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A physical model for plastic deformation

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A general theoretical model for plastic deformation is presented, which is based on considerations of the variation of internal stored energy during deformation. It is proposed that the deformation rate will always be such that the rate of energy dissipation in the deforming material is minimal. The physical justification of this principle is discussed. The model is applied to dislocation deformation in metals and the result is then compared with experimental observations in aluminium.

1. Introduction

The key problem in developing a comprehensive theory of plastic deformation in crystalline materials is to find the correct way to connect the relatively well-known behaviour of single defects with the equally well-known macroscopic deformation phenomena which result from the collective effects of a great number of events involving single defects. There are two different approaches that have been used in attempting to solve this problem. In the first, more common, approach, the starting point is the consideration of single defect interactions, the effects of which are added and averaged using a statistical method to obtain the macroscopic net effect. The other approach considers the macroscopic behaviour and regards microscopic processes within that framework. The current state of the theories of plastic deformation are described well by Argon [1] and Kocks *et al.* [2]. Since their publication there has not been much significant progress.

In the present theory the starting point is macroscopic deformation. This is connected with the microscopic process through internal state variables that should have a clear physical significance. In its general form the theory is applicable to a wide range of materials, including non-crystalline ones, even though it has been developed principally with metals in mind. Altogether the present model has been constructed in such a way that it relies on physical principles as much as possible. In this respect it differs from the model of Hart [3, 4] which is phenomenological. The present model is similar in some respects to the thermodynamic theory presented by Kratochvil and Dillon [5] and the approach of Sumino [6]. A simpler version of this model has been published by the present author [7].

In the following the model is first described in its general form and then a simple application to dislocation deformation is developed, which is fitted to the experimental data of aluminium.

2. General theory

It is assumed in this theory that a number of variables, x_i, exist that completely characterize the internal structure of the crystal, as far as it is relevant to plastic deformation. These internal state variables depend on the structural features of the crystal, such as dislocation density and arrangement, number of point defects etc. The applied external stress, σ, also has the role of a state variable in this theory: it is an external state variable. During plastic deformation the values of the state variables generally vary with time. The variations in the internal parameters, x_i, reflect changes in the structure: and the external stress is given as a function of time, $\sigma(t)$.

Together, the plastically deforming specimen and the external influences on it form a system, whose behaviour is completely determined by the current values of the state variables. It follows that the changes in the internal state of the crystal, that is, the time derivatives, $\dot{x}_i$, as well as the deformation rate, $\dot{e}$, are uniquely dependent on the state variables, σ and x_i. In this theory the

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internal stored energy plays a central role in formulating the laws that govern the behaviour of the system and ultimately the dependences of the deformation response, $\dot{e}(t)$, on the external stress, $\sigma(t)$. Here, the stored energy is understood to be a function of the state variables of the system, $U(\sigma, x_i)$, and since the values of the state variables vary with time during plastic deformation this implies that the stored energy is also a function of time: $U(t) = U[\sigma(t), x_i(t)]$.

The physical meaning of the stored energy, U, needs some clarification. According to the first law of thermodynamics the change of internal energy of a crystal undergoing plastic deformation is the difference between the external work done on the crystal and the amount of heat that is produced in the deformation. This change in the internal energy, or the associated change in enthalpy, is generally identified with the stored energy [8, 9]. All the heat produced is not, of course, immediately lost from the crystal, and the rise in temperature also contributes to the internal energy. In the present theory, however, only the part of the change in the internal energy that does not include the effects of the temperature change, is termed stored energy. In other words, here, the stored energy $U(t)$ is a function that gives the change in the internal energy after the crystal has returned to its original temperature if the deformation had been stopped at some instant, t. Consequently, the stored energy in this theory is not equal to any thermodynamic quantity, such as internal energy, except in the hypothetical case of a completely isothermal deformation.

In plastic deformation the stored energy is continuously converted to heat by various frictional processes at some rate, P, per unit volume. At the same time the external stress does work W, when the shape of the specimen changes, and the stored energy is increased by this amount. Consequently, the energy rate balance per unit volume of the crystal can be written as follows:

$$\dot{U} = \frac{\partial U}{\partial \sigma}\dot{\sigma} + \sum_i \frac{\partial U}{\partial x_i}\dot{x}_i = \dot{W} - P, \qquad (1)$$

where the dots represent differentiation with respect to time, as everywhere in the following.

It is also necessary for the development of the model to give some general statement about the rate of deformation. It is proposed in this theory that the deformation always proceeds at a rate, $\dot{e}$, such that the rate of increase of the stored energy, $\dot{U}$, is maximal. This is equivalent to saying that the amount of energy converted to heat is minimal. Written as an equation this condition is

$$\frac{\partial \dot{U}}{\partial \dot{e}} = \frac{\partial}{\partial \dot{e}}(\dot{W} - P) = 0. \qquad (2)$$

It should be noted that both $\dot{W}$ and P are predetermined functions depending generally on $\dot{e}$. The rate of external work, $\dot{W}$, is obtained from the deformation geometry, and the recovery rate, P, depends on the details of the internal microscopic processes taking place in the crystal. An argument for the physical justification of Equation 2 is made in the discussion below.

In Fig. 1 a schematic overview of the logical structure of the model is given. The function $\sigma(t)$ that is applied to the system continuously changes its state, and the response to these changes can be calculated by using Equations 1 and 2 as well as possible additional relationships which may exist between the internal state variables, x_i, or between their derivatives, $\dot{x}_i$. This response produces as an "output" a function $\dot{e}(t)$, which is the predicted deformation behaviour caused by the applied stress $\sigma(t)$.

The manner in which this model can be applied to a specific case will become clear through the following example.

3. Application to dislocation mechanism

In constructing this simple application of the general model to the deformation occurring by a dislocation mechanism, the dislocation density ρ is used as a single internal state variable. In the case of uniaxial tension the stored energy and external work rate per unit volume can be represented by the following expressions:

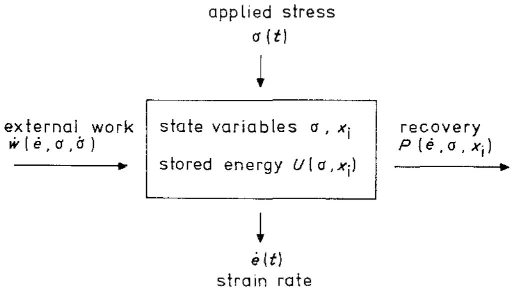

Figure 1 The principal functions and variables occurring in the model. The vertical arrows illustrate the deformation response, which is controlled by the energy flow indicated by horizontal arrows.

$$U = \frac{1}{2}\frac{\sigma^2}{E} + K\rho \qquad (3)$$

and

$$\dot{W} = \frac{\sigma}{E}\dot{\sigma} + \sigma\dot{e}, \qquad (4)$$

where E is Young's modulus and K is a constant. The direct proportionality between the dislocation density and energy in Equation 3 is a good enough approximation for the purposes of this treatment. With reference to Equation 4 it should be emphasized that $\dot{e}$ denotes only the plastic part of the total strain rate.

By substituting Equations 3 and 4 into the basic Equations 1 and 2, the following relationships are obtained:

$$\sigma\dot{e} - P(\dot{e}, \sigma, \rho) = K\dot{\rho} \qquad (5)$$

and

$$\sigma - \frac{\partial P(\dot{e}, \sigma, \rho)}{\partial \dot{e}} = 0. \qquad (6)$$

An expression for the recovery rate function $P(\dot{e}, \sigma, \rho)$ is derived in the following by considering the microscopic deformation phenomena in detail.

The inequilibrium created by the applied external stress gives rise to forces on the dislocations and these forces tend to move the disloactions in directions of lesser internal stored energy. Besides these active forces, $\bar{F}_a$, which are derived from the stored energy, there are also velocity dependent frictional forces, $\bar{F}_f$, acting on the dislocations. The velocity, $\bar{v}$, of a dislocation, at all points along it will have a value such that the vector sum of all the forces, $\bar{F}_a + \bar{F}_f$, vanishes. When a dislocation moves, the stored energy is decreased by the amount of the work which the active forces do against the frictional ones. This work is dissipated into the crystal as heat. Consequently, the rate of recovery per unit volume, P_m, due to dislocation movement can be written as

$$P_m = \rho\langle -\bar{F}_f \cdot \bar{v}\rangle, \qquad (7)$$

where the angular brackets denote the average along the dislocations.

Since the frictional force depends on the velocity, the product inside the brackets is also a function of the velocity. If we take the simplest approximation that the force is proportional to the velocity $\bar{F}_f = -\alpha\bar{v}$, the recovery rate becomes

$$P_m = \rho\alpha\langle v^2\rangle. \qquad (8)$$

The plastic deformation rate, $\dot{e}$, can be expressed by the well known formula

$$\dot{e} = \beta \mathbf{b}\rho\langle v\rangle, \qquad (9)$$

where β is a constant and $\mathbf{b}$ is the magnitude of the Burgers vector of the dislocations. The relation between the average dislocation velocity, $\langle v\rangle$, and the mean square velocity, $\langle v^2\rangle$, depends on the prevailing velocity distribution and can be formally written as

$$\langle v\rangle^2 = G(\sigma, \rho)\langle v^2\rangle, \qquad (10)$$

where the coefficient $G(\sigma, \rho)$ depends on the velocity distribution, which is determined by the state variables σ and ρ. When one part of the dislocation is stationary and others are moving, the function G gives the approximate relative proportion of the moving dislocations. Therefore it will be called a "mobility function" in the following. Its value is always between 0 and 1. Equations 8 and 9 can be combined to yield

$$P_m = \left(\frac{\alpha}{\beta^2\mathbf{b}^2 G(\sigma, \rho)}\right)\frac{\dot{e}^2}{\rho}. \qquad (11)$$

It is reasonable to assume that some recovery also occurs that does not directly result from the dislocation movement. Accordingly, an additional term is needed to obtain the total recovery rate function as follows

$$P(\dot{e}, \sigma, \rho) = \left(\frac{A}{G(\sigma, \rho)}\right)\frac{\dot{e}^2}{\rho} + R\rho^2, \qquad (12)$$

where R is a constant and $A = \alpha/\beta^2\mathbf{b}^2$. The form of the extra term $R\rho^2$, is based on experimental observations of thermal recovery, e.g. [10].

By substituting P from Equation 12 into Equations 5 and 6 we obtain the following two differential equations:

$$\dot{e} = \frac{\sigma}{2A}G(\sigma, \rho)\rho \qquad (13)$$

and

$$\dot{\rho} = \frac{\sigma^2}{4AK}G(\sigma, \rho)\rho - \frac{R}{K}\rho^2. \qquad (14)$$

The plastic deformation behaviour of the material is given by the solutions of these differential equations. Unfortunately, the solutions depend strongly on the mobility function $G(\sigma, \rho)$, which is not known with any certainty. If $G(\sigma, \rho)$ has a constant value, G_0, the solutions tend to approach the following "asymptotic" functions regardless of the initial conditions and almost regardless of the function $\sigma(t)$.

$$\rho_e(t) = \frac{\sigma(t)^2}{4RA} G_0 \tag{15}$$

and

$$\dot{e}_e(t) = \frac{\sigma(t)}{2A} G_0 \rho_e(t). \tag{16}$$

These expressions are not very useful in approximating the real solutions of Equations 13 and 14, but they can be used to obtain the stationary values at which the dislocation density and the deformation rate will settle if the stress is kept constant. When the stress is constant and the dislocation density settles to the value given by Equation 15, then the mobility function, $G(\sigma, \rho)$, is also unchanged, and Equations 15 and 16 are then valid solutions for Equations 13 and 14.

From a given mobility frunction Equations 13 and 14 can be solved by numerical methods for any applied stress, $\sigma(t)$, and for any initial conditions. The mobility function, $G(\sigma, \rho)$, can be estimated either by theoretical means or on the basis of experimental observations. Its theoretical calculation is not attempted here, but an estimate of it, for the case of aluminium at room temperature, will be presented on the basis of published experimental results.

Luthy *et al.* [11] have measured the steady state strain rate of aluminium for several different stresses. Under steady state condition, Equations 15 and 16 are valid and when the stress and strain rate are known, the corresponding dislocation density and the ratio G/A are obtained as follows

$$\rho = \left(\frac{\sigma \dot{e}}{4R}\right)^{1/2} \tag{17}$$

and

$$\frac{G}{A} = \left(4R \frac{\dot{e}}{\sigma^3}\right)^{1/2} \tag{18}$$

If the parameter R is given a value $(3.2 \times 10^{-35}\ \mu)$ $\mathrm{m}^6\ \mathrm{sec}^{-1}$ where μ is the shear modulus of aluminium, the dislocation density from Equation 17 is in agreement with the value estimated experimentally on the basis of calorimetric measurements [12]. Using these formulae the ratio G/A was calculated for five different (σ, ρ)-pairs. If the somewhat arbitrary value $(10^{11} \times 1/\mu)\ \mathrm{sec}^{-1}\ \mathrm{m}^{-2}$ is given to the parameter A, the values given in Fig. 2 are obtained for G. It is naturally not possible on the basis of solely these five data points, which lie on a line, to determine the exact course of the function $G(\sigma, \rho)$. However, by studying different possible solutions of the differential Equations 13 and 14 and with the help of some guessing it was deduced that the following expression should constitute a good analytical approximation for the mobility function:

$$G(\sigma, \rho) = \frac{1}{1 + \exp\left(\dfrac{\rho - \rho_0}{k\rho_0}\right)}, \tag{19}$$

where

$$\rho_0 = (l\sigma)^p + n, \tag{20}$$

in which k, l, p and n are parameters depending on the metal in question as well as on the temperature. In Fig. 2 the contours of equal value of this func-

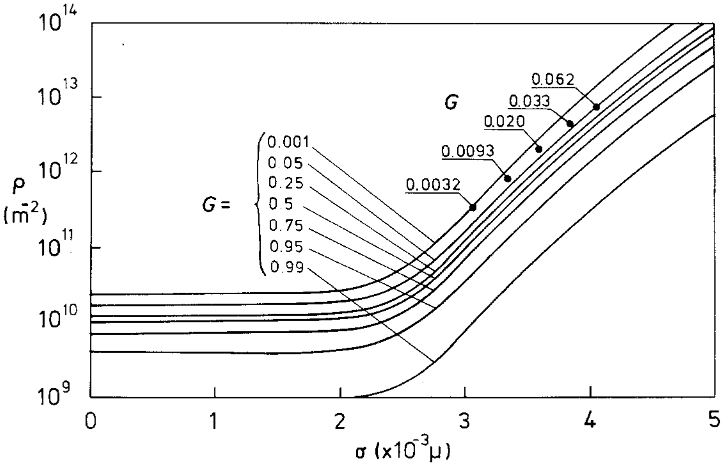

Figure 2 The mobility function $G(\sigma, \rho)$ for aluminium at room temperature as fitted to the experimental datapoints shown.

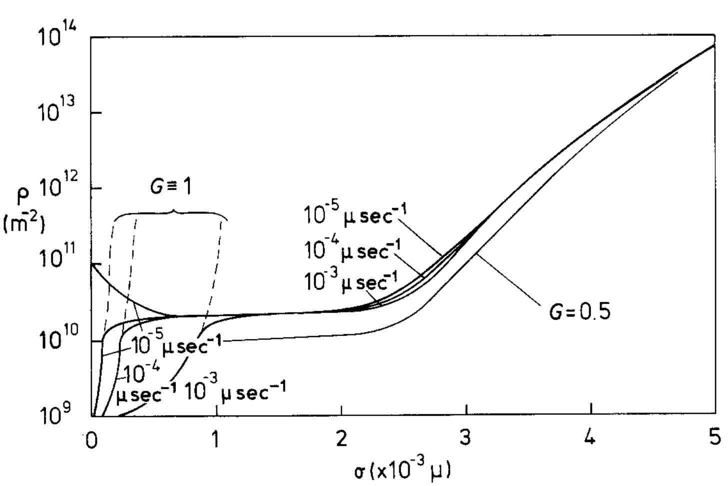

Figure 3 Numerically calculated solutions for Equation 14 in the σ–ρ-co-ordinate system for different rates of increase in the stress and for different initial conditions. The mobility function is the same as shown in Fig. 2. The solutions for constant $G(=1)$ are shown as dotted lines.

tion, $G(\sigma, \rho)$, are also shown as fitted to the data points. The fitting gives the following values to the parameters: $k = 0.2$, $l = 1.142 \times 10^7 \times 1/\mu$ m$^{-2/p}$, $p = 13$ and $n = 10^{10}$m^{-2}. This fit is by no means unique, several other choices of parameters would have resulted in a function agreeing equally well with the available data.

In Figs 3 and 4 numerically obtained solutions for the differential Equations 13 and 14 are illustrated for the case of the mobility function as constructed above. The stress, $\sigma(t)$, is taken to increase linearly at different rates. The parameters A and R have the values mentioned above and the value $(5 \times 10^{-24}\mu)$ m^4 was used for the parameter K.

It can be seen that the solution of the σ–ρ-co-ordinate system closely follows the constant G solution when $G \sim 1$ and then becomes perpendicular to the gradient of G. The stress–strain curves in Fig. 4 cannot be directly compared with experimental data, since they are calculated for a constant rate of increase in stress. Their general shape, however, seems to be the correct one.

4. Discussion

The plastic deformation is seen here as a process in which part of the external work done on the specimen, is converted to heat by the friction of defect movements or by other microscopic processes. The remainder is stored in the crystal as stored energy. The principle of minimal energy release formulated above in Equation 2 is crucial for the development of this model. According to this principle, the plastic deformation proceeds at a rate such that the energy dissipation rate is minimal at all times, i.e. the rate of increase in the stored energy, $\dot{U}$, is maximal.

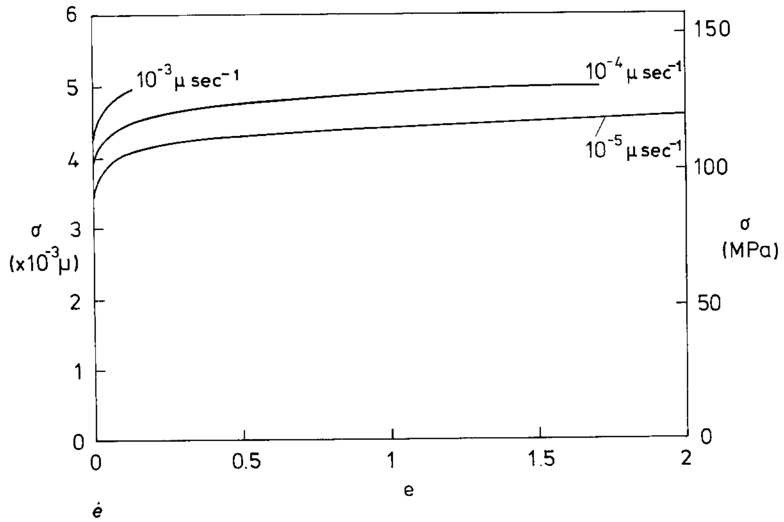

Figure 4 The stress–strain curves corresponding the solutions in Fig. 3.

In the case of the above application the rate of increase in the stored energy is the following function of the deformation rate:

$$\dot{U} = \frac{\sigma}{E}\dot{\sigma} + \sigma\dot{e} - \frac{A}{G(\sigma,\rho)}\frac{\dot{e}^2}{\rho} - R\rho^2 . \qquad (21)$$

This equation tells us what the rate of change in the stored energy would be at a deformation rate $\dot{e}$, when the crystal is in a particular internal state (particular ρ) and when there is an external stress of a particular magnitude, σ, acting on it. The rate of increase in the stored energy has a maximum according to this equation. The value of $\dot{e}$, at which the maximum is attained, is the rate at which the deformation will proceed in reality, according to the principle of minimum energy release. Fig. 5 illustrates the situation. It must be noted that the curve giving the dependence of $\dot{U}$ on $\dot{e}$ according to the above equation changes continuously and its maximum point moves accordingly. The dependence $\dot{U}(\dot{e})$, which is observed experimentally, is the track of these maximum points.

An argument for the physical justification of the principle can be made as follows:

Let us consider a relaxation experiment in which an external stress is instantly applied to the specimen and the specimen length is then kept constant. Part of the elastic strain that was instantly created by the application of the stress then slowly changes to plastic strain during relaxation. Before the application of the stress the dislocations in the specimen were in equilibrium configurations in such a way that the active forces on them vanish. The application of the external stress has two consequences: (1) the energy of the stress field inside the specimen (i.e. the stored energy) is increased instantly by a particular amount and (2) non-zero active forces are created on the dislocations. In the ensuing dislocation movement, part of the stress field energy is dissipated. The movement continues until the dislocations reach a new equilibrium configuration, after which plastic deformation ends. It seems reasonable to think that the dislocations tend to seek the closest possible new equilibrium configuration, which means that the smallest possible amount of energy is dissipated, which is the principle of minimum energy release. More complex situations, where there is a continuous influx of external work, can be regarded as generalizations of the above case.

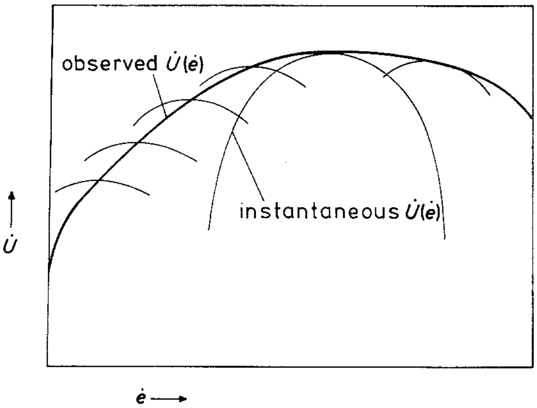

Figure 5 The dependence of the rate of increase in the stored energy on the deformation rate. At every instant during the deformation there is a potential instantaneous function $\dot{U}(\dot{e})$, whose maximum point determines the real $\dot{e}$.

The crux of the above argument is that all the external work is initially used to increase the stored energy and creates an inequilibrium situation resulting in minimal energy dissipation. It should be noted also that the principle of minimal energy release is also in agreement with the principle of smallest entropy production for stationary processes in irreversible thermodynamics. Plastic deformation does not, however, seem to be a stationary process in the thermodynamic sense.

In the application of the model to a dislocation mechanism, a number of simplifications, assumptions and approximations were made. None of them are strictly essential for the application of the theory, their purpose is to keep the treatment as simple as possible. In that sense what is presented should be regarded as a type of first approximation.

The simplification made above, that the frictional force opposing the dislocation movement is directly proportional to the velocity, is probably only true in reality for very small velocities. The exact functional relationship between the force and velocity does not, however, have any significant effect on the results obtained here. The structure of the model would stay the same, if in Equation 8 instead of $\langle v^2 \rangle$ an average of some more complicated but realistic function of the velocity appeared.

The mobility function, $G(\sigma, \rho)$, forms the link between the dislocation deformation model presented and experimental observations. It is possible to devise experiments from which the mobility function could be determined, such as, calorimetric measurements of stored energy and steady state deformation tests during which the stress is changed instantly. On the other hand, the mobility function could be calculated theoretically by considering the interactions in various dislocation configurations occurring in the deforming crystal. By comparing the experimantally determined mobility functions to the theoretically derived ones information about the microscopic deformation mechanisms could be obtained. In this way the model developed would serve as a useful tool in gathering knowledge on real plastic deformation mechanisms.

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