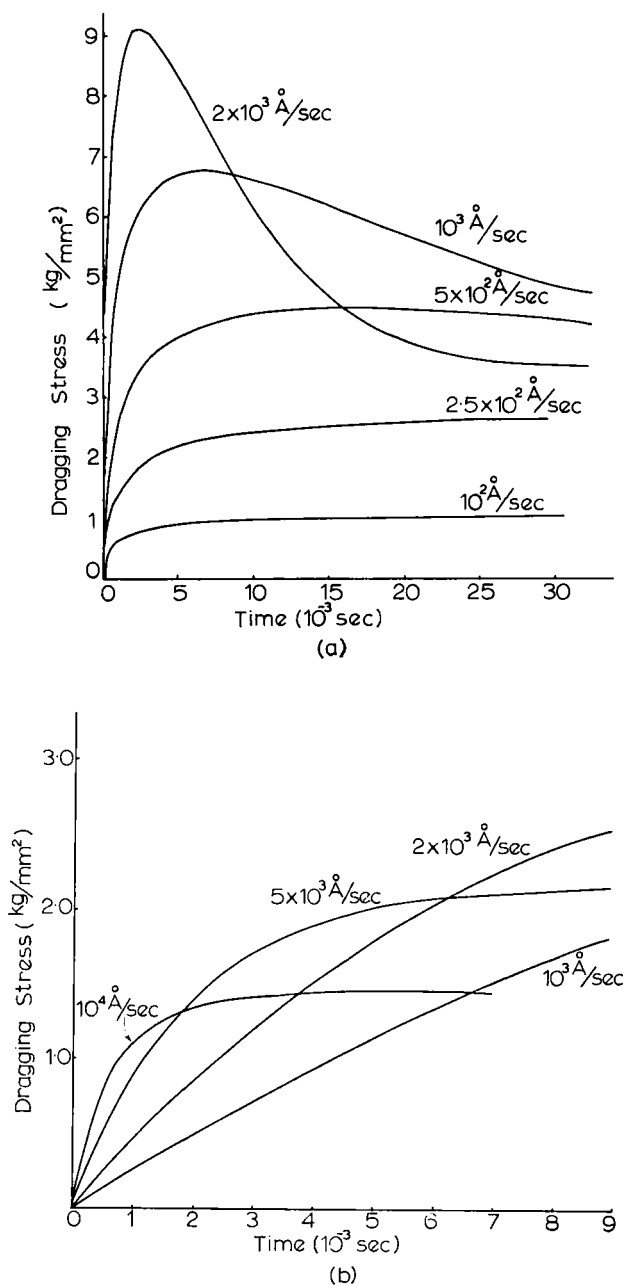
For the velocity up to about 2.5×10^2 Å/sec, the dragging stress increases monotonically to the steady state as the dislocation moves (in this lower velocity range, the steady-state atmosphere is little different from the atmosphere in thermal equilibrium for a stationary dislocation, see fig. 6), while for higher velocities, the stress is seen to increase at first but decrease, then passing through a peak gradually to the steady state (in this higher velocity range, the steady-state atmosphere is considerably weaker than that for the stationary dislocation, see fig. 6). This means that a partial unlocking occurs for these higher velocities.

On the other hand, starting from the state without atmosphere, the dragging stress increases always monotonically as a matter of course, as seen in fig. 4 (b). Further, in the earlier stage of atmosphere formation, the higher the velocity the higher the dragging stress becomes irrespective of the level of the steady state stress, because the rate of atmosphere formation on the back side of the dislocation becomes higher.

3.3. *Steady-state Atmosphere and its Dragging Stress*

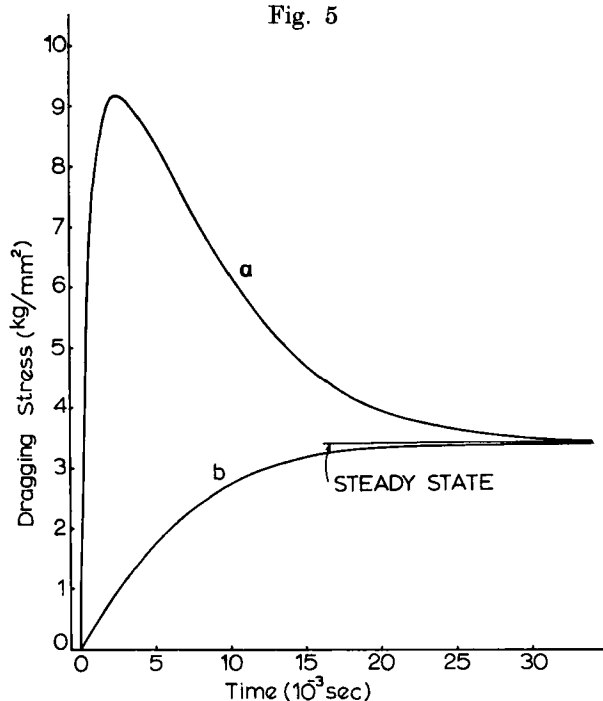
The steady-state atmosphere and its dragging stress must be determined for a given temperature and dislocation velocity irrespective of the initial conditions, but the procedure for approaching the steady state depends on the initial conditions. Starting from the atmosphere in thermal equilibrium for a stationary dislocation, the atmosphere decreases as the dislocation moves, while starting from no atmosphere, the atmosphere increases. Especially for a velocity at which the partial unlocking occurs, the dragging stress in the steady state will be approached from both sides when the two extreme initial conditions just mentioned are used. Figure 5 shows an example of this. This approaching method from both sides is useful not only to estimate the dragging stress in the steady state but also to see how near the calculated values approach to the steady state.

Fig. 4



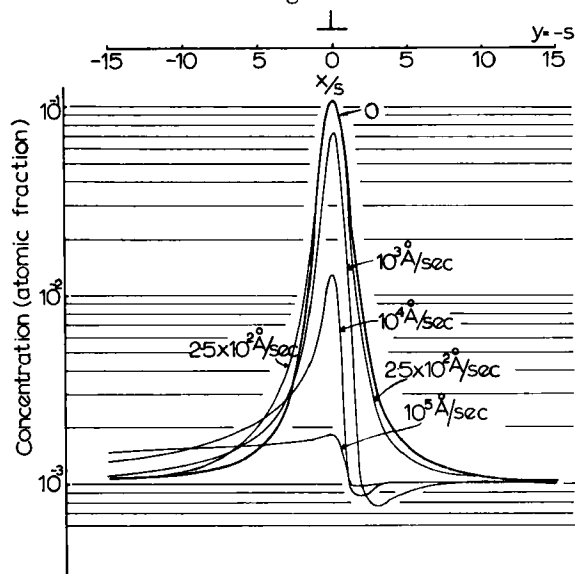
Changes of the dragging stress as the dislocation moves with various velocities indicated at 300°C. (a) The case where a stationary dislocation with the atmosphere in thermal equilibrium is forced to move. (b) The case where a dislocation with no atmosphere initially is moved.

Fig. 5



It is shown that the dragging stress in the steady state can be estimated fairly accurately by approaching from the two extreme initial conditions. Curve *a* shows the case of starting from the atmosphere in thermal equilibrium round a stationary dislocation and curve *b*, starting from no atmosphere at 300°C and for a dislocation velocity of 2×10^3 Å/sec.

Fig. 6



The concentration distributions nearly in the steady state for the various dislocation velocities indicated.

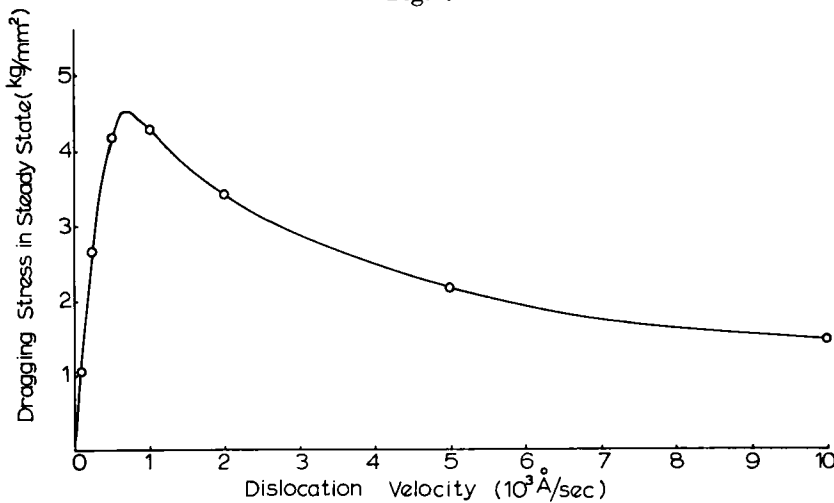
Figure 6 shows examples of the concentration distribution in the atmosphere nearly in the steady state deduced for various velocities at 300°C by this method. It is evident from this figure that the atmosphere is not very different from that for a stationary dislocation for velocities up to about 2.5×10^2 Å/sec, but considerably different above 10^3 Å/sec, i.e. the maximum concentration decreases and the atmosphere flows backward from the dislocation more significantly with increasing the velocity.

The dragging stress nearly in the steady state depends on the dislocation velocity as shown in fig. 7. When the velocity is low, the steady-state stress is seen to increase almost linearly with the velocity as predicted previously by Cottrell and Jaswon (1949), but it decreases when the velocity exceeds a critical value, v_{CH} . Cottrell (1953) showed that this critical velocity is given approximately by

$$v_{CH} = 4kTD/A, \quad \dots \dots \dots (28)$$

supposing this velocity to be the limiting one below which the concentration distribution in the steady-state atmosphere is much the same as that for a stationary dislocation. Comparing figs. 6 and 7, his presupposition is seen to be almost valid.

Fig. 7



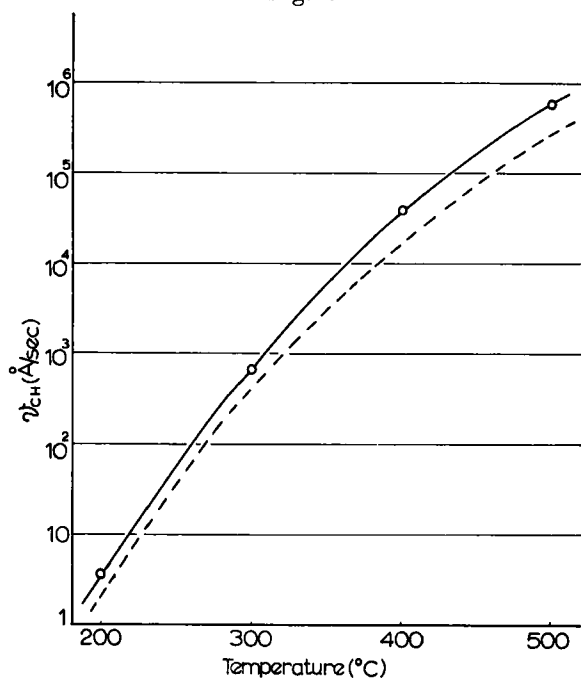
Dislocation velocity dependence of the dragging stress nearly in the steady state at 300°C.

Figure 8 shows the comparison between v_{CH} values obtained here (data points) and calculated from eqn. (28) (broken line). The values obtained here are slightly higher than those from eqn. (28), but the values can be said to agree quite well.

Further, the peak dragging stress in steady state corresponding to v_{CH} was given by Cottrell and Jaswon (1949) as

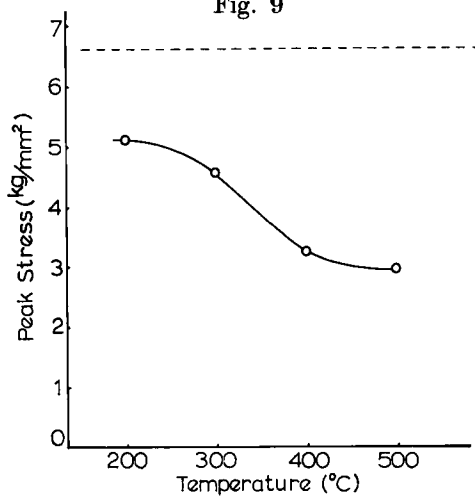
$$\tau_c = 17 A c_0 N / b \quad \dots \dots \dots (29)$$

Fig. 8



Temperature dependence of v_{CH} . The broken line is calculated from Cottrell's equation.

Fig. 9



Temperature dependence of the peak dragging stress. The broken line is calculated from Cottrell's equation.

(Cottrell 1953), where N is the total number of atoms in a unit volume, while τ_c obtained here decreases with rising temperature as shown in fig. 9, where τ_c calculated from eqn. (29) is also shown as a broken line for comparison.

It seems to follow, from the effect of the concentration dependence of the interaction energy considered in the present paper, that the τ_c values obtained here are lower than the value calculated from eqn. (29) (see § 2.2).

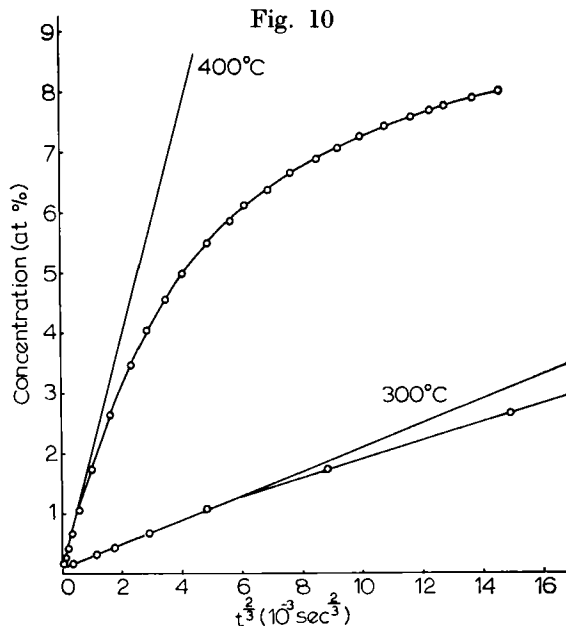
3.4. Forming Process of an Atmosphere Round a Stationary Dislocation

Cottrell and Bilby (1949) showed for the atmosphere forming process that the number of solute atoms segregated to the dislocation is proportional to $t^{2/3}$ (where t is the time elapsed). Representing their result with the concentration on the imaginary lattice point directly below the dislocation (fig. 1), we have

$$c = \left\{ 4 \times \left(\frac{\pi}{2} \right)^{1/3} \left(\frac{AD}{kT} \right)^{2/3} c_0 / s^2 \right\} t^{2/3}, \quad \quad (30)$$

where we use factor 4 instead of their 3, the reason of which was given in another paper (Yoshinaga and Morozumi 1971).

Figure 10 shows the comparison between the results obtained here (data points) and those calculated from eqn. (30) (straight lines). It is



The process of the atmosphere formation in the region directly below a stationary dislocation. Data points are calculated with the present method. The two straight lines are calculated from the equation of Cottrell and Bilby (1949). Mean concentration is 0.1 at. %.

seen that the forming process of the atmosphere begins to deviate from the $t^{2/3}$ law when the concentration directly below the dislocation exceeds 2 at. % = $20c_0$ for $c_0 = 0.1$ at. % in the material considered here. This deviation comes from the solute flow due to the concentration gradient which is not considered in eqn. (30).

§ 4. DISCUSSION

The method of calculation used here involves four major approximations in the base.

Firstly, the lattice points (fig. 1) used for the calculation are not the real sites for solute atoms but imaginary ones. However, if the concentration is low enough and the interaction energy, together with the concentration, vary gradually enough over the spacing of s , we can rewrite the right-hand side of eqn. (2) into differential forms, then we have

$$\begin{aligned}\frac{\partial c(x, y)}{\partial t} &= D \nabla^2 c + \frac{D}{kT} \nabla c \nabla V + \frac{D}{kT} c \nabla^2 V + \mathbf{v} \nabla c \\ &= -\nabla(-D \nabla c - \frac{D}{kT} c \nabla V - c \mathbf{v}) \\ &= -\nabla \mathbf{J} \dots \dots \dots (31)\end{aligned}$$

In the second form of eqn. (31), the first term in parentheses represents the solute flow due to the concentration gradient, the second term is the flow due to the interaction between solute atoms and the dislocation, i.e. Einstein's drift flow, and the third term is the apparent flow due to the dislocation moving. Then the sum of these three vectors represents the solute flow \mathbf{J} relative to the moving dislocation (Cottrell and Jaswon 1949).

Equation (31) is an equation of continuity. Accordingly, the changing rate of concentration may be obtained with sufficiently good approximation in the regions at some distance from the dislocation using eqn. (2) which has been derived from jumping frequencies of solute atoms between the imaginary lattice points. Evidently from this argument, it is not necessary in the regions far enough from the dislocation to take the imaginary lattice constant as the real jumping distance s , but the lattice constant may be taken as a distance larger than s . In the region very near to the dislocation, however, the concentration and the interaction energy vary so rapidly with the position that the approximation described above can no longer be used. To improve the approximation in such a region, the real sites for solute atoms should be considered for the calculation. However, the estimation of the interaction energy becomes difficult simultaneously in such a position close to the dislocation. Accordingly, it is difficult to estimate how far the approximation can be improved by using the real sites.

Secondly, a hole was made at the dislocation centre, simply because the interaction energy used cannot be determined there definitely. But, in the real case, the centre is not a singular point. Therefore, the calculated

atmosphere must be modified significantly in the close vicinity of the centre.

Thirdly, any anisotropy of the strain round a solute atom is not considered in estimating the interaction energy, in spite of the fact that a solute atom in an octahedral interstitial site in a b.c.c. lattice is known to produce a tetragonal strain and the interaction energy with a dislocation depends on the orientation of the principal axes of the strain. Then, the interaction energy used is more suitable for substitutional solid solutions.

If the real sites are used and the strain anisotropy is considered, the Snoek atmosphere may be calculated also, together with the Cottrell atmosphere.

Fourthly, the supposed lattice points are fixed to the dislocation and only the relative motion of the solute atoms is considered, in spite of the fact that the real sites for solute atoms move relatively to the dislocation. This approximation is similar to the first one in that the lattice points used are not real ones.

Other than the above four approximations, the interaction energy is estimated here, assuming further that the usual theory of elasticity could be applied up to a position very near to the dislocation (a position separated from the dislocation only by the jump distance of the solute atom). From this and the second approximation above, it is highly probable that we have overestimated the solute atmosphere in the vicinity of the dislocation. Further, the interaction of a solute atom with a screw dislocation is also important in b.c.c. interstitial solid solutions, but here only the hydrostatic interaction with an edge dislocation is considered.

Indeed the stress amplitude of serrations in the stress-strain curve is estimated from the calculated example described here to be about 6 kg/mm² in the maximum at 500°C, but the amplitude observed by Yoshinaga *et al.* was only 2~3 kg/mm² under test conditions nearly corresponding to the calculated example.

So it seems that the dragging stress computed here involves a considerable error due to the various approximations included, but for the temperature and dislocation-velocity dependences of the dragging stress the calculated results may be accurate enough to be compared with experimental results, because the concentration distribution round a moving dislocation may be determined mainly by the diffusing velocity of solute atoms relative to that of the dislocation.

Considering that the equation $\text{div } \mathbf{J} = 0$ holds for a steady state, Cottrell and Jaswon (1949) calculated the concentration distribution and the dragging stress due to this atmosphere, resolving analytically the above differential equation. On the other hand, the method of calculation used here is in itself for a non-steady state and the steady state is obtainable as the limit approaching from these non-steady states, as shown in figs. 4 and 5.

Accordingly, the present method is suitable to calculate a changing process in the non-steady state such as the forming process of a solute

atmosphere round a dislocation (figs. 2 (b), 4 (b) and 10) or the breaking process of a dislocation from its atmosphere when the velocity of the dislocation is accelerated (Yoshinaga and Morozumi 1971, and figs. 2 (a) and 4 (a)).

§ 5. SUMMARY

Considering an imaginary tetragonal lattice round a dislocation, the solute atmosphere formation round a dislocation moving with an arbitrary velocity and the dragging stress effected on the dislocation by this atmosphere were calculated with a high-speed computer, repeating the calculation of the concentration change at each imaginary lattice point in a very small time interval from jumping frequencies of solute atoms between these lattice points under the interaction with the dislocation. Since this method is for a non-steady state, the forming process of a solute atmosphere round a dislocation or the decreasing process of the atmosphere when the velocity of the dislocation is accelerated can be calculated with this method. The steady state is also obtainable as a limiting case of non-steady states.

Applying this calculation method to vanadium containing 0.1 at. % carbon, the following results were obtained.

1. There is a critical dislocation velocity v_{CH} , which depends on temperature. Below this critical velocity, the dragging stress τ in steady state increases with increasing velocity, while the stress decreases contrarily for $v > v_{CH}$. The values of v_{CH} obtained here are only slightly higher than those calculated from Cottrell's eqn. (28), and τ increases almost proportionally to v up to the vicinity of v_{CH} as predicted by Cottrell and Jaswon (1949). The steady-state atmosphere is much the same as that for a stationary dislocation up to about v_{CH} , as assumed by Cottrell (1953) in his estimation of the dragging stress, but it decreases significantly with increasing dislocation velocity in the range $v > v_{CH}$ (fig. 6).

2. When a stationary dislocation with the atmosphere in thermal equilibrium is forced to move with a velocity v , the dragging stress increases monotonically to the value in the steady state for v considerably lower than v_{CH} , while for higher velocities a partial unlocking occurs and the dragging stress decreases after passing through a peak to that in steady state, because the atmosphere becomes considerably weaker than that of a stationary dislocation (fig. 4 (a)).

3. Even if $v > v_{CH}$, the dragging stress increases with increasing dislocation velocity in the process of atmosphere formation (fig. 4 (b)).

4. For the forming process of the atmosphere round a stationary dislocation, eqn. (30) derived by Cottrell and Bilby (1949) is obeyed in its earlier stage, but the process begins to deviate from their $t^{2/3}$ law when the concentration in the region directly below the dislocation exceeds about 2 at. % = $20 c_0$.

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