CHAPTER IX *THERMAL ACTIVATED DISLOCATION MOTION*

9.1 Introduction

The speed of plastic deformation of a crystal sample is related to the density of mobile dislocations, Λm, to their mean speed by the Orowan relation (6.17):

$$\dot{\varepsilon} = \Lambda_m b \bar{V}$$

If the dislocations moved freely in the crystal—without friction, obstacles, or mutual interactions—their velocity would approach the speed of sound, and the strain rate would then be controlled primarily by Λm. However, in real crystalline materials, dislocations interact with numerous forms of resistance, including:

- internal lattice friction,
- elastic interactions with other dislocations,
- interactions with point defects, impurities, and precipitates.

Under these conditions, the strain rate is governed less by Λm (which varies only slightly) and more by the average dislocation velocity, ($\bar{\bar{V}}$). This velocity is limited by the time required for a dislocation to bypass or overcome obstacles. When these obstacles are localized—meaning they involve only a small group of atoms—thermal activation can help overcome the associated energy barriers, reducing the applied stress required to sustain deformation at higher temperatures.

This thermally assisted deformation is significant at elevated temperatures and under sustained stress, where materials can undergo creep. The creep response typically evolves through three stages: primary creep, during which strain hardening causes a gradual decrease in strain rate; secondary creep, where a balance between hardening and recovery leads to a nearly constant, minimum creep rate; and tertiary creep, marked by the initiation and growth of cavities and microcracks, resulting in accelerated deformation and eventual rupture. The minimum (steady-state) creep rate is strongly dependent on stress and temperature, and often follows an Arrhenius-type relationship, allowing determination of the activation energy associated with the controlling creep mechanism.

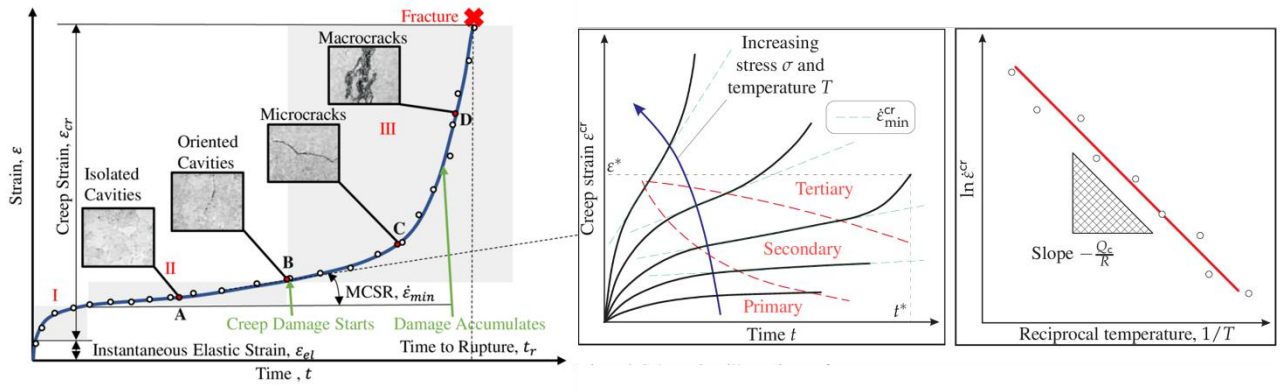
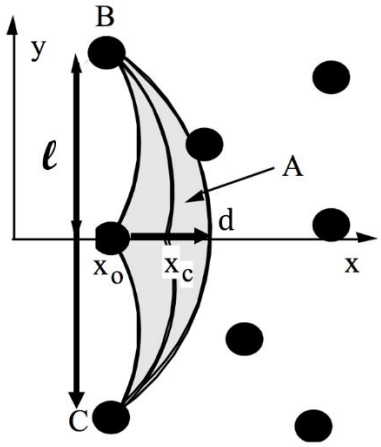


Figure 9-1: *Stages of creep damage as a function of creep strain and time, which are thermally activated processes*

This chapter is dedicated to the thermodynamics of the thermally activated motion of dislocations. After reviewing the expression of the strain rate as a function of the frequency at which the dislocations cross the obstacles, the Gibbs free energy related to overcoming energy barriers is defined. The activation volume derived from this relationship represents the number of atoms involved. We then present some experimental techniques that allow us to access those parameters. Finally, dislocation climb is explained as a vacancy-mediated process, which, by definition, is a thermally activated phenomenon.

9.2 Strain rate



In the classic framework of thermal activation theory, we generally consider that the time of flight" (or glide time in this notation) between two obstacles is short compared to the average time necessary to cross an obstacle (escape time):

$$t_g \ll t_e$$

We can perform "in situ" electron microscopy to observe how dislocations move with a "jerky-type" profile.

Figure 9-1: *Area swept by a dislocation during the crossing of an obstacle*

If *d* is the total distance of dislocation motion (during and after the activation process), the average speed of the dislocation can be written:

$$\bar{V} \approx \frac{d}{t_e + t_g} \approx \frac{d}{t_e} \approx \frac{A}{l}\frac{1}{t_e} \tag{9.1}$$

where *l* is the dislocation line length, and *A* is the total area swept by the dislocation during and after the crossing of the obstacle (Figure 9-1). In several cases, the obstacles controlling dislocation motion can be represented by energy barriers ΔG_o of the order of 1 eV. In these conditions, the thermal energy can facilitate the traversing of these obstacles.

Considering the dislocation comprises N atoms as a group of harmonic oscillators with fundamental frequency ν_0, $\nu_0 = \nu_D(b/l)$ where ν_D is Debye frequency, we obtain from statistic mechanics theory that the probability of success per unit time of a coherent motion by thermal activation is given by (*Granato et al., J. Appl. Phys. 35 (1964) p.2732)*:

$$P \approx \nu_0 \exp\left(-\frac{\Delta G}{kT}\right) \tag{9.2}$$

where $\Delta G = \Delta G(\sigma, T)$ is the minimum variation of free energy necessary to move the dislocation reversibly from the equilibrium position *R(0)* to the local maximum position $R_2(c)$ (Figure 9-3a). This energy is taken from the thermal vibration of the lattice. It is lower the higher the stress applied, because work is done by stress and temperature. Considering that all obstacles are identical and they are crossed independently, we have:

$$Pt_e = 1$$

So the expression for the mean speed is: $\bar{V} = \left(\frac{A}{l}\right)P$

From this, we finally have the following:

$$\dot{\varepsilon} \approx \Lambda_m A v_D \left(\frac{b}{l}\right)^2 \exp\left(-\frac{\Delta G}{kT}\right) = \dot{\varepsilon}_0 \exp\left(-\frac{\Delta G}{kT}\right) \tag{9.3}$$

Remark:

Inverting relation (9.3), we have:

$$\Delta G = kT log\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right) \tag{9.4}$$

where the pre-exponential term $\dot{\varepsilon}_o$ depends essentially on the substructure of dislocations and on the quantities Λ_m, ***l,*** and *A.* These evolve in general slowly with the temperature *T* and the stress σ during strain tests at an imposed strain rate, i.e., for $\dot{\varepsilon} \approx$constant:

$$\Delta G = \alpha kT \tag{9.5}$$

where $\alpha = log(\dot{\varepsilon}_0 / \dot{\varepsilon})$ has a typical value ranging from 20 to 30. Taking for example $A \sim l^2$, we have $\dot{\varepsilon}_0 = \Lambda_m b^2 v_D$ and as typical values $\Lambda_m = 10^{12}$ m/m^3, b=3·10^{-10} m, v_D = 10^{13} s^{-1} and $\dot{\varepsilon} = 10^{-4}$ s^{-1}, we obtain:

$$\alpha = ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right) \approx 23 \tag{9.6}$$

9.3 Gibbs free energy calculation during the crossing of an obstacle

To find the expression for the variation in Gibbs free energy a dislocation incurs crossing an obstacle, we follow subsections of the fundamental articles by Schoeck (*Phys. Stat. Sol. 8 (1965) p. 499)* and by Hirth and Nix*(Phys. Stat. Sol. 35 (1969) p. 177)* and describe them below.

9.3.1 Analysis in terms of applied stress

a) Gibbs free energy is required for crossing an obstacle.

Consider the simplified case in which the crystal contains only two dislocations, (1) and (2). The position and configuration are represented symbolically by *R1* and *R2.* The dislocation (2) represents the mobile dislocation, whereas (1) represents the origin of internal stresses f_i and is assumed sessile while dislocation (2) moves. The thermodynamic system considered here includes the crystal and the external sources to which it is linked. We then fix the force F_a, the temperature *T,* and the pressure *P* applied to the crystal. Let a length ***l*** of dislocation (2) move by *dR2* in a quasistatic and isothermal manner. We assume here that ***l*** is constant. We also suppose that dislocation (2) crosses a local "obstacle" during the displacement, in which a force f0 represents the interaction force. The work done by the system to displace the mobile dislocation (2), in other words, the work needed to move the two margins of the cut surface, one with respect to the other, is given by the following expression:

$$dW = f_0(T, R_2, \sigma_a)dR_2 + f_i(R_1, R_2)dR_2 - \sigma_a(T, R_2)bldR_2 + F_a(T)dx - PdV \tag{9.7}$$

In this expression:

- $f_0(T, R_2, \sigma_a)dR_2$ is the variation of elastic energy due to the obstacle. The force f_0 is a way to model the interaction of dislocation (2) with the obstacle. Suppose f0 has a meaning in the case of a purely elastic interaction. In that case, it only represents an image of mechanisms such as jog deformation and dislocation deviations.

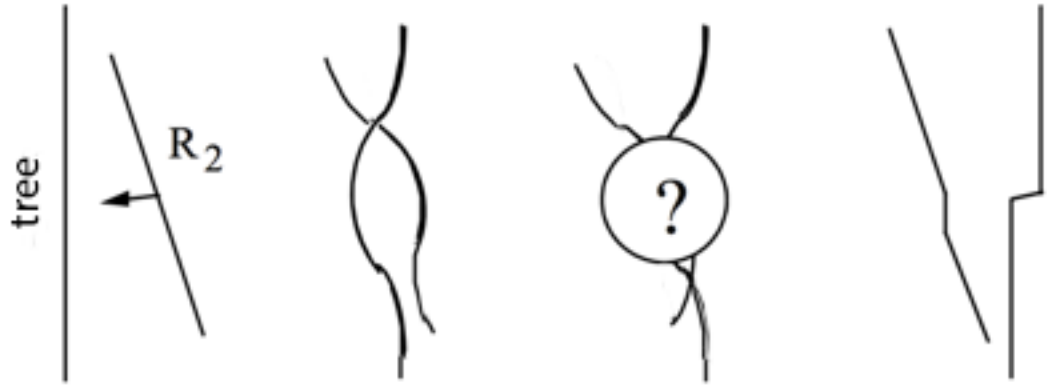


Figure 9-2: *Diagram of the interaction with a dislocation of the forest*

- $f_i(R_1, R_2)dR_2$ is the work due to the internal stresses acting on the cut surface in the direction opposed to *b*. Because of its delocalized character, the force f_i cannot correspond to any thermal activation. It does not explicitly depend on temperature T, but it could implicitly depend on it through R_1.
- $\sigma_a(T, R_2)bldR_2$ is the work of the external force F_a on the cut surface in the direction of *b* according to the Peach and Koehler equation (7.31). This term has a negative sign because its internal energy decreases when the dislocation exits the crystal.
- PdV is the work of the external pressure (if the displacement creates a change in the volume of the crystal)
- $F_a(T)dx$ is the work of the external force F_a if its application point moves by *dx* due to the dislocation (2) displacement.

We can prove (Colonnetti's theorem) that:

$$F_a(T)dx - \sigma_a(T, R_2)bldR_2 = 0 \tag{9.8}$$

This means that in practice, and without friction, the crystal's energy variation is zero when the dislocation is extracted. However, if the displacement of dislocation (2) occurs in a reversible and isothermal way, the internal energy variation of the crystal is:

$$dE = TdS + dW = TdS + f_i dR_2 + f_0 dR_2 - PdV \tag{9.9}$$

where *dS* is the entropy variation of the system due to the change in the volume of the crystal and to the change in the vibrational states caused by the introduction of f_i and f_0.

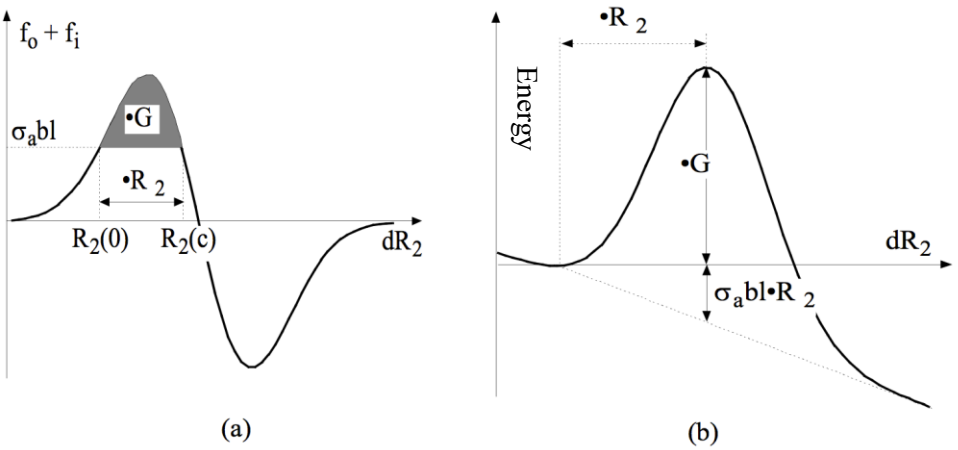


Figure 9-3: *Force-displacement (a) and energy-displacement diagram (b) during the crossing of an energy barrier*

The Gibbs Free energy of the system is defined by:

$$G_a = E + PV - TS - F_a x \tag{9.10}$$

Its variation is then, by using the previous relations and with the conditions: $F_a = const$, $P = const$, $T = const$, $R_1 = const$:

$$dG_a = f_0 dR_2 + f_i dR_2 - \sigma_a bl dR_2 \tag{9.11}$$

By comparing this expression with equation (9.9), we note that the dislocation displacement (without friction) does not change the internal energy but the free energy. Consider now the case in which dislocation (2) goes from an equilibrium position $R_2(0)$ to a local maximum position $R_2(c)$, and we have the following relations:

$$\Delta G_a = \int_{R_2(0)}^{R_2(c)} \left(\frac{\partial G_a}{\partial R_2} \right) dR_2 = \int_{R_2(0)}^{R_2(c)} [f_0 + f_i - \sigma_a bl] dR_2$$

or

$$\Delta G_a = \int_{R_2(0)}^{R_2(c)} (f_0 + f_i) dR_2 - \sigma_a bl \Delta R_2 \tag{9.12}$$

where $\Delta R_2 = R_2(c) - R_2(0)$

b) The activation volume

Considering the state variables σ_a and T, we can write:

$$d(\Delta G_a) = \left. \frac{\partial \Delta G_a}{\partial \sigma_a} \right|_{T,P,R_1} d\sigma_a + \left. \frac{\partial \Delta G_a}{\partial T} \right|_{\sigma_a,P,R_1} dT \tag{9.13}$$

The quantity $(\Delta G_a)/\sigma_a$ being homogeneous to a volume, we define thus an activation volume:

$$V_a = -\left. \frac{\partial \Delta G_a}{\partial \sigma_a} \right|_{T,P,R_1} \tag{9.14}$$

By expression (9.12) for ΔG_a:

$$V_a = -\frac{\partial}{\partial \sigma_a}\left(\int_{R_2(0)}^{R_2(c)} [f_0 + f_i - \sigma_a bl] dR_2\right) \tag{9.15}$$

Using Leibniz formula

$$\frac{\partial}{\partial y}\left(\int_{a_0(y)}^{a_1(y)} g(x,y)dx\right) = g(a_1,y)\frac{\partial a_1}{\partial y} - g(a_0,y)\frac{\partial a_0}{\partial y} + \int_{a_0}^{a_1}\frac{\partial g(x,y)}{\partial y}dx \tag{9.16}$$

We obtain:

$$V_a = -\left.\frac{\partial \Delta G_a}{\partial R_2}\right|_{R_2(c)}\frac{\partial R_2(c)}{\partial R_2} + \left.\frac{\partial \Delta G_a}{\partial R_2}\right|_{R_2(0)}\frac{dR_2(0)}{d\sigma_a} - \int_0^c \frac{\partial}{\partial \sigma_a}[f_0 + f_i - \sigma_a bl]dR_2 \tag{9.17}$$

The first two terms of (9.17) are zero because $R_2(0)$ and $R_2(c)$ are equilibrium points (maxima or minima), and thus $\left(\frac{\partial \Delta G_a}{\partial R_2}\right)_{F_a,P,T,R_1} = 0$

Therefore:

$$V_a = bl\Delta R_2 - \int_0^c \frac{\partial f_0}{\partial \sigma_a}dR_2 \tag{9.18}$$

In the case of a rigid obstacle - in other words- when the interaction force between the obstacle and the dislocation does not depend on the applied stress σ_a, or when the form of the energy barrier (Figure 9-3b) does not depend on σ_a, we have:

$$V_a = bl\Delta R_2 \tag{9.19}$$

where $l\Delta R_2$ represents the area swept by the dislocation during the activation (Figure 9-1).

Remarks:

- When V_a is expressed in b^3 units (~ atomic volume), this represents essentially the number of atoms the activation involves.
- The variation of Gibbs free energy can be written in a first-order approximation as:

$$\Delta G_a = \Delta G_0 + \sigma_a\left(\frac{\partial \Delta G_a}{\partial \sigma_a}\right) = \Delta G_0 - \sigma_a V_a \tag{9.20}$$

or

$$\Delta G_0 = \sigma_a V_a + kT\ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right) \tag{9.21}$$

The first term on the right of (9.21) represents the portion associated with the work done by the applied stress, and the second term represents the thermal energy contribution.

During the process of crossing an obstacle, stress and temperature share the work." Suppose, in principle, that dislocations can cross any obstacle only by applying stress (i.e., a sufficiently strong force below the decohesion force of the crystal). Moreover, it is not always the case that overcoming an obstacle is facilitated by increasing temperature. The number of atoms involved in overcoming obstacles should not be too high because the probability of exciting them simultaneously by thermal agitation is low. Therefore, the thermal activation theory applies only to small obstacles and is thus very localized. For thermal activation to have a significant impact, the two previous contributions must be of the same magnitude. That is, for $\Delta G_o \sim 1$ eV, we must be within a temperature range such that (see equations (9.6) and (9.21)):

$$25\ kT \sim 0.5\ eV \rightarrow T \sim 230\ K \quad \text{(let s say below } T_{amb}\text{)}$$

and a stress range:

$$\sigma_a V_a = 0.5\ eV \sim 0.1\ \mu b^3$$

That is to say $\sigma_a \sim 10^{-2}\ \mu$ for $V_a = 10\ b^3$ to $\sigma_a \sim 10^{-4}\ \mu$ for $V_a = 1000\ b^3$.

Remarks:

- V_a is not the true thermodynamic activation volume ΔV defined by:

$$\Delta V = -\left.\frac{\partial \Delta G_a}{\partial P}\right|_{T, F_a} \tag{9.22}$$

In fact, V_a does not correspond to a real volume change but a shape change.

- σ_a has an impact on ΔG_a only through the force per unit length $\sigma_a b$, and thus V_a always has the absolute value of the Burgers vector b as a factor. To avoid any confusion, we often define an activation area:

$$A_a = -\left.\frac{1}{b}\frac{\partial G_a}{\partial \sigma_a}\right|_{T, P, R_1} \tag{9.23}$$

The entropy change or activation entropy is defined by:

$$\Delta S_a = -\left.\frac{\partial \Delta G_a}{\partial T}\right|_{\sigma_a, P, R_1} \tag{9.24}$$

and the variation of activation internal enthalpy is:

$$\Delta H_a = \Delta G_a + T\Delta S_a = \Delta G_a - T\left.\frac{\partial \Delta G_a}{\partial T}\right|_{\sigma_a, P, R_1} = \left.\frac{\partial (\Delta G_a / T)}{\partial (1/T)}\right|_{\sigma_a, P, R_1} \tag{9.25}$$

ΔH_a defined in (9.25) only differs from the free enthalpy variation ΔG_a when the latter depends on T. The sources of entropy come from the dependency of ΔG_a with temperature and are essentially the following:

- The variation of the elastic constants C_{ij} constitutes the most significant contribution (*Basinski, Phil. Mag. 4 (1958) p. 393*).
- the creation of point defects, $\Delta S_a \sim k$ (see 4.43), which is then generally negligible.

- The variation of the vibration frequencies of the neighboring atoms of the dislocation when the dislocation crosses the obstacle. This term is poorly known.
- The thermal dilatation of the lattice is typically an order of magnitude smaller than the one due to the change in elastic constants (*Surek et al., Scripta Met. 7 (1973) p. 1131).*

We again use the Leibniz relation (9.16) and the fact that we consider σ_a to be constant, we have:

$$\Delta S_a = -\int_0^c \frac{\partial}{\partial T}[f_0 + f_i]dR_2$$

In the majority of cases, f_0 and f_i are proportional to the shear modulus μ and vary with temperature as μ(T), so that we can write:

$$f_0(T, \sigma_a, R_2) = \mu h(\sigma_a, R_2) \text{ and } f_i(R_1, R_2) = \mu f_\mu(R_2)$$

where *h* and f_μ do not explicitly depend on temperature, so that:

$$\Delta S_a = -\frac{\partial \mu}{\partial T}\int_0^c [h + f_m u]dR_2$$

From which expression (see (9.12) and (9.20)):

$$\Delta S_a = \frac{\Delta H_a + \frac{T}{\mu}\frac{\partial \mu}{\partial T}(\sigma_a V_a)}{1 - \frac{T}{\mu}\frac{\partial \mu}{\partial T}} \tag{9.26}$$

Finally, the activation parameters previously defined must satisfy the compatibility relations:

$$\left.\frac{\partial V_a}{\partial T}\right|_{\sigma_a, P, R_1} = \left.\frac{\partial \Delta S_a}{\partial \sigma_a}\right|_{T, P, R_1} \tag{9.27}$$

$$\left.\frac{\partial \Delta H_a}{\partial T}\right|_{\sigma_a, P, R_1} = T\left.\frac{\partial \Delta S_a}{\partial T}\right|_{\sigma_a, P, R_1} \tag{9.28}$$

9.3.2 Analysis in terms of effective stress

a) Introduction to an internal athermal" stress

Expression (9.21) of the energy barrier ΔG_o implies that, in a strain test at a constant strain rate, the elastic yield strength σ_a must vary with the temperature *T* following the relation:

$$\sigma_a = \frac{\Delta G_0}{V_a} - \frac{kT}{V_a}\ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)$$

This expression leads to the conclusion that beyond a specific critical temperature T_c equal to:

$$T_c(\dot{\varepsilon}) = \frac{\Delta G_0}{k\ln\left(\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}}\right)} \tag{9.29}$$

We must have $\sigma_a = 0$. At such temperatures, thermal energy is sufficient to overcome the energy barrier without the need for applied stress; the obstacles of height do not offer any resistance to the gliding of the dislocation. On the contrary, experience rather indicates a variation $\sigma_a(T)$ with a nonzero athermal asymptote. This suggests writing σ_a as the sum of two stresses (Seeger, *Dislocations and Mechanical Properties of Crystals*, John Wiley and Sons, (1957) p. 271):

• One is due to the localized obstacles, σ^* that is called the effective stress, which varies with temperature by thermal activation;
• The other is due to the internal" stress fields at long range, called internal stresses, which are responsible for the athermal asymptote.

$$\sigma^* = \sigma_a - \sigma_i \tag{9.30}$$

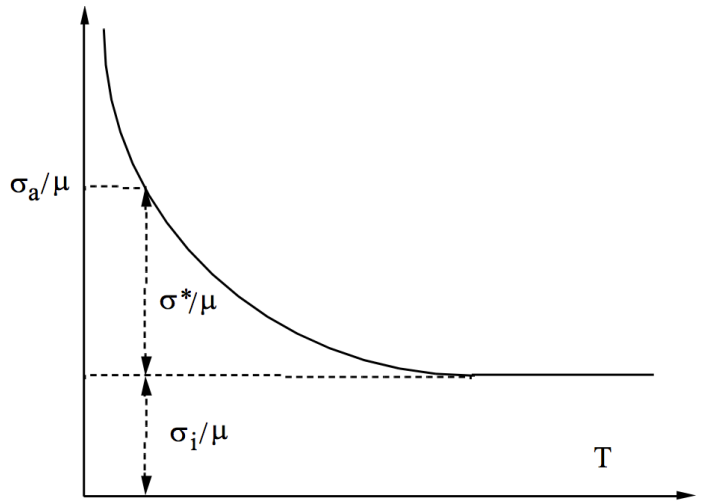


Figure 9-4: *Evolution of the elastic yield stress (normalized) or flow stress as a function of temperature. We can notice an athermal asymptote σ_i/μ.*

Remarks:

• Adding an effective stress σ^* and internal stress σ_i we can determine the applied stress σ_a implicitly, assuming that the stress fields of these two kinds of obstacles superpose in the crystal (Figure 9-5), i.e., the stress σ_i is essentially nonlocalized as opposed to σ^* .

• Consequently, the internal stress σ_i cannot correspond to any thermal activation. In other words, σ_i is explicitly independent of temperature. Nevertheless, σ_i can depend implicitly on temperature through the shear modulus μ, to which σ_i is proportional. We often measure then σ_i/μ by taking the value of the athermal asymptote of the curve σ_a/μ as a function of *T*.

• The internal stress σ_i can also depend on temperature, as the structure of the dislocation distribution varies with *T*. However, this dependency should be weak since the statistical character of σ_i is little affected by the details of this distribution.

• The internal stress σ_i, opposed to the displacement of the dislocations, is assumed constant, which is a reasonable assumption for a mobile dislocation having a displacement at least of the order of ***l*** (the size of the lattice parameter). As discussed in the previous chapters, the internal stress σ_i can be schematically represented as a stress field oscillating in space around a zero mean value, with a two-dimensional period of the order of ***l*** and amplitude (see 7.5.6):

$$\sigma_i \approx \alpha \frac{\mu b}{l}$$

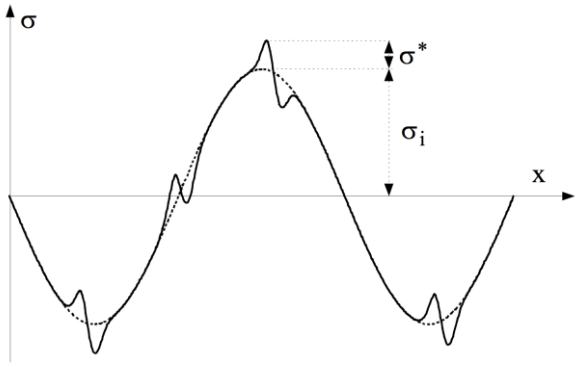


Figure 9-5: *Variation of the stress field as a function of dislocation displacement. Effective stress and internal stresses superpose.*

In this stress field, the dislocation has a curvature R^{-1} sufficient to avoid the zones of maximum σ_i

$$R \approx \frac{l}{\alpha} \quad \text{for a line tension } \tau = \mu b^2$$

For a displacement over a distance larger than or equal to l, it's difficult to cross zones where the stress σ_i is maximum. It is prevalent in studies on elastic yield stress and flow stress. In other studies for which the strains are small (the distances covered by the moving dislocations are small compared to the size of the Frank network), one must consider the internal effective" stress σ_i , which smooths those local variations.

9.4 Measure of thermodynamic quantities

Different experimental setups can determine the thermodynamic quantities at variable temperatures, stresses, or strain rates. In general, to minimize structural variations in the samples, we use techniques in which parameters can be readily varied or held constant.

Here, we consider the thermodynamic system of the entire sample, corresponding to the variables ($\dot{\varepsilon}, T$ and σ_a), on which the experimenter can act directly. These variables are measured using different tests, such as strain, one-dimensional axial tensile or compressive tests, or bending tests. Two principal tests exist: creep tests, in which we observe the strain rate as a function of time at several temperatures and stresses (held constant and referred to as dead-load tests), and strain tests at an imposed strain rate, in which we observe the stress as a function of the strain. These experiments can provide three kinds of parameters:

$$\left.\frac{\partial ln\dot{\varepsilon}}{\partial \sigma_a}\right|_T, \left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a}, \left.\frac{\partial \sigma_a}{\partial T}\right|_{\dot{\varepsilon}}$$

a) variation of the applied stress $\left.\frac{\partial ln\dot{\varepsilon}}{\partial \sigma_a}\right|_T$.

This parameter can be measured:

- by jumps in the strain rates (Figure 9-6a) or in the relaxation of the stress (Figure 9-6b) during strain tests done at imposed constant strain rates;
- by jumps in the stress during creep tests at constant temperature and stress (Figure 9-6c).

The kinetics of plastic deformation previously introduced are:

$$\Delta G_a = kT \ln \frac{\dot{\varepsilon}_0}{\dot{\varepsilon}} \qquad \text{that is} \qquad \ln \dot{\varepsilon} = -\frac{\Delta G_a}{kT} + \ln \dot{\varepsilon}_0$$

Recalling the expression of the activation volume V_a:

$$V_a = -\left.\frac{\partial \Delta G_a}{\partial \sigma_a}\right|_T$$

We can state that the quantity $V_{exp,}$ which is measured by strain rate jumps or stress jumps σ_a during a creep test, is:

$$V_{\exp} = kT \left.\frac{\partial \ln \dot{\varepsilon}}{\partial \sigma_a}\right)_T = V_a + kT \left.\frac{\partial \ln \dot{\varepsilon}_0}{\partial \sigma_a}\right)_T \tag{9.31}$$

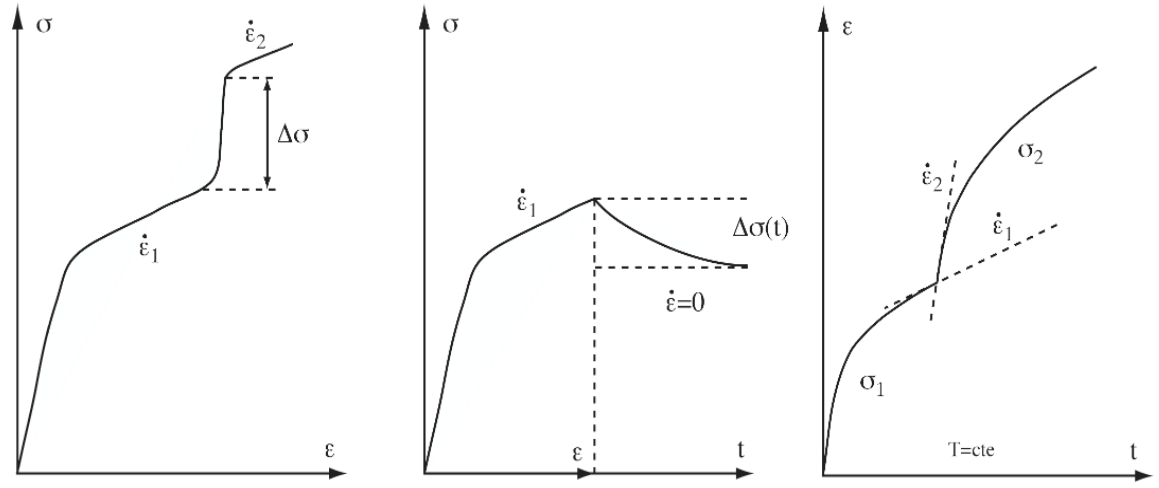


Figure 9-6: *Measure of the sensibility of the strain rate to the stress during imposed strain rate tensile testing: (a) by a jump in the strain rate, (b) by relaxation of the stress, (c) by a jump in the flow stress.*

Thus, the activation volume that is determined experimentally, V_{exp}, is only equal to the thermodynamic volume, V_a, when the pre-exponential term $\dot{\varepsilon}_o$ is often expressed as:

$$\dot{\varepsilon}_0 = B\sigma_a^m$$

With this assumption:

$$V_{exp} = V_a + kT\left(\frac{m}{\sigma_a}\right) \tag{9.32}$$

V_a is only accessible when the term $m\ kT/\sigma_a$ is negligible, i.e., generally far from the athermal plateau (where σ_a becomes small).

b) Temperature variations $\left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a}$

This parameter can be measured during tests at imposed stress (creep):

• by a jump in temperature (Figure 9-7a);

• by conventional tests done at different temperatures (Figure 9-7b)

During a creep test, we obtain for a temperature jump type measurement:

$$\left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a} = -\frac{1}{k}\left.\frac{\partial(\Delta G_a/T)}{\partial T}\right|_{\sigma_a} + \left.\frac{\partial ln\dot{\varepsilon}_0}{\partial T}\right|_{\sigma_a}$$

Now, we have that:

$$-\frac{1}{k}\left.\frac{\partial(\Delta G_a/T)}{\partial T}\right|_{\sigma_a} = \frac{1}{kT^2}\left.\frac{\partial(\Delta G_a/T)}{\partial(1/T)}\right|_{\sigma_a} = \frac{\Delta H_a}{kT^2}$$

We then measure the following:

$$\left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a} = \frac{\Delta H_a}{kT^2} + \left.\frac{\partial ln\dot{\varepsilon}_0}{\partial T}\right|_{\sigma_a}$$

With:

$$\Delta H_{exp} = kT^2\left.\frac{\partial ln\dot{\varepsilon}}{\partial T}\right|_{\sigma_a}$$

$$\Delta H_{exp} = \Delta H_a + kT^2\left.\frac{d\ln\dot{\varepsilon}_0}{dT}\right|_{\sigma_a} \qquad (9.33)$$

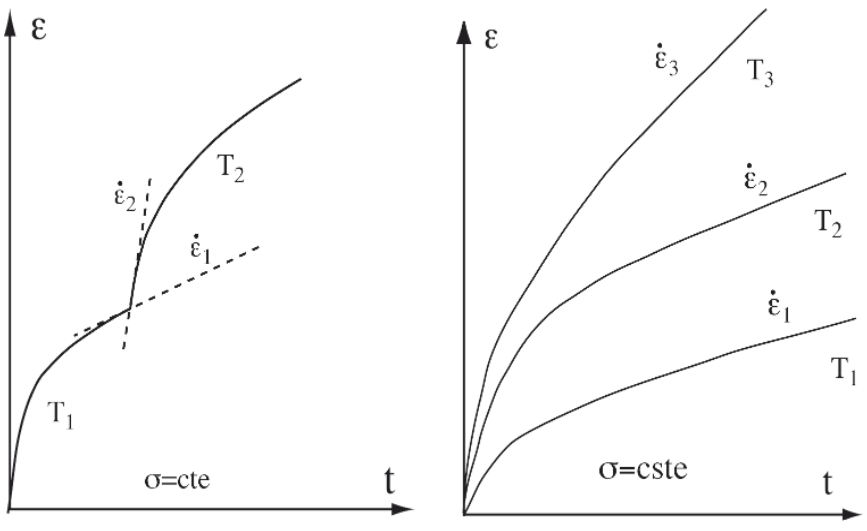


Figure 9-7: *Variation in the creep speed realized during tests at imposed stress (creep) (a) by stress jump and (b) by temperature jump*

9.5 Climb of dislocations

9.5.1 Introduction

For edge dislocations to move outside their glide plane, matter must be removed or added to its extra half-plane (Figure 9-8) and (Figure 9-9). Nevertheless, the formation energy of an interstitial, in general, is very high compared to that of a vacancy. As such, dislocation climb is exclusively mitigated by vacancy absorption or emission. The mechanism of dislocation climb can be deduced from the study of different fluxes of vacancies between the dislocation and potential sources or sinks of vacancies, which are a free external surfaces, grain boundaries, and dislocations. These fluxes obey Fick's law and can be driven by differences in concentration or the chemical potential of vacancies between different crystal sources.

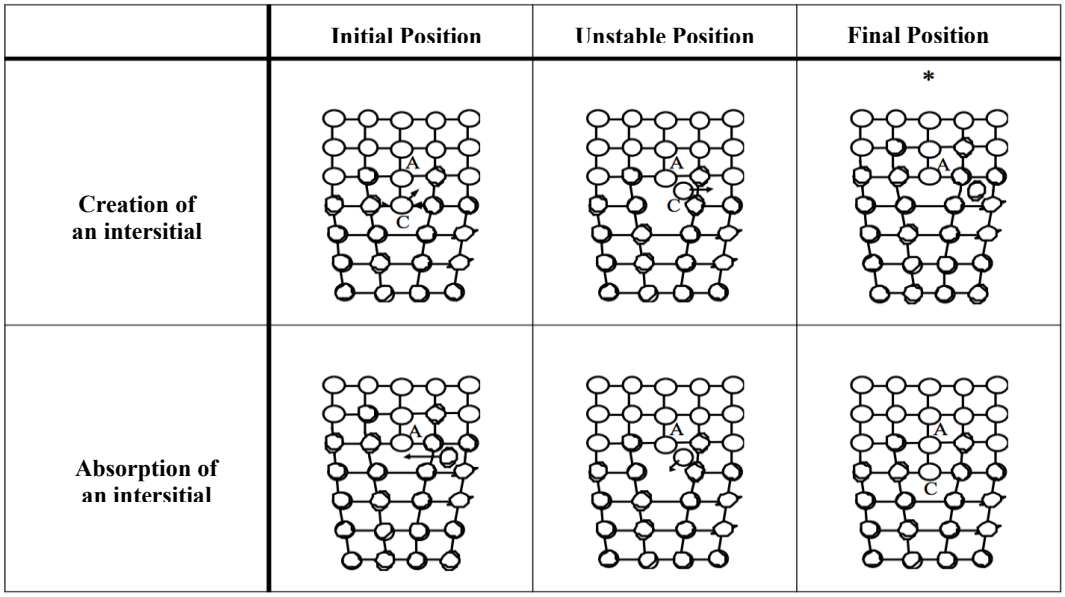


Figure 9-8: *Climb by interstitial mechanism (* indicates the metastable position)*

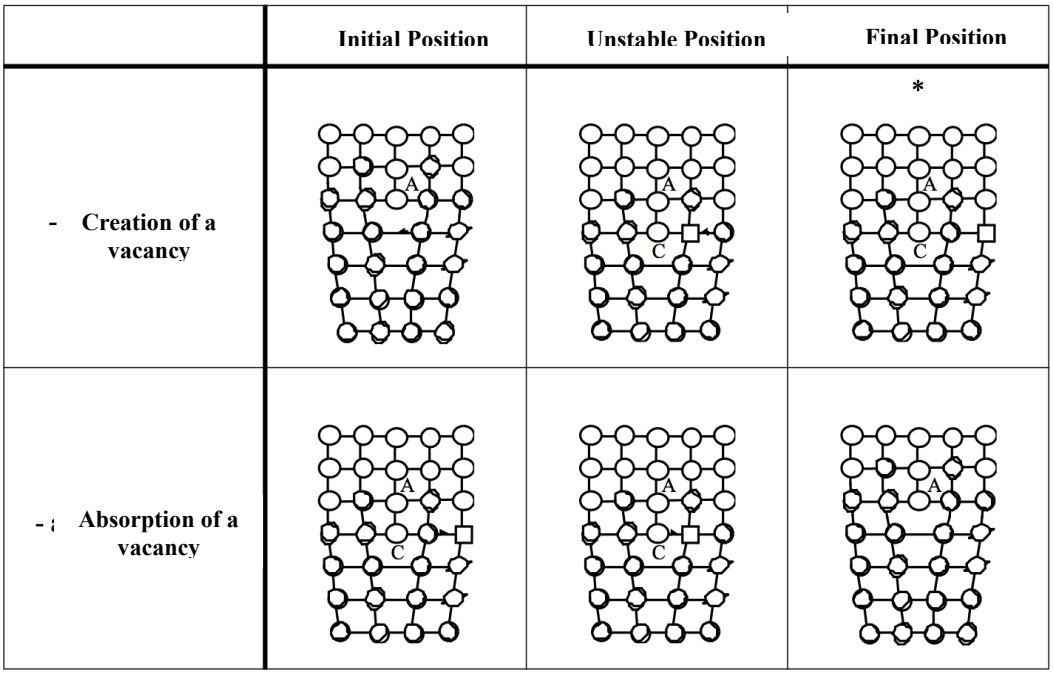


Figure 9-9: *Climb by vacancy mechanism (* indicates the metastable position)*

9.5.2 Geometric aspect of the climb

Any dislocation with an edge character can be considered the limit of an extra half-plane," even though the corresponding atoms are not all located in the same plane. Thus, the dislocation climb corresponds to the removal (or the supply) of a given number of atoms equal to the volume bounded between the two half-planes and by the dislocation line with thickness b, equal to the Burgers vector of the dislocation (Figure 9-10).

If the dislocation line L, with length $\boldsymbol{l}$, forms an angle ψ with its Burgers vector ($(\vec{\xi},\vec{b}) = \cos\psi$) and it moves perpendicularly to its glide plane (GP in the Figure) by a distance b, the volume of the absorbed (or emitted) atoms is:

$$V = (\ell\vec{\xi} \wedge \vec{b})\cdot\vec{b}'$$

We can understand this by considering the two extreme cases of an edge dislocation and a screw dislocation. In the first case, one atom is absorbed at each atomic site; in the second case, there is no need to absorb atoms, and there is no climb, only gliding.

To keep the notation simple, we suppose $b = b$ in what follows, and thus:

$$V_a = \ell b^2 \sin\psi$$

corresponding to the number of atoms N in the volume $\Omega = b^3$:

$$N = \frac{\ell}{b}\sin\psi$$

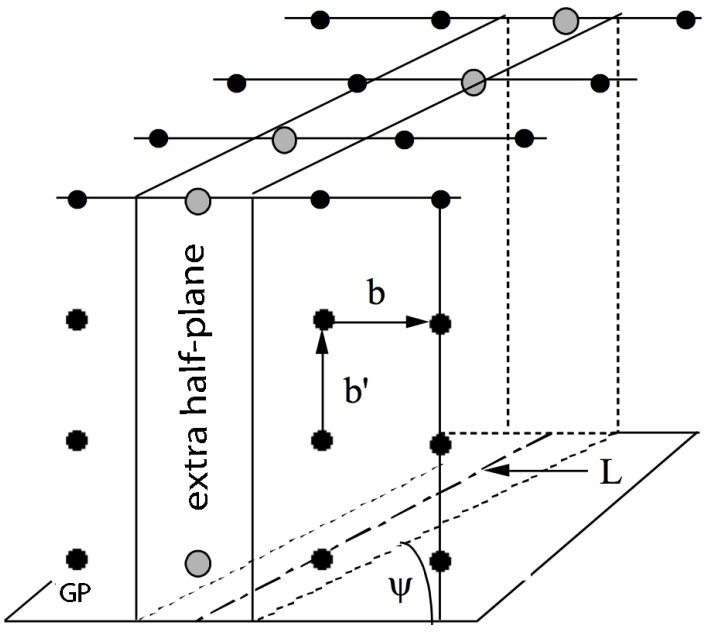


Figure 9-10: *Atoms and atomic planes involved in the climb of a dislocation*

The absorption (or the emission) of vacancies is principally done at the level of the existing jogs, which have a concentration C_j equal to the number of jogs on the line over the number of possible sites, that is:

$$C_j = \frac{n_j}{\left(\frac{\ell}{b/\sin\psi}\right)} = \frac{n_j b}{\ell \sin\psi} \tag{9.34}$$

Remark:

The distance $b/(\sin\psi)$ represents the displacement of a jog during the absorption (or the emission) of a vacancy. Nevertheless, only a distance of the order of b corresponds effectively to the vacancy's absorption (or emission) during the displacement. The rest corresponds to a simple jog sliding (see 9.5.5). In what follows, we consider an edge dislocation as simply $\sin\psi = 1$.

9.5.3 Forces on a Dislocation

The total force on a dislocation is obtained starting from the free energy of a crystal during the emission of the vacancy by the dislocation. The dislocation is a source of vacancies with potential μ_{Vd} (the chemical potential of vacancies on the dislocation), which becomes μ_{Vc} in the crystal, giving a change in free enthalpy:

$$dG = \mu_{Vc} - \mu_{Vd}$$

Several factors can influence this potential:

• Vacancy concentration C in the crystal is different from the equilibrium concentration C_V (4.28), which varies the source potential by: $kT \ln\left(\frac{C}{C_V}\right)$

• Application of a stress σ on the crystal. This creates an elastic force $F_e = \sigma b dl$ on the dislocation. We note that F_e represents the Peach-Koehler force components in the climb plane of the dislocation. It corresponds, for example, to a compression of the crystal, which pushes up the extra plane of an edge dislocation, like a wet bar of soap squeezed in your hand. We usually consider Fe to be positive if it promotes the emission of vacancies from the dislocation. The work of the force F_e during the creation of vacancies is given (see section (7.5.1)) by the product of the force σb and the swept area dA during the displacement of a jog:

$$dA = b^2 \tag{9.35}$$

We then have the following:

$$\sigma b^3 \tag{9.36}$$

• Line tension. A dislocation showing a local curvature radius R, taken with a negative sign if the center of curvature is located in the extra half-plane, tends to emit vacancies to regain its equilibrium position. In this case, the line tension τ helps the formation of vacancies in the crystal. We know that $R = \tau/\sigma b$ (7.36). Thus, the chemical potential of the vacancy in the crystal decreases by a value equal to $(\tau b^2)/R$.

To summarize, if μ_{Vc} is the chemical potential of a vacancy in the crystal, we have:

$$\mu_{Vc} - \mu_{Vd} = kTln\left(\frac{C}{C_V}\right) - \sigma b^3 - \frac{\tau b^2}{R} \tag{9.37}$$

In the case of a straight dislocation, the variation of free energy during the creation of a vacancy is then:

$$dG = \mu_{Vc} - \mu_{Vd} = kTln\left(\frac{C}{C_V}\right) - \sigma b^3 \tag{9.38}$$

whereas the area swept by the line during this event equals:

$$dA = b^2$$

The quantity *dG/dA* has the units of a force per unit length and must then be considered as the force *F* per unit length applied on the dislocation line in its climb plane, that is, in this case:

$$\frac{F}{d\ell} = \sigma b - \frac{kT}{b^2}\ln\left(\frac{C}{C_V}\right) = F_e - F_s$$

where the first term, F_e, represents the force due to the stresses, and the second term comes from the over- or under-concentration of vacancies and is called oversaturation or chemical force:

$$\frac{F_s}{d\ell} = \frac{kT}{b^2}\ln\left(\frac{C}{C_V}\right) \tag{9.39}$$

The dislocation is in equilibrium when the force *F* is zero, which corresponds to a concentration of vacancies surrounding the dislocation equal to:

$$C = C_V \exp\left(\frac{\sigma b^3}{kT}\right) \tag{9.40}$$

and when the force *F* is nonzero, the dislocation moves in its climb plane. In the absence of thermal activation (*T*=0 K), the condition on the stress σ necessary for dislocation climb can be calculated by setting the work of the force *F* and the formation energy of a vacancy equal to each other, as follows:

$$\sigma b^3 = \Delta G_V^F$$

From which with $\mu b^3 \sim 5\,eV$ and $\Delta G_V^F \sim 1\,eV$ we get a stress σ within an order of a magnitude:

$$\sigma \approx \frac{\Delta G_V^F}{b^3} \approx \frac{\mu}{5}$$

That is close to the theoretical elastic yield stress (except for the dislocations closer to the screw type). We can deduce from this that the climb of dislocations is possible only via thermal activation. Therefore, it is a relevant phenomenon only at high temperatures.

9.5.4 Bardeen-Herring sources

We now consider the case in which the dislocation is bent without applying any force to the sample during the inflow of vacancies. The variation in free energy is given this time by:

$$dG = \mu_{Vc} - \mu_{Vd} = kT \ln\left(\frac{C}{C_V}\right) - \frac{\tau b^2}{R}$$

As before, *dG/dA* gives the force per unit length being applied on the dislocation:

$$\frac{F}{d\ell} = \frac{-kT}{b^2} \ln\left(\frac{C}{C_V}\right) + \frac{\tau}{R}$$

The line tension tends to bring back the dislocation to a straight configuration. Thus, the condition for which the dislocation can climb by the inflow of vacancies is only when:

$$\frac{\tau}{R} < \frac{kT}{b^2} \ln\left(\frac{C}{C_V}\right)$$

This mechanism is analogous to Frank-Read sources, but the oversaturation of vacancies does the climb. Thus, as already seen in 7.5.6b, taking $\tau = \alpha\mu b^2$ and $R \geq \frac{\ell}{2}$, we will have:

$$\ln\left(\frac{C}{C_V}\right) \geq \frac{2\alpha\mu b^4}{\ell kT} \tag{9.41}$$

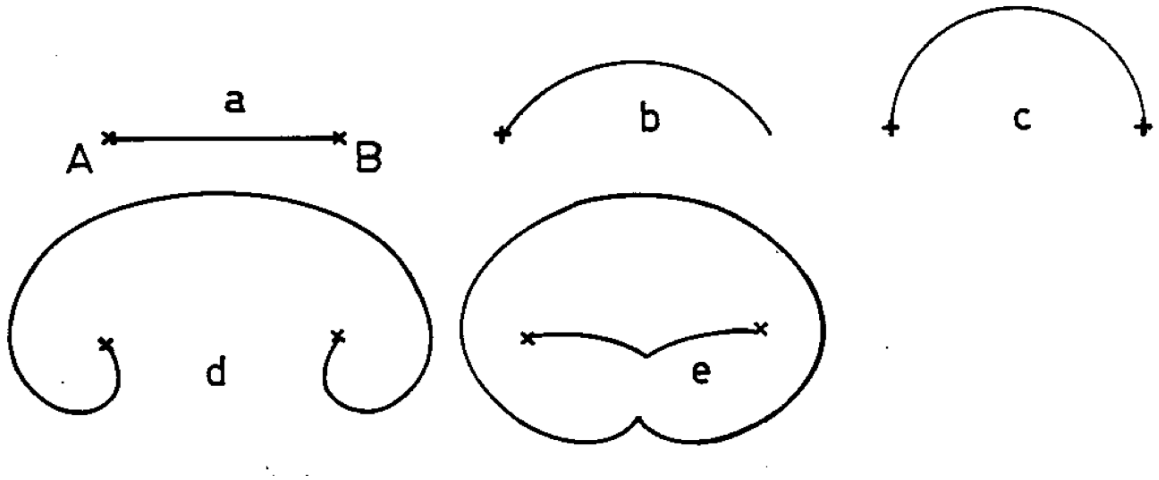


Figure 9-11: *Bardeen-Herring source by the climb of dislocations: the climb plane lies in the plane of the page*

Application

Aluminum: $\mu = 25\,[GPa], b = 2.3\,[\text{Å}], \ell = 10^{-6}\,[m], T = 500\,[K]$ implies $\frac{C}{C_V} \approx 1.02$. Thus, an oversaturation of 2% of vacancies can activate the sources with a length of 1 μm.

9.5.5 Velocity of the climb of a dislocation

We have seen that vacancies' absorption or emission occurs principally at the jogs. Therefore, we expect the dislocation climb velocity to be determined by the jog velocity.

a) General case

When a jog moves along a dislocation of length ***l***, the dislocation moves by a distance *b* in its climb plane (Figure 9-12).

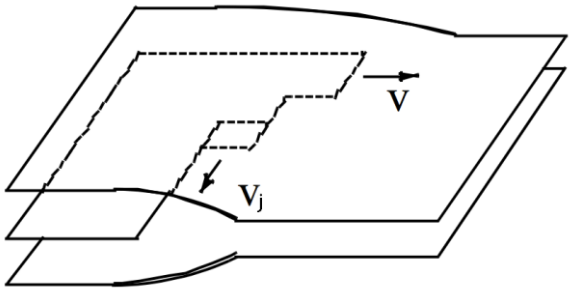


Figure 9-12: *Climb of dislocation by the forward motion of a jog*

If V_j is the displacement velocity of the jog, the climb velocity of dislocation V is given by:

$$V = \frac{b}{(\ell / V_j)} = \frac{bV_j}{\ell}$$

This result must be multiplied by the number of jogs (nj) along the dislocation line, that is, (see (9.34)):

$$V = \frac{bV_j n_j}{\ell} = C_j V_j \qquad (9.42)$$

In this formulation, the problem reduces to finding the velocity of the jogs. Then, each time that these absorb or emit a vacancy, they move by a distance *b* corresponding to a velocity:

$$V_j = b\Delta\nu \qquad (9.43)$$

where $\Delta\nu$ is the difference between the vacancy emission frequency and absorption frequency, $\Delta\nu = \nu_e - \nu_a$, hence:

$$V = bC_j\Delta\nu$$

We must then evaluate Δν. This calculation is performed for a pure edge dislocation, as an additional screw component would complicate the analysis.

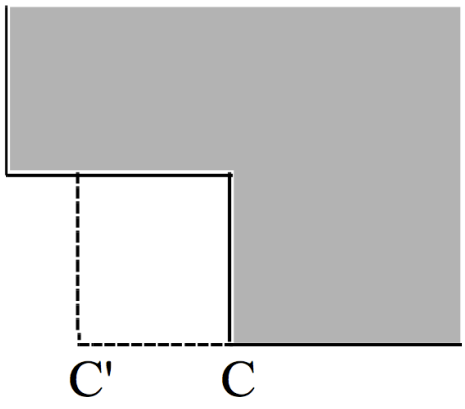


Figure 9-13: *Jog moving from C to C'*

b) Case of a jog on an edge dislocation

The emission frequency of vacancies is related to the enthalpy necessary for a jog to emit a vacancy.

This requires the jog to move from position C to position C (Figure 9-13), which requires a formation energy /.

In the presence of a force F_e, this energy decreases by σb^3 (the work the applied stress does when C goes to C).

In this unstable situation (Figure 9-9), the vacancy must switch sites with an atom from the lattice, resulting in an additional migration energy: ΔG_V^m. We can now obtain the emission frequency:

$$\nu_e = \exp\left[\frac{-\Delta G_V^F - \sigma b^3}{kT}\right] z\nu_D exp\left[\frac{-\Delta G_V^m}{kT}\right] \tag{9.44}$$

For a jog to absorb a vacancy, the latter must be on a neighboring site for the switch to occur. The absorption frequency then equals the frequency of the jumps times the probability of finding a vacancy in an adjacent site, which gives:

$$\nu_a = Cz\nu_D \exp\left[-\frac{\Delta G_V^m}{kT}\right] \tag{9.45}$$

In the absence of stress, we must have $\Delta\nu = 0$ at equilibrium, hence:

$$\exp\left[-\frac{\Delta G_V^F}{kT}\right] - C = 0$$

corresponding to an equilibrium concentration of:

$$C = C_V = exp\left[-\frac{\Delta G_V^F}{kT}\right]$$

If the concentration C is different from the equilibrium concentration C_V, we have (9.39):

$$C = C_V \exp\left[\frac{\frac{F_s}{d\ell} b^2}{kT}\right]$$

$$\nu_e - \nu_a = z\nu_D \exp\left[-\frac{\Delta G_V^m}{kT}\right]\left\{\exp\left[-\frac{\Delta G_V^F - \sigma b^3}{kT}\right] - C\right\} \tag{9.46}$$

Considering that (5.14):

$$z\nu_D \exp\left[-\frac{\Delta G_V^m}{kT}\right]\exp\left[-\frac{\Delta G_V^F}{kT}\right] = 6D_{SD}/b^2$$

We finally get:

$$\Delta\nu = \frac{6D_{SD}}{b^2}\left\{\exp\left[\frac{\sigma b^3}{kT}\right] - \exp\left[\frac{\frac{F_s}{d\ell} b^2}{kT}\right]\right\} \tag{9.47}$$

where D_{SD} is the self-diffusion coefficient.

Several cases can occur according to the values of σb^3 and $(F_s/d\ell)b^2$ with respect to kT.

i) σb^3 and $(F_s/d\ell)b^2 << kT$

By expanding the exponentials, we get the following:

$$\Delta v = 6D_{SD}\frac{\sigma b - F_s/(d\ell)}{kT} \quad \text{or else} \quad V = \frac{6D_{SD}C_j(\sigma b^2 - (F_s b)/(d\ell))}{kT} \tag{9.48}$$

It is Einstein s relation (see chapter 5.4). In this case, the activation energy is equal to the self-diffusion energy, possibly increased by the formation energy of jogs ($\Delta G_j \sim 0.1\,eV$).

ii) $\sigma b^3 >> kT$ and $(F_s/d\ell)b^2 << kT$

We have:

$$\Delta v = \frac{6D_{SD}}{b^2}\exp\left[\frac{\sigma b^3}{kT}\right] \quad \text{or else} \quad V = \frac{6D_{SD}C_j}{b}\exp\left[\frac{\sigma b^3}{kT}\right] \tag{9.49}$$

This case results in significant elastic forces, like those found at the front of a pileup of dislocations or those due to substantial dislocation concentrations. The activation energy is equal here to the self-diffusion energy minus the term σb^3 and possibly increased by the formation energy of a jog.

iii) $\sigma b^3 << kT$ and $(F_s/d\ell)b^2 >> kT$

In this case, we have:

$$\Delta v = -\frac{6D_{SD}}{b^2}\exp\left[\frac{b^2F_s/(d\ell)}{kT}\right] \quad \text{or else} \quad V = -\frac{6D_{SD}C_j}{b}\exp\left[\frac{b^2F_s/(d\ell)}{kT}\right] \tag{9.50}$$

We are here in the presence of an oversaturation of vacancies, Δv is negative, and the activation energy is reduced to the self-diffusion energy, possibly even decreased by the oversaturation term.

c) Particular case: jogs on a screw dislocation

If we consider jogs (outside the climb plane) on an edge dislocation, we can see that they cannot affect the dislocation's motion. On the contrary, for screw dislocations, jogs always have an edge character, and as a consequence, they can only move by climb if they are to preserve their Burgers vector. However, if the dislocations move in another plane, they can drag the jog segment, leaving a line of vacancies or interstitial defects, depending on the jog's sign.

If we consider the case in Figure 9-14, we can implement the form used in § 9.5.5a by taking into account that this time, the external stress acts on jogs of length ***l*** and, as a consequence $F_e = \sigma \ell \mathrm{b}$

$$\Delta v = \frac{D_{SD}}{b^2}\left\{\exp\left[\frac{\sigma \ell\, \mathrm{b}^2}{kT}\right] - \exp\left[\frac{b^2F_s/(d\ell)}{kT}\right]\right\} \tag{9.51}$$

If σb^3 and $(F_s/d\ell)b^2 << kT$, we have a relation of Einstein s kind:

$$\Delta v = \frac{D_{SD}}{b^2}\frac{\sigma b^2 \ell - \mathrm{b}^2F_s/(d\ell)}{kT} \quad \text{or else} \quad V = \frac{D_{SD}C_j b(\sigma \ell - F_S/(d\ell))}{kT} \tag{9.52}$$

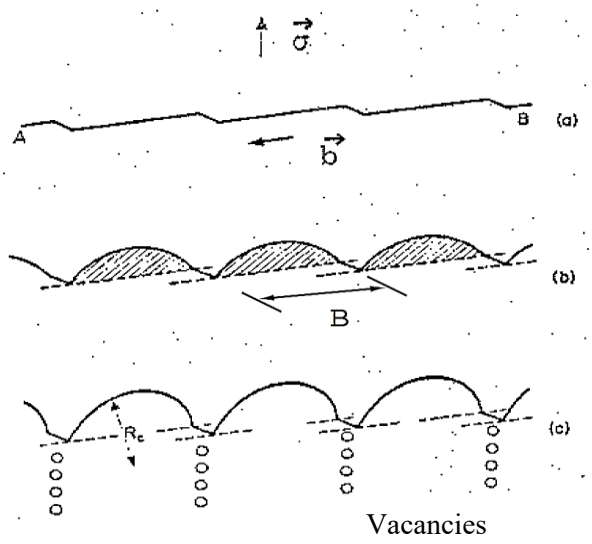


Figure 9-14: *Climb of a screw dislocation with jogs*

9.5.6 Climb governed by diffusion in the crystal

Until now, we have essentially considered that the absorption or the emission of vacancies by jogs controls the climb velocity of a dislocation. However, these velocities were relatively low compared to their arrival or departure speeds.

Inverting this approach, we can ask ourselves. What happens when the absorption velocity of vacancies is high compared to their arrival velocity? In this case, we can show that the climb of the dislocation depends on the self-diffusion coefficient and the activation volume of a vacancy σb^3.

We consider this a straight-edge dislocation in a crystal, and we suppose the vacancies have their equilibrium concentration C_V on a cylinder with a radius R_2 around the dislocation. In a radius R_1 of some multiples of b, the probability of absorbing the vacancy is assumed to be 1.

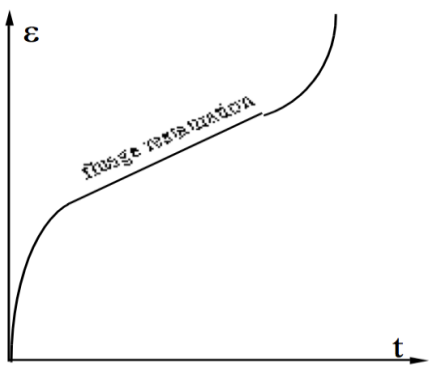
We get:

$$V = \frac{2\pi R_2 D_V C_V}{bR_1} \frac{\left(1-\exp\left(\frac{\sigma_n b^3}{kT}\right)\right)}{\ln\left(\frac{R_2}{R_1}\right)}$$

σ_n being the stress in the climb plane. Assuming $\sigma_n b^3 << kT$ (which is often a good approximation) and taking $R_1 \sim b$, we get:

$$V = \frac{2\pi D_V C_V}{bkT} \frac{\sigma_n b^3}{\ln\left(\frac{R_2}{R_1}\right)} = \frac{2\pi D_{SD}}{bkT} \frac{\sigma_n b^3}{\ln\left(\frac{R_2}{b}\right)} \tag{9.53}$$

9.5.7 Application to stationary creep



What we call stationary creep corresponds to the linear part of Figure 9-15. It occurs at higher stresses than in Nabarro-Herring creep (see exercise 6).

Most of the strain comes from the gliding of dislocations, during which obstacles progressively impede their motion. The climb of edge dislocations with non-screw character (or cross-slip for screw dislocations) can help release them and glide until the next obstacle.

Figure 9-15: *Creep curve*

The steady-state creep results in a dynamic equilibrium between blocking and releasing, meaning that the t_e gliding of dislocations is controlled by climb (or cross-slip) at the obstacles (Figure 9-16).

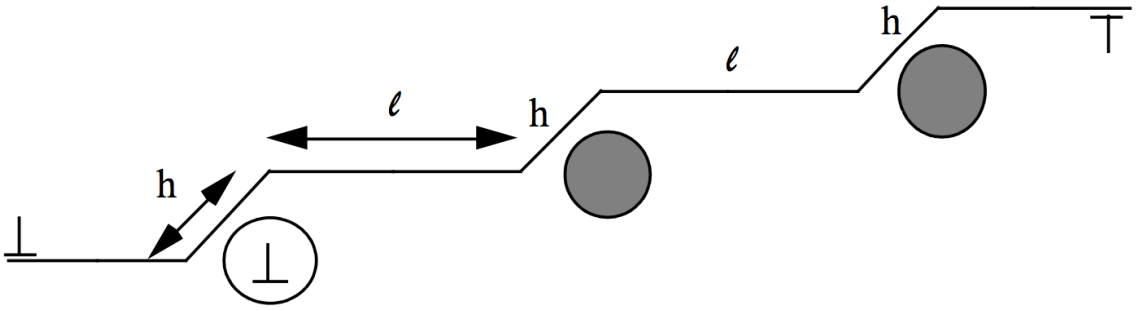


Figure 9-16: *Glide scheme of a dislocation crossing obstacles by climb motion*

The flight time or glide time t_g between two obstacles is very short compared to the escape time. On the other hand, the distance ***l*** between obstacles is larger than the distance *h* to be covered by climb (or cross-slip). The average velocity is then written as:

$$\bar{V} \approx \frac{\ell}{t_r + t_g} \approx \frac{\ell}{t_r} = \ell \frac{V_e}{h}$$

where $V_e = h/t_r$ is the escape velocity, a characteristic of the mechanism controlling dislocation release. Orowan s law gives here a strain rate of:

$$\dot{\varepsilon} = \Lambda_m b \ell \frac{V_e}{h} \tag{9.54}$$

If we consider that the obstacles are the dislocations of the forest and that the density ρ_m of mobile dislocations is a constant fraction of the total dislocation density Λ, and that the same goes for the forest s density Λ_m, then.

$$\Lambda_m \propto \Lambda_f \propto \Lambda \approx \frac{1}{\ell^2}$$

where ℓ is the mean distance between the obstacles. At steady state, we have:

$$\sigma \cong \sigma_i \propto \sqrt{\Lambda} \propto \sqrt{\Lambda_m}$$

which can be written in a non-dimensional form as a function of σ/μ:

$$\Lambda_m \propto \left(\frac{\sigma}{\mu}\right)^2 \tag{9.55}$$

We get the following:

$$\dot{\varepsilon} \propto \left(\frac{\sigma}{\mu}\right)^2 \ell \frac{V_r}{h} b$$

If finally, we admit that - even though ***l*** and *h* could depend on σ, (ℓ / h) does not:

$$\dot{\varepsilon} \propto \left(\frac{\sigma}{\mu}\right)^2 V_r b$$

This expression depends on the escape velocity V_e (this value was previously calculated for climb velocities). For example, in the case in which the relaxation mechanism is controlled by climb, governed by the diffusion in the crystal (9.53):

$$V = \frac{2\pi D_{SD}}{bkT} \frac{\sigma_n b^3}{\ln\left(\frac{R}{b}\right)}$$

We then get:

$$\dot{\varepsilon} = A \frac{\sigma^3}{kT} \exp\left(-\frac{H_{SD}}{kT}\right) \tag{9.56}$$

This type of creep is only an example. More refined assumptions can lead to equations that generally have the form (Dorn law):

$$\dot{\varepsilon} = A\sigma^n \exp\left(-\frac{H}{kT}\right) \tag{9.57}$$

with exponents for the stress that could be different than $n = 3$.