Philosophical Magazine
First published in 1798

One-dimensional models of thermal activation under shear stress

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ABSTRACT

The analysis of thermal activation under shear stress in three- and even two-dimensional models presents unresolved problems. The analysis of one-dimensional models presented here may illuminate the study of more realistic models. For the model in which as many dislocations are poised for backward jumps as for forward jumps, the experimental activation volume $V^{\dagger e}(\sigma_a)$ under applied stresses close to σ_a is different from the true activation volume $V(\sigma)$ evaluated at $\sigma = \sigma_a$. The relations between the two are developed. A model is then discussed in which fewer dislocations are available for backward than for forward jumps. Finally, the appropriateness of the hyperbolic sine approximation for moderately low stresses is defined and shown to be very limited.

§ 1. INTRODUCTION

A formal general theory of thermal activation of deformation by the motion of dislocations under a shear stress was presented for example by Kocks *et al.* (1975). In practice the process is usually three dimensional, but the analysis in three dimensions is still intractable. There has been more success in a two-dimensional model (Kocks 1984), with an analysis that relates closely to the experimental observations. Nevertheless, the difficulties of even a two-dimensional model are apparent. It is not completely analytic; an important parameter, the ratio of the average spacing of 'hard' groups of point obstacles to the average spacing of these point obstacles is derived from a computer simulation. The simulation itself is hardly realistic, since (Labusch 1970) the finite widths of real obstacles to dislocation motion usually lead to a behaviour substantially different from that in the presence of point obstacles. While a one-dimensional model is physically unrealistic, its behaviour can be studied with some precision and may indicate some considerations which will be relevant in more realistic models.

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In §2 the conventional theory of the activation volume, or, in one dimension, the activation distance, is outlined. This analysis holds when dislocations are driven forwards over obstacles by the applied stress, and backward jumps may be neglected. This leads to the idea of the experimental activation volume defined by equation (6). In §3 the conventional theory at low stresses, where backward jumps are also considered, is developed. In general, the true activation volume depends on the stress σ as $V(\sigma)$. The experimental activation volume $V^{\dagger e}(\sigma_a)$ measured in the neighbourhood of an applied stress σ_a then differs from $V(\sigma_a)$, as shown in equation (12). In principle, $V(\sigma_a)$ may be derived from a series of measurements of $V^{\dagger e}(\sigma)$ between $\sigma = 0$ and $\sigma = \sigma_a$ by means of equation (21).

The conventional model of dislocations jumping forwards and backwards over isolated obstacles is not physically realistic. There is no steady state. A dislocation which has jumped forward over its obstacle runs away to infinity, and there are no dislocations poised to jump backwards. A more realistic model pictures a periodic sequence of isolated obstacles, as envisaged by Evans and Rawlings (1969). In a quasistatic steady state, the same thermal energy which activates dislocations over obstacles ensures that some dislocations will be poised for backward jumps. This situation is analysed in §4. Finally, §5 confirms the statement of Schoeck (1965) that 'the indiscriminate use of a sinh function to take account of the back fluctuations . . . is not . . . justified'.

§2. THE EXPERIMENTAL ACTIVATION VOLUME

As Cahn and Nabarro (2001) have shown, the activation volume is actually a tensor quantity $V_{ij}^{\dagger}$ but, if the applied stress has only the two components $\sigma_{ij} = \sigma_{ji}$, the suffices i and j may be dropped. We consider only the case of a system which is described by a single reaction coordinate x. The potential energy of the system $U(x)$ has a hump at $x = 0$ (figure 1), and the system experiences a force

$$F(x) = \frac{\mathrm{d}U(x)}{\mathrm{d}x} \tag{1}$$

opposing its forward motion. This force has a maximum value F_m, and a force F_a is applied to the system. It is assumed that $F(x)$ is negligibly small when $|x| > x_m$. It is convenient to shift the origin of coordinates so that the new coordinate X is zero where $\mathrm{d}F(X)/\mathrm{d}X = 0$. Then the system is in stable equilibrium at $X = X_-(F_a)$ and in unstable equilibrium at the saddle point $X = X_+(F_a)$.

We define the activation distance $L^{\dagger}(F_a)$ by

$$L^{\dagger}(F_a) = X_+(F_a) - X(F_a), \tag{2}$$

and the activation enthalpy for a forward jump is

$$H_+^{\dagger}(F_a) = \int_{F_a}^{F_m} L^{\dagger}(F_a)\,\mathrm{d}F_a. \tag{3}$$

For a three-dimensional problem described by a single reaction coordinate, $L_+^{\dagger}$ is replaced by an activation volume $V^{\dagger}$. In the case of a dislocation segment approaching an obstacle on its glide plane, $V^{\dagger}$ is the product of the magnitude b of the Burgers vector and the area of the glide plane swept by the segment during the
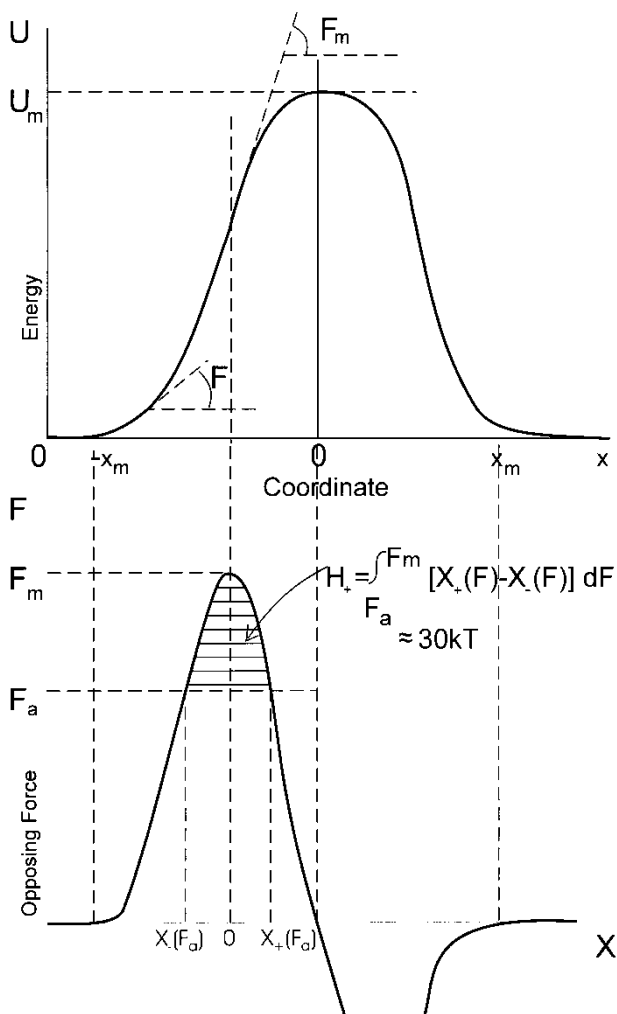
Figure 1. In the upper half of the figure, the energy U is plotted as a function of the coordinate x, with $x = 0$ at the position of maximum energy. In the lower part, the opposing force F is plotted as a function of the coordinate X, with $X = 0$ at the position of maximum opposing force.

activation process, while F_a is the product of b, the resolved shear stress σ_a and the length ℓ of the dislocation segment. Then

$$H_+^{\dagger}(\sigma_a) = \int_{\sigma_a}^{\sigma_m} V_+^{\dagger}(\sigma)\, d\sigma. \tag{4}$$

The rate $\dot{\varepsilon}$ of plastic deformation as a result of the activation of forward jumps may be written

$$\dot{\varepsilon}(\sigma_a) = \dot{\varepsilon}_0 \exp\left(\frac{-H_+^{\dagger}(\sigma_a)}{kT}\right). \tag{5}$$

We define the experimental activation volume $V^{\dagger\mathrm{e}}$ by

$$V^{\dagger\mathrm{e}}(\sigma_{\mathrm{a}}) = kT\left(\frac{\partial \ln \dot{\varepsilon}}{\partial \sigma_{\mathrm{a}}}\right)_T. \tag{6}$$

If $\dot{\varepsilon}_0$ depends negligibly on σ_{a}, this leads to

$$V^{\dagger\mathrm{e}}(\sigma_{\mathrm{a}}) = V^{\dagger}_{+}(\sigma_{\mathrm{a}}). \tag{7}$$

§3. BEHAVIOUR AT LOW STRESSES

Equation (5) cannot hold at low applied stresses, whatever physical model is considered. This would imply a steady directed process in the absence of an applied stress, contrary to the principle of detailed balance, and a forward strain rate under a small backward stress, contrary to the laws of thermodynamics. The theory must incorporate the possibility that backward jumps will occur as well as forward jumps. If we assume the systems to be symmetrical, and that backward and forward jumps can be treated on the same basis, the rate of strain is given by

$$\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} = \exp\left(\frac{-H^{\dagger}_{+}(\sigma_{\mathrm{a}})}{kT}\right) - \exp\left(\frac{-H^{\dagger}_{-}(\sigma_{\mathrm{a}})}{kT}\right) \tag{8}$$

where

$$H^{\dagger}_{-}(\sigma_{\mathrm{a}}) = \int_{-\sigma_{\mathrm{m}}}^{\sigma_{\mathrm{a}}} V(\sigma)\,\mathrm{d}\sigma. \tag{9}$$

The symmetry of the potential $V(\sigma)$ allows $H^{\dagger}_{+}$ and $H^{\dagger}_{-}$ to be written in the forms

$$H^{\dagger}_{+}(\sigma_{\mathrm{a}}) = \int_{0}^{\sigma_{\mathrm{m}}} V(\sigma)\,\mathrm{d}\sigma - \int_{0}^{\sigma_{\mathrm{a}}} V(\sigma)\,\mathrm{d}\sigma \tag{10 a}$$

and

$$H^{\dagger}_{-}(\sigma_{\mathrm{a}}) = \int_{0}^{\sigma_{\mathrm{m}}} V(\sigma)\,\mathrm{d}\sigma + \int_{0}^{\sigma_{\mathrm{a}}} V(\sigma)\,\mathrm{d}\sigma. \tag{10 b}$$

It follows that

$$\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \exp\left(\int_{0}^{\sigma_{\mathrm{m}}} \frac{V(\sigma)}{kT}\,\mathrm{d}\sigma\right) = 2\sinh\left(\int_{0}^{\sigma_{\mathrm{a}}} \frac{V(\sigma)}{kT}\,\mathrm{d}\sigma\right). \tag{11}$$

As was made clear by Argon (1996), equation (7) holds only when σ_{a} is so close to σ_{m} that the frequency of backward jumps can be neglected in comparison with that of forward jumps. When this is not the case, equation (7) is replaced by

$$V^{\dagger\mathrm{e}}(\sigma_{\mathrm{a}}) = V(\sigma_{\mathrm{a}}) \coth\left(\int_{0}^{\sigma_{\mathrm{a}}} \frac{V(\sigma)}{kT}\,\mathrm{d}\sigma\right). \tag{12}$$

If $V^{\dagger}(\sigma)$ tends to a constant value $V^{\dagger}(0)$ as σ_{a} tends to zero, the integral in equation (12) tends to $\sigma_{\mathrm{a}} V^{\dagger}(0)/kT$, and equation (8) becomes

$$V^{\dagger\mathrm{e}}(\sigma_{\mathrm{a}}) = \frac{kT}{\sigma_{\mathrm{a}}}. \tag{13}$$

Experimental observations often fit a power-law relationship

$$\dot{\varepsilon} \propto \sigma_\mathrm{a}^n. \tag{14}$$

Except for the cases when $n = 1$ and $n = 3$, there are no simple theoretical models for this formula. If equation (6) is applied to equation (14), the result is

$$V^{\dagger\mathrm{e}}(\sigma_\mathrm{a}) = \frac{nkT}{\sigma_\mathrm{a}}. \tag{15}$$

This result has two unexpected features. Firstly, $V^{\dagger\mathrm{e}}$ tends to infinity as σ_a tends to zero. This behaviour, although incompatible with the initial assumption that $V^\dagger$ tends to the finite value $V^\dagger(0)$, is not unrealistic. Figure 1 illustrates an obstacle with a finite range x_n. A real isolated defect will have a small effect even at very large distances and, when the applied stress is very small, the stable and unstable equilibrium values of the reaction coordinate will be very large. In practice, the dislocation segment or other lattice displacement will, when the reaction coordinate is large, interact more strongly with other lattice defects than with the obstacle that is about to be overcome. The analysis above does not consider such many-centre potential fields. Secondly, $V^{\dagger\mathrm{e}}$ depends only on σ_a, and is independent of $V^\dagger(0)$. This implies the extraordinary result that the experimental activation volume for any system at low stresses does not depend on the nature of the system under observation. It is less surprising that $V^\dagger(0)$ cannot be determined by stress-dip experiments in the Newtonian range. The difference between the rates of forward and backward jumps is proportional to $V^\dagger(0)\sigma_\mathrm{a}$, but the observed strain rate $\dot{\varepsilon}(\sigma_\mathrm{a})$ is multiplied by the unknown factor $\dot{\varepsilon}_0$.

In the general case, it is possible to invert equation (12) and to express the true activation volume $V^\S(\sigma)$ in terms of the experimental activation volume $V^{\S\mathrm{e}}(\sigma)$.

If we write

$$Z^\mathrm{e}(\sigma_\mathrm{a}) = \int_0^{\sigma_\mathrm{a}} \frac{V^{\dagger\mathrm{e}}(\sigma_\mathrm{a})}{kT} \, \mathrm{d}\sigma \tag{16}$$

and

$$Z(\sigma_\mathrm{a}) = \int_0^{\sigma_\mathrm{a}} \frac{V(\sigma)}{kT} \, \mathrm{d}\sigma, \tag{17}$$

equation (12) becomes

$$\frac{\mathrm{d}Z^\mathrm{e}}{\mathrm{d}\sigma_\mathrm{a}} = \frac{\mathrm{d}Z}{\mathrm{d}\sigma_\mathrm{a}} \coth Z, \tag{18}$$

which integrates to give

$$Z^\mathrm{e} = \ln(\sinh Z) \tag{19}$$

or

$$Z = \operatorname{arcsinh}(\exp Z^\mathrm{e}). \tag{20}$$

Hence

$$
\begin{aligned}
V(\sigma_a) &= \frac{kT \, \mathrm{d}Z}{\mathrm{d}\sigma_a} \\
&= kT \frac{\mathrm{d}}{\mathrm{d}\sigma_a} \left\{ \operatorname{arcsinh} \left[\exp\left(\int_0^{\sigma_a} \frac{V^{\dagger e}(\sigma)}{kT} \mathrm{d}\sigma \right) \right] \right\}.
\end{aligned}
\tag{21}
$$

§4. A one-dimensional statistical model

The analysis of §2 is based on the implicit assumption that each particle or dislocation segment poised to jump in the direction of the applied force or stress is matched by another, poised to jump in the opposite direction. This will not be the case if the activation events are isolated. Once a particle has jumped over an obstacle in the direction of the applied force, it will move indefinitely in the direction of the force, acquiring an unbounded negative enthalpy. It will never return to the position from which it can make a backward jump. However, if it comes to rest against another obstacle at a finite distance, it will have a finite negative enthalpy, and thermal activation may return it to the edge of the initial obstacle. We analyse the behaviour of a one-dimensional array of non-interacting particles moving under a force F_a in a potential field in which isolated obstacles of width $L^\dagger(0)$ and activation enthalpy under zero force $H^\dagger(0)$ are separated by distances $\Lambda \gg L^\dagger(0)$. The analysis for the case of dislocation segments is similar, provided that they are so dilute that their interactions may be neglected.

The potential energy of a particle at a distance X forward of an obstacle is $-F_a X$. At a temperature T, the density of particles at X is proportional to $\exp(F_a X / kT)$. If the mean linear density of particles is ρ, independent of F_a, then the density $\rho(X)$ at X is

$$
\rho(X) = \frac{F_a \Lambda \rho}{kT} \frac{\exp(F_a X / kT)}{\exp(F_a \Lambda / kT) - 1}.
\tag{22}
$$

In particular,

$$
\rho\left[-\tfrac{1}{2} L^\dagger(0)\right] \approx \frac{F_a \Lambda \rho}{kT} \frac{\exp(F_a \Lambda / kT)}{\exp(F_a \Lambda / kT) - 1}
\tag{23}
$$

and

$$
\rho\left[+\tfrac{1}{2} L^\dagger(0)\right] \approx \frac{F_a \Lambda \rho}{kT} \frac{1}{\exp(F_0 \Lambda / kT) - 1}.
\tag{24}
$$

Equation (8) is now replaced by

$$
\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} = \frac{F_a \Lambda \rho}{kT[\exp(F_a \Lambda / kT) - 1]} \left[\exp\left(\frac{F_a \Lambda - H_+^\dagger(F_a)}{kT} \right) - \exp\left(\frac{-H_-^\dagger(F_0)}{kT} \right) \right]
\tag{25}
$$

where equations (10 a) and (10 b) are replaced by

$$
H_+^\dagger(F_a) = H_-^\dagger(0) - \int_0^{F_a} L^\dagger(F_a) \, \mathrm{d}F_a
\tag{26 a}
$$

and

$$H_-^\dagger(F_a) = H^\dagger(0) + \int_0^{F_a} L^\dagger(F_a)\, dF_a. \tag{26 b}$$

Then equation (11) is replaced by

$$\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \exp\left(\frac{H^\dagger(0)}{kT}\right) = 2\rho\, \frac{\sinh\left\{\left[F_a \Lambda + 2\int_0^{F_a} L^\dagger(F_a)\, dF_a\right]\middle/ 2kT\right\}}{(2kT/F_a\Lambda)\sinh\left(F_a\Lambda/2kT\right)}. \tag{27}$$

Equation (27) bridges the gap from small to large F_a. We note that

$$\int_0^{F_a} L^\dagger(F_a)\, dF_a < \int_0^{F_a} L^\dagger(0)\, dF_a = L^\dagger(0) F_a \ll \Lambda F_a. \tag{28}$$

The formula simplifies in certain ranges of F_a. If $F_a \Lambda/2kT$ is small, it becomes

$$\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \exp\left(\frac{H^\dagger(0)}{kT}\right) = \frac{F_a \Lambda \rho}{kT}, \tag{29}$$

with Newtonian flow. The same result holds if $F_a\Lambda/2kT$ is neither large nor small, and the integral in equation (28) is small.

If $F_a\Lambda/2kT$ is large, equation (27) becomes

$$\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \exp\left(\frac{H^\dagger(0)}{kT}\right) = \frac{F_a \Lambda \rho}{kT} \exp\left(\frac{\int_0^{F_a} L^\dagger(F_a)\, dF_a}{kT}\right) \tag{30}$$

The additional proportionality to F_a arises because the applied force compresses the gas of particles against the obstacles. The corresponding experimental activation distance is

$$L^{\dagger e}(F_a) = L^\dagger(F_a) + \frac{kT}{F_a}. \tag{31}$$

Since activation processes are usually observed under conditions where $F_a L^\dagger(F_a) \approx 30kT$, the second term in equation (31) represents only a small correction.

§5. The appropriateness of the hyperbolic sine approximation

At very low stresses the strain rate $\dot{\varepsilon}$ is expected to be linearly proportional to the applied stress σ_a. It is often suggested that at somewhat higher stresses an expression of the form

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \sinh\left(\frac{\sigma_a}{\bar{\sigma}}\right) \tag{32}$$

will be appropriate.

Some analysis of the word 'appropriate' is necessary. Equation (32) may be expanded as

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \frac{\sigma_a}{\bar{\sigma}} + \frac{1}{6}\dot{\varepsilon}_0\left(\frac{\sigma_a}{\bar{\sigma}}\right)^3 + \frac{1}{120}\dot{\varepsilon}\left(\frac{\sigma_a}{\bar{\sigma}}\right)^5 + \cdots. \tag{33}$$

The experimental observations may be expanded in the form

$$\dot{\varepsilon} = a_1\sigma_a + a_3\sigma_a^3 + a_5\sigma_a^5 + \cdots. \tag{34}$$

Comparison of equations (33) and (34) requires that

$$a_1 = \frac{\dot{\varepsilon}_0}{\overline{\sigma}},$$

$$a_3 = \frac{\dot{\varepsilon}_0}{6\overline{\sigma}^3}$$

and

$$a_5 = \frac{\dot{\varepsilon}_0}{120\overline{\sigma}^5}, \tag{35}$$

so that

$$\frac{a_1 a_5}{a_3^2} = \frac{3}{10}. \tag{36}$$

The hyperbolic sine approximation is appropriate if this relation is satisfied.

To apply this analysis to equation (11), we note that, for a symmetrical potential, $V(\sigma)$ may be expanded at a fixed temperature T in the form

$$V(\sigma) = c_0 kT + 3c_2 kT\sigma^2 + 5c_4 kT\sigma^4 + \cdots, \tag{37}$$

so that

$$\int_0^{\sigma_a} \frac{V(\sigma)}{kT}\,\mathrm{d}\sigma = c_0\sigma_a + c_2\sigma_a^3 + c_4\sigma_a^5 + \cdots \tag{38}$$

and

$$\dot{\varepsilon} \propto c_0\sigma_a + c_2\sigma_a^3 + c_4\sigma_a^5 + \frac{1}{6}(c_0\sigma_a + c_2\sigma_a^3)^3 + \frac{1}{120}c_0^5\sigma_a^5 + \cdots$$

$$= c_0\sigma_a + \left(\frac{1}{6}c_0^3 + c_2\right)\sigma_a^3 + \left(\frac{1}{120}c_0^5 + \frac{1}{2}c_0^2 c_2 + c_4\right)\sigma_a^5 + \cdots, \tag{39}$$

which clearly does not satisfy equations (34) and (36).

The hyperbolic sine approximation is not appropriate even for the simple model leading to equation (11).

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