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A PHYSICAL THEORY OF THE FINITE ELASTIC-VISCOPLASTIC BEHAVIOUR OF SINGLE CRYSTALS

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The aim of this paper is to review some of the main results concerning the mycrodynamics of dislocation motion in single crystals and to construct a finite phenomenological theory of the elastic-plastic behaviour on the basis of these results. The physical research done in the last forty years has shown that plasticity and viscoplasticity are typical properties of crystalline materials and that the motion of crystal defects (dislocations, point defects, grain and phase boundaries) is the main elementary process that is macroscopically observed as viscoplastic deformation. However, the real physical microscopic process is so complex that any macroscopic theory, derived by applying certain averaging procedures, has to focus on merely the main aspects of the process, in the hope of clarifying their relative importance in various regimes of loading, temperature, and crystal conditions. This paper is intended to give a sufficient general description of the elastic-viscoplastic behaviour of single crystals. However, anelastic deformation, viscoelastic deformation produced by the motion of point defects, as well as recovery processes are not taken into account, and unloading is considered as purely elastic(¹). The first three sections review the main present knowledge concerning the microdynamics of viscoplastic flow, in order to get some guidance for the macroscopic theory, which is developed in the last five sections of the paper, and which is based on previous work by KRÖNER and TEODOSIU [4] and TEODOSIU [5].

1. THERMALLY ACTIVATED MOTION OF DISLOCATIONS IN SINGLE CRYSTALS

When a dislocation glides, it generally encounters two types of obstacles:

(i) *extended obstacles* such as dislocation pile-ups, large precipitates or second-phase particles, etc.;

(ii) *local obstacles*, such as impurity atoms, forest dislocations (dislocations threading the glide plane), jogs in gliding dislocations, etc.

Extended obstacles produce a long-range stress field, which varies only slowly with the position of the dislocation in the glide plane. The resolved shear stress(²) generated by extended obstacles is usually denoted by τ_μ because it is proportional in the isotropic approximation to the shear modulus, μ, and depends on temperature only through the temperature dependence of the elastic constants. The mean wavelength, Λ, of τ_μ is so large that thermal fluctuations cannot assist the resolved shear stress produced by external forces, τ, to move the dislocations past extended obstacles; therefore, such obstacles are also termed *athermal* obstacles.

(¹) For recent work relaxing some of these restrictive assumptions see, e.g., PERZYNA [1, 2] and TEODOSIU and SIDOROFF [3].

(²) The resolved shear stress is the component of the stress tensor acting on the glide plane and in the glide direction.

Local obstacles produce short-range stress fields, which act over a few atomic distances. Such obstacles are also called *thermal* obstacles, for they can be overcome by the action of the *effective stress*,

$$\tau^* = \tau - \tau_\mu, \tag{1.1}$$

assisted by thermal fluctuations(³).

The resolved shear stress experienced by a dislocation segment during its glide is schematically represented in Fig. 1, where a positive long-range stress is considered to oppose the applied stress and a negative long-range stress to assist it in moving the dislocation past local obstacles. For a dislocation segment to surmount the strongest local obstacle at 0°K, τ should equal τ_0. However, at some temperature above 0°K thermal fluctuations will assist the applied stress, and dislocation glide can occur at a stress $\tau < \tau_0$. As temperature increases, τ can decrease until it becomes equal to the amplitude of the long-range stress field. Further increase in temperature does not give any additional significant decrease in the applied stress, since the energy barrier is too extended for thermal fluctuations to make a significant contribution. Alternatively, if the applied stress grows beyond τ_0, the dislocation segment can overcome the local obstacle with no thermal aid: local obstacles become penetrable to the dislocation motion. Thus, the stress regime corresponding to the thermally-activated dislocation glide is defined by

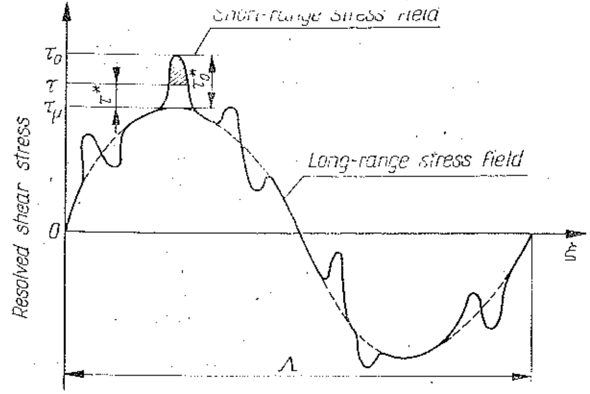

Fig. 1. Resolved shear stresses acting on a gliding dislocation

$$\tau_\mu < \tau < \tau_0 \quad \text{or} \quad 0 < \tau^* < \tau_0^*, \tag{1.2}$$

where $\tau_0^* = \tau_0 - \tau_\mu$.

When a dislocation moves through an array of local obstacles, its velocity is determined by the wait time, t_W, which is required to cut or bypass obstacles,

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(³) The Peierls stress, which represents the inherent resistance of the crystal lattice to the dislocation motion, is a short-range stress field, too. However, if the dislocation glide is controlled by overcoming the Peierls barriers, the effective stress should be considered as $\tau^* = \tau + \tau_\mu$, since this process takes place preferentially by thermal formation of double kinks at places where τ_μ aids τ in overcoming the barrier [6, 7].

and by the flight or traverse time, t_F, which is required to move from one obstacle to another. Hence, if l_F denotes the mean separation distance between two successive obstacles, the average velocity of a dislocation segment is given by

$$v = l_F/(t_W + t_F)\,. \tag{1.3}$$

The relative magnitudes of the times t_W and t_F depend strongly on the loading and crystal conditions. Thus, for strain rates and single crystals used in routine tensile tests one finds $t_W > t_F$ or even $t_W \gg t_F$. On the contrary, for very high strain rates [8] and/or high purity single crystals [9] one finds $t_W < t_F$ or even $t_W \ll t_F$. Therefore, both times must be considered in a general treatment of the problem [10].

Since the dislocation has a negligible inertia, after overcoming an obstacle it accelerates in a negligible time (⁴) to a flight velocity, v_F, which is limited by some drag mechanism. During the steady-state motion of the dislocation, the dissipative force acting on it equals the driving one, which leads for a unit dislocation length to the balance equation

$$Bv_F = b\tau^*\,, \tag{1.4}$$

where B is the drag coefficient, and b is the magnitude of the Burgers vector. The magnitude of B is of the order of 10^{-4} cgs at room temperature and decreases to about 10^{-5} cgs at 4.2°K [11]. There are a number of mechanisms that are responsible for the dislocation drag [12]. However, experiments carried out in the last few years on various metals with closed-packed atomic structures over wide ranges of temperatures and dislocation velocities have shown that interaction with thermal phonons and conduction electrons gives rise to the most part of energy dissipation for moving dislocations.

A still open problem is the upper limit to dislocation velocity. Continuum linear elasticity theory predicts that the total energy and effective mass of a dislocation grow to infinity as the dislocation velocity approaches the minimum sound velocity of the material. On the other hand, when the discrete nature of the lattice is considered, supplementary dispersion effects occur, which are very sensitive to the dislocation core, and the lattice seems to support supersonic dislocation motion. For mechanical tests, however, even under shock conditions, the dislocation velocity is generally less than 1/10 of the minimum sound velocity, c. It has been shown [11] that under such conditions, B can be taken in a first approximation as constant being corrected only for high dislocation speeds by a "relativistic" factor of the form

$$B = B_0\,[1-(v_F/c)^2]^{-n}\,,$$

where $0 < n \leqslant 1$. From Eq. (1.4) it follows that

$$t_F = l_F/v_F = l_F\,B/(b\tau^*)\,. \tag{1.5}$$

(⁴) The acceleration time is as small as 10^{-10} to 10^{-11} sec at room temperature for close-packed metals and increases by about one order of magnitude at 4.2°K. This shows that dislocation velocities are practically in phase with the effective stress even for very rapid loadings and high dislocation velocities [11].

As pointed out by FROST and ASHBY [13], drag also operates as the dislocation bows out between obstacles before it overcomes them; thus, in a more accurate approach, it should be taken into account when calculating t_W, too. However, in a first approximation, we shall derive the expression of the wait time by the usual approach of the rate theory applied to thermally activated aprocesses.

The reciprocal value of the wait time of a dislocation segment in front of a local obstacle is given by

$$1/t_W = \nu_{\text{eff}}^+ - \nu_{\text{eff}}^-, \tag{1.6}$$

where ν_{eff}^+ and ν_{eff}^- are, respectively, the effective frequencies of the forward and backward jumps over the obstacle. According to the rate theory [14 – 16], these frequencies can be calculated by multiplying the corresponding attempt frequencies ν_0^+ and ν_0^- by a Boltzmann factor, which depends on the free enthalpy of activation and gives the probablity of the co-operative thermal motion of atoms making an attempt successful. Thus,

$$\nu_{\text{eff}}^+ = \nu_0^+ \exp(-\Delta G^+/k\theta), \quad \nu_{\text{eff}}^- = \nu_0^- \exp(-\Delta G^-/k\theta), \tag{1.7}$$

where $k = 1.38 \times 10^{-23}$ J/mol °K is Boltzmann's constant, and ΔG^+ and ΔG^- are, respectively, the differences in the free enthalpy between the configuration of the dislocation segment in the saddle point and in the ground state for forward and backward jumps and depend on structure, applied stress, and temperature (see Sec. 2). It is generally assumed that the two attempt frequencies are equal and that they are proportional to the fundamental frequency of the dislocation segment, i.e.,

$$\nu_0^+ = \nu_0^- = k_1 \nu_D b/(2l), \tag{1.8}$$

where $\nu_D \approx 8 \times 10^{12}$ sec^{-1} is the Debye frequency, l is the mean separation distance between neighbouring barriers along the dislocation line, and $k_1 \approx 1.8 - 2$ is a factor which depends weakly on structure [17]. Taking $k_1 = 2$ and combining the Eqs. (1.6) – (1.8) yields

$$1/t_W = (\nu_D b/l)\,[\exp(-\Delta G^+/k\theta) - \exp(-\Delta G^-/k\theta)]. \tag{1.9}$$

The equation (1.9) has been derived in a more rigorous way by GRANATO *et al.* [18] by using statistical mechanics for temperatures higher than the Debye temperature, for which classical partition functions may be used. Their result can be shown to reduce to Eq. (1.9) when the activation entropy is conveniently defined [19].

Assuming now that all local obstacles have the same strength and are disposed in a square array, i.e., $l \approx l_F$, we deduce from the Eqs. (1.2), (1.5), and (1.9) that

$$v = b\nu_D \{[\exp(-\Delta G^+/k\theta) - \exp(-\Delta G^-/k\theta)]^{-1} + B\nu_D/\tau^*\}^{-1}. \tag{1.10}$$

To obtain a more explicit expression of the dislocation velocity, the activation free enthalpy should be evaluated as a function of structure, applied stress, and temperature.

2. INTERACTION POTENTIALS ASSOCIATED WITH VARIOUS TYPES OF LOCAL OBSTACLES

The first systematic description of the thermally-activated dislocation glide has been given by SEEGER [6, 20, 21]. Subsequently, two different approaches for the thermodynamic analysis of dislocation motion have been developed. Thus CONRAD and WIEDERSICH [22] and LI [23 - 25] employed as independent thermodynamic variables the effective stress, τ^*, and the absolute temperature, θ, while BAŚIŃSKI [26, 27], GIBBS [28 - 30], and SCHOECK [7] proposed the use of τ and θ. Although these alternative descriptions seem to eliminate each other, HIRTH and NIX [31] have been able to prove their mutual compatibility: the (τ, θ)-approach describes the behaviour of an *actual* thermodynamic system, namely the whole crystal acted on by external forces, while the (τ^*, θ)-approach uses a hypothetical *local* system (a small region around a particular pinned dislocation segment), which models the real one in a self-consistent way. However, the first approach, which will be adopted in the following, seems more natural, because it is the entire crystal rather than a local region which adopts the minimum free enthalpy configuration consistent with the imposed structure.

Let us take as thermodynamic system a single crystal containing mobile dislocations, local obstacles, and sources of long-range stress fields. Consider a dislocation segment of length $2l$, which is pinned at its ends and at the midpoint by local obstacles. Denote as before by τ and τ_μ the resolved shear stresses produced by external forces and long-range sources, respectively. The dislocation segment is bowed out under the action of the effective stress $\tau^* = \tau - \tau_\mu$. Let us denote by ξ_1' and ξ_1 the midpoint position of stable equilibrium under zero effective stress and under τ^*, respectively, and by ξ_2' and ξ_2 the corresponding positions of unstable equilibrium (Fig. 2).

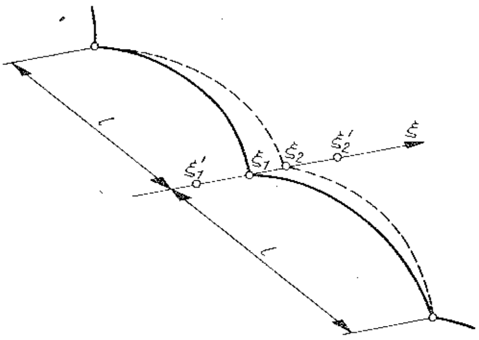

Fig. 2. Equilibrium positions of a dislocation segment pinned by a local obstacle

By thermal activation the dislocation segment can overcome the central obstacle and move in the direction of τ until it is stopped by the next obstacle. Since this elementary event takes place within a very short time, the applied stress, the temperature, and the long-range stress field can be considered as constant. Therefore, the equilibrium positions, ξ_1 and ξ_2, will correspond to the minimum and the maximum free enthalpy, respectively, considered as a function of the displacement ξ of the midpoint in the glide direction. Denoting by $\delta\xi$ the virtual displacement of the midpoint, the abscissas of the ground-state and saddle-point positions, ξ_1 and ξ_2, are the roots of the equation

$$\delta G(\xi) = \delta F_i(\xi) - \tau^* bl\delta\xi = 0, \tag{2.1}$$

where $\delta F_i(\xi)$ is the variation of the dislocation-obstacle interaction free energy and $\tau^* bl\,\delta\xi$ is the reversible work done by the effective stress (Fig. 3a). Equation (2.1) can be obviously rewritten as

$$G'(\xi)=F_i'(\xi)-\tau^* bl=0\,. \tag{2.2}$$

If ξ_1 and ξ_2 denote the roots of this equation, then the activation free enthalpy is given by

$$\Delta G=G(\xi_2)-G(\xi_1)\,. \tag{2.3}$$

The equations (2.2) and (2.3) may be also interpreted in terms of the forces undergone by the dislocation segment. Putting $f(\xi)\equiv G'(\xi)$ and $f_i(\xi)\equiv F_i'(\xi)$, we see from (2.2) that the dislocation segment is acted on by the force

$$f(\xi)=f_i(\xi)-\tau^* bl\,. \tag{2.4}$$

The two terms on the right-hand side give the forces exerted by the local obstacle and the effective stress, respectively. In view of (2.2), we deduce that ξ_1 and ξ_2 satisfy the equation $f(\xi)=0$, and hence they are the abscissas of the points where the graph of $f_i(\xi)$ is intersected by a line denoting the constant force $\tau^* bl$ (Fig. 3b).

From (2.2) and (2.3) it follows that

$$\Delta G=\int_{\xi_1}^{\xi_2} f(\xi)\,d\xi=\int_{\xi_1}^{\xi_2} f_i(\xi)\,d\xi-\tau^* bl\Delta\xi\,, \tag{2.5}$$

with $\Delta\xi=\xi_2-\xi_1$, and hence ΔG equals the shaded area in Fig. 3b. The quantity

$$\Delta g=\int_{\xi_1}^{\xi_2} f_i(\xi)\,d\xi \tag{2.6}$$

equals the area under the graph of $f_i(\xi)$ bounded by the ξ-axis and the lines $\xi=\xi_1$ and $\xi=\xi_2$; it obviously depends on τ^* and represents the contribution to ΔG of the atomic misfit produced by the local obstacle.

The quantities ΔV^* and ΔA^* defined by

$$\Delta V^*=b\Delta A^*=bl\Delta\xi\,, \tag{2.7}$$

which have the dimensions of a volume and an area, respectively, are commonly termed *activation volume* and *activation area*. However, ΔV^* is not a volume change of the system, for dislocation glide does not alter the crystal volume.

With the notions (2.6) and (2.7), the Eq. (2.5) becomes

$$\Delta G=\Delta g-\tau^*\Delta V^*\,. \tag{2.8}$$

Calculating the explicit dependence of ΔG on τ^*, θ, and structure requires the knowledge of the functions $F_i(\xi)$ or $f_i(\xi)$, which characterize the dislocation-obstacle interaction. In this respect distinction should be made between the so-called "rigid" and "deformable" free energy profiles [19].

A rigid energy profile is given by a single dependence of F_i on ξ, irrespective of the value of τ^*; it characterizes the interaction between an undissociated dislocation and a rigid obstacle (such as a precipitate particle). On the contrary, a deformable energy profile is represented by a function $F_i(\xi)$ that depends on τ^*; it characterizes the interaction between the gliding dislocation and a deformable obstacle (such as a forest dislocation), or the interaction between a dissociated dislocation and an obstacle, whether the latter is rigid or deformable. An accurate discussion of deformable energy profiles would require the consideration of non-linear elastic and core effects arising from the change of the atomic bonds in the deformable obstacle as the gliding dislocation moves to its equilibrium position ξ_1. That is why, for the sake of simplicity, only rigid energy profiles will be considered in what follows.

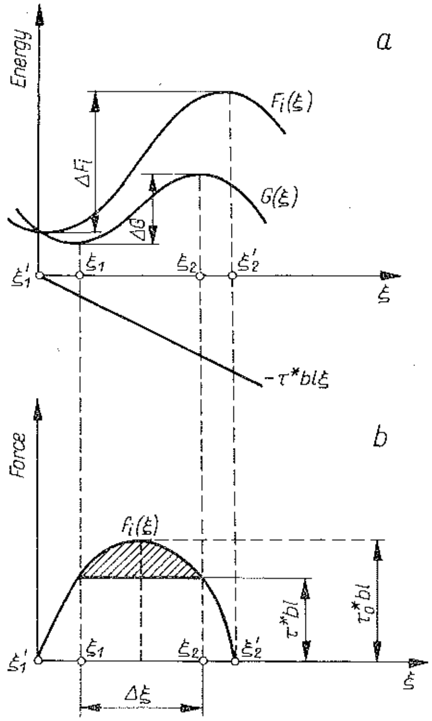

Fig. 3. Schematic representation of the energies and forces associated with the overcoming of a local obstacle by a dislocation segment

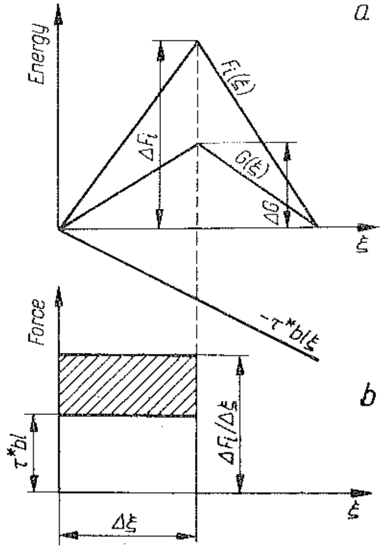

Fig. 4. SEEGER's triangular potential and its corresponding force — distance curve

The activation volume, ΔV^*, depends on τ^* through both $\Delta\xi$ and l. In the original treatment of the thermally-activated dislocation glide given by SEEGER [32,6], it was assumed for simplicity that the profile $F_i(\xi)$ is rigid and that $\Delta\xi$ and l do *not* depend on τ^* and θ. This is equivalent to assuming a triangular free energy profile or a rectangular force-distance curve (Fig. 4). Such a potential is believed to give a reasonable approximation for defect-emitting jogs.

A more intricate interaction potential, which, however, seems to be adequate for a broader class of rigid obstacles, is the sinusoidal potential proposed by MOTT and NABARRO [33]. Choosing for convenience the origin of the ξ-axis in the ground-state point for zero effective stress, as shown in Fig. 3a, the free energy profile is given by the equation

$$F_i(\xi)=(\Delta F_i/2)\,[1-\cos(\pi\xi/\xi_2')]\,, \tag{2.9}$$

whence, by (2.1) and (2.3),

$$\Delta G=(\Delta F_i/2)\,[\cos(\pi\xi_2/\xi_2')-\cos(\pi\xi_1/\xi_2')]-\tau^* bl\Delta\xi\,. \tag{2.10}$$

In view of (2.2), the abscissas ξ_1 and ξ_2 are the roots of the equation

$$\sin(\pi\xi/\xi_2')=2\xi_2' bl\tau^*/(\pi\Delta F_i)\,, \tag{2.11}$$

and hence

$$\xi_1=(\xi_2'/\pi)\,\sin^{-1}[2\xi_2' bl\tau^*/(\pi\Delta F_i)]\,,\qquad \xi_2=\xi_2'-\xi_1\,. \tag{2.12}$$

It then follows that

$$\Delta\xi=\xi_2-\xi_1=\xi_2'\,\{1-(2/\pi)\sin^{-1}[2\xi_2' bl\tau^*/(\pi\Delta F_i)]\}\,. \tag{2.13}$$

Substituting now (2.12) into (2.10) yields

$$\Delta G=\Delta F_i\,\{1-[2\xi_2' bl\tau^*/(\pi\Delta F_i)]^2\}^{1/2}-\tau^* bl\Delta\xi\,. \tag{2.14}$$

Under the action of the local effective stress, τ^*, the dislocation segment bows out between obstacles, which increases the probability of the contact with other obstacles. The amount of bowing out depends on τ^* and on the line tension, and hence also on the shear modulus, μ. Consequently, the average spacing l of the obstacles along a dislocation line depends on τ^* and θ (through the temperature dependence of μ). From the statistics of dislocation-obstacle interactions FRIEDEL [34] deduced that, for not too small and not too large values of τ^*, l is given by the relation

$$l=(\mu bA/\tau^*)^{1/3}\,, \tag{2.15}$$

where A is the average area swept out by a gliding dislocation during an activation event, which is assumed independent of τ^* and θ.

Introducing (2.15) into (2.13) gives

$$\Delta\xi=(2\xi_2'/\pi)\,[\pi/2-\sin^{-1}(\tau^*/\tau_0^*)^{2/3}]\,, \tag{2.16}$$

where

$$\tau_0^*=[\pi\Delta F_i/(2\xi_2' b^2)]\,[\pi\Delta F_i/(2\xi_2'\mu A)]^{1/2} \tag{2.17}$$

is the value of τ^* corresponding to $\Delta\xi=0$, i.e., the minimum value of τ^* for which the dislocation segment can overcome the local obstacle without thermal activation.

From (2.14) - (2.17) we finally obtain

$$\Delta G=\Delta F_i\,\{[1-(\tau^*/\tau_0^*)^{4/3}]^{1/2}-(\tau^*/\tau_0^*)^{2/3}\,[\pi/2-\sin^{-1}(\tau^*/\tau_0^*)^{2/3}]\}\,. \tag{2.18}$$

The plot of $\Delta G/\Delta F_i$ versus τ^*/τ_0^* is shown in Fig. 5.

Although the sinusoidal potential has been originally proposed for describing the interaction between dislocations and precipitates, it gives a reasonable intuitive interaction potential for other types of rigid obstacles, too. On the other hand, for large values of τ^* for which the ratio τ^*/τ_0^* approaches unity, the Eq. (2.18) yields

$$\Delta G = \Delta F_i \, 2^{1/2} [1 - (\tau^*/\tau_0^*)^{2/3}]^{3/2}, \tag{2.19}$$

a dependence obtained as high-stress limit also for other intuitive potentials. Thus, for the interaction potential

$$F_i(\xi) = \Delta F_i \exp(\xi/\xi_0)/[1 + \exp(\xi/\xi_0)], \tag{2.20}$$

which has been introduced by SEEGER [35] in connexion with the theory of irradiation hardening, one obtains after a similar calculation

$$\Delta\xi = 2\xi_0 \log \frac{1 + [1 - (\tau^*/\tau_0^*)^{2/3}]^{1/2}}{1 - [1 - (\tau^*/\tau_0^*)^{2/3}]^{1/2}}, \tag{2.21}$$

$$\tau_0^* = \frac{\Delta F_i}{8b^2 \xi_0} [\Delta F_i/(\xi_0 \mu A)]^{1/2}, \tag{2.22}$$

$$\Delta G = \Delta F_i \{[1 - (\tau^*/\tau_0^*)^{2/3}]^{1/2} - \\ - (\tau^*/\tau_0^*)^{2/3} \Delta\xi/(4\xi_0)\}, \tag{2.23}$$

and the last equation yields for τ^*/τ_0^* close to unity

$$\Delta G = (2\Delta F_i/3) [1 - (\tau^*/\tau_0^*)^{2/3}]^{3/2}, \tag{2.24}$$

i.e., the same functional dependence of ΔG on τ^* as that found in the high-stress limit for the sinusoidal potential.

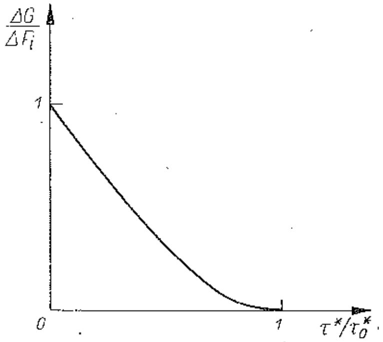

Fig. 5. Variation of the activation free enthalpy with the effective stress

Before closing this section we note that, in view of (2.8) and assuming that the quantities Δg and ΔV^* are approximately equal for forward and backward jumps over local barriers, we can write

$$\Delta G^+ = \Delta g - \tau^* \Delta V^*, \quad \Delta G^- = \Delta g + \tau^* \Delta V^*. \tag{2.25}$$

Substituting now (2.25) into (1.10) leads to

$$v = b\nu_D \{\exp(\Delta g/k\theta) [2 \operatorname{sh}(\tau^* \Delta V^*/k\theta)]^{-1} + B\nu_D/\tau^*\}^{-1}. \tag{2.26}$$

Various simplified forms of this equation, corresponding to various stress and strain-rate regimes, will be analyzed in the next section. We note here only that, as expected, v vanishes together with the effective stress, τ^*.

It has been already mentioned that drag operates not only during dislocation flight, but also as the dislocation bows out between obstacles before overcoming them. As pointed out by JONAS [36], since drag reduces the velocity of the dislocation during activation, the apparent activation free enthalpy will be $\Delta G' = \Delta G + \Delta G^D$, where ΔG^D is the energy dissipated during activation. Therefore, experimental activation energies can be expected to be higher than theoretical ones for a given class of obstacles by an amount which increases with the velocity of the dislocation during activation.

3. THE MACROSCOPIC VISCOPLASTIC STRAIN RATE

We will analyze now the relation between the microscopic dislocation motion and the macroscopic viscoplastic strain rate. Assume for simplicity that a single glide system is active and that glide is macroscopically homogeneous in the whole crystal.

Let α_M be the *mobile dislocation density*, i.e., the length of all mobile dislocation lines per unit volume in the active system, at a given time, t. From these glide dislocations only a small fraction, say α_F, are moving between obstacles with the flight velocity, v_F. The other glide dislocations (density α_W) are waiting at each local obstacle a mean wait time, t_W, before overcoming it by thermal activation (Fig. 6).

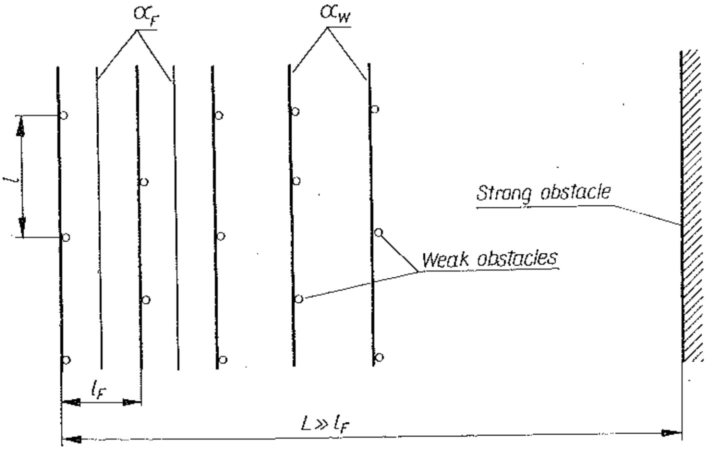

Fig. 6. Schematic representation of waiting and flying dislocations

The macroscopic viscoplastic strain rate, $\dot{a}$, is given by OROWAN's relation [37](5),

$$\dot{a} = b\alpha_F v_F . \tag{3.1}$$

The flight motion is said to be *quasi-stationary*(6) if

$$\alpha_F \approx \text{const}. \tag{3.2}$$

during the mean flight time, t_F. This requirement is fulfiled if no essential changes in the stress, temperature, and structure conditions take place during the time t_F, i.e., if

$$\dot{\tau} t_F \ll \tau , \quad \dot{\theta} t_F \ll \theta , \quad \dot{c} t_F \ll c , \quad \dot{\alpha} t_F \ll \alpha , \tag{3.3}$$

where α is the *total dislocation density* and c is the *concentration of point defects.*

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(5) For a rigorous proof of OROWAN's relation in the case of a finite elastic-plastic deformation see [4].

(6) The notion of quasi-stationarity of the dislocation motion has been independently introduced by MECKING [38] and by de ROSSET and GRANATO [10], being further discussed by MECKING and LÜCKE [39], NEUHÄUSER *et al.* [40], and others.

Since t_F is as small as 10^{-6} sec [38], conditions (3.3) are certainly satisfied for all macroscopic routine tests.

Differentiating (3.2) with respect to t gives

$$\dot{\alpha}_F = \alpha_W/t_W - \alpha_F/t_F = 0, \tag{3.4}$$

where α_W/t_W is the mobilization rate of the waiting dislocations and α_F/t_F is the immobilization rate of the flying dislocations. Since $\alpha_M = \alpha_W + \alpha_F$, the Eq. (3.4) yields

$$\alpha_F/t_F = \alpha_W/t_W = \alpha_M/(t_W + t_F), \tag{3.5}$$

and hence

$$\alpha_F v_F = \alpha_M l_F/(t_W + t_F) = \alpha_M v, \tag{3.6}$$

where $l_F = v_F t_F$ is the mean distance between obstacles and

$$v = l_F/(t_W + t_F) \tag{3.7}$$

is the mean dislocation velocity. From (3.1) and (3.6) it results that

$$\dot{a} = b\alpha_M v, \tag{3.8}$$

where α_M means, as already mentioned, the total mobile dislocation density, which includes flying and waiting dislocations as well.

Assume now that during the viscoplastic deformation stronger obstacles (such as Lomer-Cottrell barriers) are generated that can no longer be overcome by thermal activation. Let us denote by $L \gg l_F$ the average spacing between these obstacles, i.e., the mean free path of the dislocations before their final immobilization, and by t_L the mean life time of a mobile dislocation. The entire dislocation motion is said to be *quasi-stationary* if

$$\alpha_M \approx \text{const} \tag{3.9}$$

during the life time t_L. This condition is satisfied if the stress, temperature, and structure conditions do not significantly change within the time t_L, i.e., if

$$\dot{\tau} t_L \ll \tau, \quad \dot{\theta} t_L \ll \theta, \quad \dot{c} t_L \ll c, \quad \dot{\alpha} t_L \ll \alpha. \tag{3.10}$$

As t_L is of the order of one second, condition (3.10) is always fulfiled for low and moderate strain rates. On the contrary, sudden changes in temperature or strain rate cause a transitory behaviour until a new quasi-stationary state is attained [38, 39].

Differentiating (3.9) with respect to t yields

$$\dot{\alpha}_M = r_P - r_I = r_P - \alpha_M/t_L = r_P - \alpha_M v/L = 0, \tag{3.11}$$

where r_P and r_I are, respectively, the *production rate* and the *immobilization rate*, of the mobile dislocations. Hence,

$$\alpha_M v = r_P L, \tag{3.12}$$

and the Eq. (3.8) may be written as

$$\dot{a} = b r_P L. \tag{3.13}$$

Finally, if the immobilization of the dislocations by strong barriers is definitive (no recovery takes place), then the production rate of the mobile dislocations equals the rate of the total dislocation density, i.e., $r_P = \dot{\alpha}$, and hence

$$\dot{a} = b\dot{\alpha}L. \tag{3.14}$$

This equation has been repeatedly used in the literature [32, 41, 42]. If the variation of L with α is known, then the Eq. (3.14) expresses the viscoplastic strain rate in terms of quantities characterizing the dislocation multiplication and motion.

The analysis of thermally-activated dislocation glide undertaken in the preceding sections enables us to replace the velocity v in (3.8) by the expression (2.26), thus obtaining

$$\dot{a} = b^2 \alpha_M \nu_D \{\exp(\Delta g/k\theta)\,[2\,\mathrm{sh}\,(\tau^* \Delta V^*/k\theta)]^{-1} + B\nu_D/\tau^*\}^{-1}. \tag{3.15}$$

It should be noted, however, that passing from (2.26) to (3.15) requires averaging over all dislocation segments moving through the crystal. Therefore, when using the Eq. (3.15) for the interpretation of macroscopic experiments, the quantities Δg, τ^*, ΔV^*, and α_M should be regarded as phenomenological parameters, which correspond to those denoted by the same symbols in the Eq. (2.26) only in special circumstances [19, 31]. Nevertheless, the Eq. (3.15) has the merit of suggesting the right macroscopic variables to be included in the continuum theory and will be used to this aim in what follows.

In order to investigate the influence of various parameters on the viscoplastic strain rate, the dependence (3.15) has been studied by means of digital computer technique [43]. It was assumed for simplicity, like in SEEGER's original treatment of thermally-activated glide, that Δg and ΔV^* do not depend on τ^*. Denoting as before by

$$\tau_0^* = \Delta g/\Delta V^*$$

the effective stress for which local obstacles become penetrable without thermal activation, the Eq. (3.15) can be rewritten in the equivalent form

$$\dot{a} = \frac{b^2 \alpha_M \nu_D}{\{\exp[-\Delta g(1-\tau^*/\tau_0^*)/k\theta] - \exp[-\Delta g(1+\tau^*/\tau_0^*)/k\theta]\}^{-1} + B\nu_D/\tau^*}. \tag{3.16}$$

The following typical values of the parameters have been chosen for illustration:

$$b = 3\times 10^{-8}\,\mathrm{cm}, \quad b^2\alpha_M\nu_D = 10^6\,\mathrm{sec}^{-1}, \quad \Delta g = 1\,eV = 1.6\times 10^{-12}\,\mathrm{erg},$$

$$\Delta V^* = 1.000\,b^3, \quad \tau_0^* = 0.6\times 10^8\,\mathrm{dyn/cm}^2, \quad B\nu_D/\tau_0^* = 60.$$

For details concerning the graphical illustration of the relations between the parameters $\dot{a}$, θ, and τ^*/τ_0^*, when one of them is considered as constant, we refer to [43] and [5]. We content ourselves here with indicating that the numerical analysis of (3.16) reveals that the general relation (3.15) may be given several simplified forms depending on the prescribed stress or strain-rate regime:

i) For *low effective stresses*, i.e., for $0 < \tau^*/\tau_0^* \lesssim 0.1$, the glide is obstacle-controlled. The hyperbolic sine in the Eq. (3.15) can be replaced by its argument, and the flight time can be neglected against the wait time, thus obtaining a linear dependence,

$$\dot{a}=(2b^2\alpha_M\nu_D\Delta V^*/k\theta)\tau^*\exp(-\Delta g/k\theta), \tag{3.17}$$

between the strain rate and the effective stress.

ii) For *moderate effective stresses*, i.e., for $0.1<\tau^*/\tau_0^*\lesssim 0.7$, the glide is still obstacle -controlled. The hyperbolic sine can be replaced by an exponential function, and the flight time can be further neglected against the wait time. It results that

$$\dot{a}=b^2\alpha_M\nu_D\exp[-(\Delta g-\tau^*\Delta V^*)/(k\theta)]. \tag{3.18}$$

iii) For *high effective stresses*, i.e., for $0.7\leqslant\tau^*/\tau_0^*\lesssim 1$, the glide is both obstacle and drag-controlled. The hyperbolic sine can be still replaced by an exponential function, but both wait and flight time have to be taken into consideration, and hence

$$\dot{a}=b^2\alpha_M\nu_D\{\exp[(\Delta g-\tau^*\Delta V^*)/(k\theta)]+B\nu_D/\tau^*\}^{-1}. \tag{3.19}$$

iv) Finally, for *very high effective stresses*, i.e., for $\tau^*/\tau_0^*\geqslant 1$, the glide is only drag-controlled, and "relativistic" effects should eventually be taken into account through a velocity-dependent drag coefficient (cf. Sec. 1). The wait time vanishes, which again leads to a linear strain rate vs. effective stress dependence:

$$\dot{a}=b^2\alpha_M\tau^*/B. \tag{3.20}$$

We return now to the problem of obtaining macroscopic equations by averaging procedures from microscopic ones. A rigorous averaging should include the statistical representation of the long-range stress field as well as of the short-range barriers.

Unfortunately, none of these are known in detail. In order to evaluate the effect of the long-range stresses, some assumption must be made about their form and distribution.

Since long-range stresses are produced by internal sources, their mean value on each section of the crystal is zero. Therefore, the simplest possible assumption is that the long-range stress field, $\tau_\mu(\xi)$, varies sinusoidally, with an amplitude τ_μ and a wavelength Λ (Fig. 1). Accordingly, the effective stress field, $\tau^*(\xi)$, is given by

$$\tau^*(\xi)=\tau+\tau_\mu\sin(2\pi\xi/\Lambda), \tag{3.21}$$

where τ is the applied stress, assumed as being uniform throughout the crystal.

Various treatments of the effect of a periodic long-range stress have been carried out by CHEN *et al.* [44], ARSENAULT and LI [45], ADAMS [46], LI [47], ARGON [48], NIX *et al.* [49], SOLOMON and NIX[50,] and LUTON and JONAS [51].

Accounting for fluctuations in the long-range stress is rather important, since these markedly decrease the average velocity of the dislocations; indeed, more time is lost in the low stress regions than is gained as high stress regions are traversed. To illustrate this effect, we will make use of a linear velocity-effective stress dependence, which is typical for very low or very high effective stresses. In this case, again neglecting all inertia effects, the instantaneous velocity is given by

$$v(x)=v_0\,[1+(\tau_\mu/\tau)\sin(2\pi\xi/\Lambda)], \tag{3.22}$$

where v_0 is the velocity of the unimpeded dislocation under the applied stress τ.

Following the approach of CHEN *et al.* [44], the average velocity, $\bar{v}$, is given by

$$\bar{v}=\Lambda\left[\int_0^\Lambda \frac{d\xi}{v(\xi)}\right]^{-1}. \tag{3.23}$$

Substituting (3.29) into (3.23) and setting $\alpha=2\pi\xi/\Lambda$ gives

$$\bar{v}=2\pi v_0\left[\int_0^{2\pi} \frac{d\alpha}{1+(\tau_\mu/\tau)\sin\alpha}\right]^{-1}.$$

This integral can be calculated by residue theorem [50], thus obtaining

$$\bar{v}=v_0\,[1-(\tau_\mu/\tau)^2]^{1/2}<v_0\,. \tag{3.24}$$

Similar calculations have been carried out for power and hyperbolic sine velocity--effective stress laws (see, e.g. [48, 51]).

Another important problem connected with the macroscopic averaging, which stirs up an ever increasing interest, is that of the dislocation movement through random arrays of obtacles, which has been approached by using both analytic solutions and/or computer simulations [13, 52 – 66].

The critical stress required to move a dislocation through a random array of short-range barriers at zero absolute temperature has been determined by FOREMAN and MAKIN [55] and by KOCKS [56 – 58]. They observed that the stress required is less than that necessary to move a dislocation through a square array of the same concentration of short-range barriers.

A very complex *one-dimensional stochastic model* of the dislocation glide, with random barrier height and spacing has been studied by FORMAN [66]. It consists of a series of obstacles with quadratic dislocation-barrier interaction potentials that the dislocation must overcome by thermal activation and between which it moves subject to both inertial and viscous drag forces. In addition, the model allows for multiple jumps occurring when the dislocation, after traversing the interbarrier distance from the $(n-1)^{\text{th}}$ barrier, has an energy still greater than the n^{th} barrier. Computer simulations using this model led to the following conclusions:

i) The effect of the random spacing is negligible for all values of stress.

ii) The effect of the random distribution of barrier strengths is important only in the low stress, obstacle-controlled regime ($t_W \gg t_F$). It leads to a decrease in the dislocation velocity in comparison with a model with uniform barrier heights equal to the mean value of the random distribution. This is so because the larger-than average barrier heights increase the wait time much more than the smaller-than--average barrier heights decrease it.

iii) The coupling between barriers becomes important in the transition regime ($t_W \approx t_F$). Its neglection would be physically unrealistic in the high stress, drag-controlled regime, for the dislocation ought to be stopped at every barrier. It is worth noting that multiple jumps become frequent from about $\tau^*/\tau_0^* = 0.6$ to 0.7, in accordance with the beginning of the transition regime found above by using a simplified deterministic model.

Two-dimensional models of the dislocation glide are, of course, more complicated, but they have the advantage of accounting for some important aspects arising from the two degrees of freedom of the dislocation in the glide plane, such as kink formation, curvature effects and unzipping (sideways motion of the dislocation). Computer simulations using such models have been obtained by FROST and ASHBY [13] and by CADMAN and ARSENAULT [65]. The latter showed that, as the shape of the mobile dislocations is concerned, there are two possible types of gliding, depending on the stress, temperature, and structure conditions. If the stress is large or the temperature is high, the dislocation moves at the drag velocity and traverses the glide plane as a straight line. If the stress is reduced or the temperature is lowered so that some short-range barriers become effective, the dislocation does not remain straight; it bulges out at several places, these bulge outs grow until they link together, and the dislocation moves, forward in this manner. The magnitude of the bulge out increases with the ratio between the applied stress and the obstacle strength.

Although much work has to be done towards a complete statistical description of the elementary glide processes, the results obtained so far seem most promising for a future improved macroscopic theory based upon the understanding of the microdynamics of viscoplastic flow and of its statistics (see also [4, 67]).

4. KINEMATICS OF THE ELASTIC-VISCOPLASTIC DEFORMATION AND ITS RELATION TO THE DISLOCATION MOTION

Consider a single crystal $\mathscr{C}$ at time t_0, free of any surface tractions and body forces, at a uniform absolute temperature θ_0, and choose this configuration, say (k_0), as *reference configuration* of $\mathscr{C}$.

Assume that the crystal is imperfect. Then, a global natural configuration, i.e., a stress-free configuration of the whole crystal, does not exist. Let X be an arbitrary particle of $\mathscr{C}$ and denote by $N(X)$ a material neighbourhood of X whose diameter in (k_0) is small with respect to that of $\mathscr{C}$ but large in comparison with the mean separation distance between crystal defects. To determine the residual macroscopic elastic deformation of $N(X)$ in (k_0) we may, at least in principle, cut out this neighbourhood and release it under fixed positions of all crystal defects(⁷). Let $(\tilde{k}_0)$ denote the configuration of $N(X)$ obtained in this way. We then call the

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(⁷) For thin specimens, this requirement can practically be fulfilled by irradiating the crystal with fast neutrons before load-removal thus pinning the dislocations in their under-load positions (see MUGHRABI [68, 69]). However, the configuration $(\tilde{k}_0)$ plays in our considerations only the role of an ideal configuration, which need not be achieved by any real experiment.

deformation of $N(X)$ from $(\tilde{k})_0$ to (k_0) the *residual elastic deformation* of $N(X)$ in the unloaded reference configuration (k_0).

Assume now that the crystal undergoes an elastic-viscoplastic deformation under the action of external loads and of an inhomogeneous temperature field. Let (k) denote its current configuration at time t, and let $\mathbf{x}_0$ and $\mathbf{x}$ be the position vectors of the material point X in the configurations (k_0) and (k), respectively. The *motion* of the crystal is given by the one-parameter family of mappings

$$\mathbf{x}=\mathbf{x}(\mathbf{x}_0, t) \tag{4.1}$$

and the *velocity* field by

$$\dot{\mathbf{x}}=\frac{\partial \mathbf{x}(\mathbf{x}_0, t)}{\partial t}. \tag{4.2}$$

The *deformation gradient* associated with the motion (4.1) is

$$\mathbf{F}=\frac{\partial \mathbf{x}(\mathbf{x}_0, t)}{\partial \mathbf{x}_0}. \tag{4.3}$$

To determine the thermoelastic deformation undergone by $N(X)$ at time t, we may repeat the cutting out procedure used at time t_0. Let $(\tilde{k})$ be the configuration of the material neighbourhood $N(X)$ obtained by cutting it out at time t, suddenly reducing its temperature to θ_0, and releasing it from the constraints exerted on it by the remaining part of the crystal, all crystal defects being again considered as fixed. Then, the deformation of $N(X)$ from $(\tilde{k})$ to (k) will be called the *thermoelastic deformation* of $N(X)$ at time t.

Like $(\tilde{k}_0)$, the local configuration $(\tilde{k})$ is a natural state only for the macroscopic stress produced by the external loads, the inhomogeneous temperature field, and the incompatibility of the viscoplastic deformation. To remove also the microscopic stress produced by dislocations it would be necessary to cut the crystal into even smaller pieces with diameters comparable to the mean separation distance between the dislocation lines. According to our definition of the configurations $(\tilde{k}_0)$ and $(\tilde{k})$ we shall always understand by stresses and strains the corresponding macroscopic quantities, i.e., mean values calculated over macroscopic surface and volume elements which, therefore, do not contain microscopic fluctuations.

The configurations $(\tilde{k}_0)$ and $(\tilde{k})$ have been obviously defined to within a rigid-body rotation. We now remove this indeterminancy by requiring that the mean lattice orientation, as defined at points far from crystal defects, be the same throughout the motion and for all particles $X \in \mathscr{C}$. According to this convention, the glide directions and planes in the configuration $(\tilde{k})$ will be parallel to those in the configuration $(\tilde{k}_0)$ for any X and t. Then the deformation of $N(X)$ from $(\tilde{k}_0)$ to $(\tilde{k})$ is called the *viscoplastic deformation* of $N(X)$ *at time* t(⁸).

Let now Y be another particle of $N(X)$, and let $d\mathbf{x}$, $d\mathbf{x}_0$, $d\tilde{\mathbf{x}}$, $d\tilde{\mathbf{x}}_0$, denote the position vectors of Y with respect to X in the configurations (k), (k_0), $(\tilde{k})$, and $(\tilde{k}_0)$,

---

(⁸) This definition is justified by the fact that dislocation glide leaves unchanged the mean lattice orientation of the crystal.

respectively (Fig. 7). We define the *thermoelastic distortion*, $\mathbf{A}$, the *residual elastic distortion* $\mathbf{A}_0$, and the *viscoplastic distortion*, $\mathbf{P}$, by the relations

$$d\mathbf{x} = \mathbf{A}\,d\tilde{\mathbf{x}}, \quad d\mathbf{x}_0 = \mathbf{A}_0\,d\tilde{\mathbf{x}}_0, \quad d\tilde{\mathbf{x}} = \mathbf{P}\,d\tilde{\mathbf{x}}_0. \tag{4.4}$$

We also assume, that, for sufficiently small neighbourhoods $N(X)$, the so-defined values of the distortions at X do not depend on the choice of the neighbourhood $N(X)$ and of the material point $Y \in N(X)$. Consequently, by repeating the same procedure for all particles $X \in \mathscr{C}$ and times t, we may define the fields $\mathbf{A}(\mathbf{x}, t)$, $\mathbf{A}_0(\mathbf{x}_0)$, and $\mathbf{P}(\mathbf{x}, t)$(9).

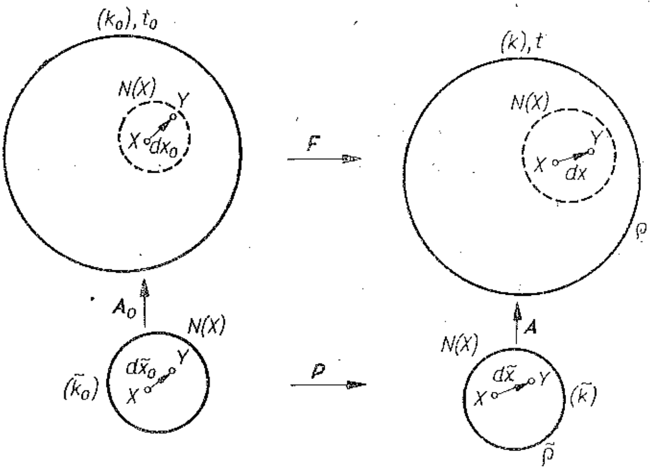

Fig. 7. On the definition of various distortions and configurations associated with the elastic-viscoplastic deformation

Suppose now that the tensor fields $\mathbf{F}$, $\mathbf{A}$, and $\mathbf{P}$ are continuously differentiable and admit for any *fixed* time t the inverses $\mathbf{F}^{-1}$, $\mathbf{A}^{-1}$, and $\mathbf{P}^{-1}$. Since, by (4.3),

$$d\mathbf{x} = \mathbf{F}\,d\mathbf{x}_0, \tag{4.5}$$

it follows from (4.4) that

$$\mathbf{F} = \mathbf{A}\mathbf{P}\mathbf{A}_0^{-1}. \tag{4.6}$$

From (4.2) and (4.3) we deduce that

$$\dot{\mathbf{F}} = \partial\dot{\mathbf{x}}/\partial\mathbf{x}_0 = (\operatorname{grad}\dot{\mathbf{x}})\,\mathbf{F},$$

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(9) Eckart [70] was the first to use time-dependent, local natural configurations, like $(\tilde{k})$, in order to separate the elastic from the inelastic part of the total deformation. The non-linear composition rule (4.6) of the distortions was independently introduced by Lee and Liu [71] and Fox [72, 73] in the special case $\mathbf{A}_0 = \mathbf{1}$, and by Teodosiu [74] and Rice [75] in the general case. The special choice of the orientation of the configuration $(\tilde{k})$ made in this paper was first used by Teodosiu [74], and independently considered by Rice [75] and Mandel [76]. As pointed out by Lee [77] and Mandel [76], the configuration $(\tilde{k})$ may be uniquely defined only if the macroscopic stress tensor, $\mathbf{T}$, is uniquely determined by the current values of $\mathbf{A}$ and θ, being independent of the defect content of the crystal. This simplifying assumption is based upon the low sensitivity of the elastic constants to the viscoplastic deformation, which has been revealed by various experiments. It can be expressed mathematically by the additive decomposition of the free energy density into a thermoelastic and a dislocation-dependent part [Eq. (5.6) below].

where a superposed dot denotes the time derivative for $\mathbf{x}_0=\text{const}$, and grad denotes $\partial/\partial\mathbf{x}$ for $t=\text{const}$. The last equation can be written in the equivalent form

$$\text{grad}\,\dot{\mathbf{x}}=\dot{\mathbf{F}}\mathbf{F}^{-1}, \tag{4.7}$$

from which, by making use of (4.6), we obtain

$$\text{grad}\,\dot{\mathbf{x}}=\dot{\mathbf{A}}\mathbf{A}^{-1}+\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{P}^{-1}. \tag{4.8}$$

This relation shows that in the non-linear case the velocity gradient cannot be decomposed into a purely elastic and a purely plastic part, unless elastic strains and rotations are small enough to allow the replacement of **A** by **1** in the last term of the Eq. (4.8).

Let n be the number of the (potential) glide systems of the crystal, and denote by $\mathbf{g}^{(s)}$ and $\mathbf{n}^{(s)}$, $s=1, \ldots, n$, the unit vectors of the glide direction and of the normal to the associated glide plane of the s^{th} glide system in the configuration $(\tilde{k})$. It can be shown [4] that (^{10})

$$\dot{\mathbf{P}}\mathbf{P}^{-1}=\sum_{s}\dot{a}^{(s)}\mathbf{g}^{(s)}\otimes\mathbf{n}^{(s)}, \tag{4.9}$$

where

$$\dot{a}^{(s)}=b^{(s)}\,\alpha_M^{(s)}\,v^{(s)} \tag{4.10}$$

is the viscoplastic shear rate in the glide system (s) measured with respect to the vectors $\mathbf{g}^{(s)}$ and $\mathbf{n}^{(s)}$, and the sum in (4.9) extends to all active glide systems. In (4.10), $b^{(s)}$ is the magnitude of the true Burgers vector, $\alpha_M^{(s)}$ is the total length of the mobile dislocation lines at time t per unit volume in the configuration $(\tilde{k})$, and $v^{(s)}$ is the mean expansion velocity of the dislocation loops, i.e., the mean value of the dislocation advance per unit time, measured on the outward normal to the loop in the configuration $(\tilde{k})$ and in the s^{th} glide system. The quantities $a^{(s)}$, $\dot{a}^{(s)}$ are assumed non-negative for any s. Consequently, we distinguish two glide systems that correspond to opposite glide directions for each crystallographically potential glide system.

The equation (4.9) relates the macroscopic kinematic equation (4.8) to quantities characterizing the dislocation motion. It may be viewed as a generalization of OROWAN'S relation (cf. Sec. 3) to the case of the finite elastic-viscoplastic deformation.

5. THERMODYNAMICS OF THE ELASTIC-VISCOPLASTIC DEFORMATION

Before passing to this section, a word on the thermodynamic aspects of plasticity may be appropriate. As is well known, the entropy, as a measure of the degree of order, plays a decisive role in thermodynamic considerations. In our problem,

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(^{10}) In [4], the quantities associated with the configuration $(\tilde{k})$ are distinguished from the corresponding quantities associated with the configuration $(\tilde{k})$ by a superposed tilde. In the present paper, all kinematic quantities involved in the Eqs. (4.9) and (4.10) are referred to the configuration $(\tilde{k})$ and, therefore, no tildes are used to label them.

the interest is not only in the degree of order as determined by heat vibrations, but also in that of the dislocation arrangement, which is responsible to a very large extent for the instantaneous state of the body. It seems, therefore, that the development of an accurate method for describing the internal state and its evolution has to be more complex than the application of classical thermodynamics [4]. However, due to the high complexity of the problem, we content ourselves in the following with applying the common concepts of continuum thermodynamics, in agreement with the level of accuracy adopted for the kinematical description of the deformation.

The thermodynamic process must be compatible with the laws of *balance of linear and angular momenta*

$$\operatorname{div}\mathbf{T}+\rho\mathbf{f}=\rho\ddot{\mathbf{x}}, \qquad \mathbf{T}=\mathbf{T}^T, \tag{5.1}$$

and the *balance of energy*

$$\rho\dot{\varepsilon}=\mathbf{T}\cdot\operatorname{grad}\dot{\mathbf{x}}-\operatorname{div}\mathbf{q}+\rho r. \tag{5.2}$$

Here **T** is the stress tensor, **f** is the specific *body force* per unit mass, ε is the *internal energy density* per unit mass, **q** is the *heat flux* vector, and r is the *heat supply* per unit mass and unit time.

Along with Eq. (5.2), which expresses the first principle of thermodynamics, we shall use the second principle in the form of the *Clausius-Duhem inequality*

$$\rho\dot{\eta}\geqslant-\operatorname{div}(\mathbf{q}/\theta)+\rho r/\theta, \tag{5.3}$$

where η is the *entropy density* per unit mass.

Eliminating r between the Eqs. (5.2) and (5.3), and taking into account (4.8), we obtain

$$\rho\dot{\eta}\theta\geqslant\rho\dot{\varepsilon}-(\dot{\mathbf{A}}\mathbf{A}^{-1}+\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}A^{-1})\cdot\mathbf{T}+(1/\theta)\mathbf{q}\cdot\operatorname{grad}\theta.$$

Finally, by introducing the *free energy density*

$$\psi=\varepsilon-\eta\theta, \tag{5.4}$$

the last inequality becomes

$$-\rho\dot{\psi}-\rho\eta\dot{\theta}+(\dot{\mathbf{A}}\mathbf{A}^{-1}+\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1})\cdot\mathbf{T}-(1/\theta)\mathbf{q}\cdot\operatorname{grad}\theta\geqslant0. \tag{5.5}$$

We adopt now a set of constitutive equations, by taking as independent variables besides the classical thermoelastic variables **A**, θ, and grad θ, a set of internal (or structural) state variables, namely the total dislocation densitites $\alpha^{(1)}, \ldots, \alpha^{(n)}$, and the concentrations $c^{(1)}, \ldots, c^{(r)}$ of various point defects per unit mass(¹¹). These constitutive equations are

$$\begin{gathered}
\psi=\hat{\psi}(\mathbf{A},\theta,\boldsymbol{\alpha},\mathbf{c})=\tilde{\psi}(\mathbf{A},\theta)+\bar{\psi}(\theta,\boldsymbol{\alpha},\mathbf{c}),\\
\mathbf{T}=\hat{\mathbf{T}}(\mathbf{A},\theta,\boldsymbol{\alpha},\mathbf{c}), \qquad \eta=\hat{\eta}(\mathbf{A},\theta,\boldsymbol{\alpha},\mathbf{c}),\\
\mathbf{q}=\hat{\mathbf{q}}(\mathbf{A},\theta,\operatorname{grad}\theta,\boldsymbol{\alpha},\mathbf{c}),
\end{gathered} \tag{5.6}$$

(¹¹) There exists an extensive literature concerning the thermodynamics of materials with internal state variables (see, e.g., [1–5, 74–99]). Some of the papers on this topic discuss also the physical significance of the internal state variables in the case of the viscoplastic deformation [1–5, 84–86, 88–91, 94, 95, 99].

where

$$\boldsymbol{\alpha}=\{\alpha^{(1)}, \ldots, \alpha^{(n)}\}, \qquad \mathbf{c}=\{c^{(1)}, \ldots, c^{(r)}\}. \tag{5.7}$$

denote the vectors of the structural state variables.

The particular additive form adopted for ψ assures the independence of the thermoelastic constants on the defect content of the crystal (cf. footnote p. 34); $\bar{\psi}\,(\theta, \boldsymbol{\alpha}, \mathbf{c})$ may be interpreted as residual free energy density in the configuration $(\tilde{k})$. Including grad θ as independent variable into the first three equations (4.6) proves to be incompatible with the Clausius-Duhem inequality and, therefore, it has been omitted from the very beginning.

Let us now investigate the restriction imposed by the Clausius-Duhem inequality on the possible form of the constitutive equations. From $(5.6)_1$ we find

$$\dot{\psi}=\frac{\partial\tilde{\psi}}{\partial\mathbf{A}}\cdot\dot{\mathbf{A}}+\frac{\partial\hat{\psi}}{\partial\theta}\dot{\theta}+\frac{\partial\bar{\psi}}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}}+\frac{\partial\bar{\psi}}{\partial\mathbf{c}}\cdot\dot{\mathbf{c}}.$$

Introducing this expression into (5.5) gives after some manipulation

$$\begin{aligned}\left\{\mathbf{T}(\mathbf{A}^{-1})^{T}-\rho\frac{\partial\tilde{\psi}}{\partial\mathbf{A}}\right\}\cdot\dot{\mathbf{A}}-\rho\left(\eta+\frac{\partial\hat{\psi}}{\partial\theta}\right)\dot{\theta}-\rho\frac{\partial\bar{\psi}}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}}-\rho\frac{\partial\bar{\psi}}{\partial\mathbf{c}}\cdot\dot{\mathbf{c}}+&\\ +(\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1})\cdot\mathbf{T}+(1/\theta)\mathbf{q}\cdot\operatorname{grad}\theta\geqslant 0.&\end{aligned} \tag{5.8}$$

It may be shown that there always exists a real thermodynamic process for which $\dot{\mathbf{A}}$ and $\dot{\theta}$ take arbitrarily prescribed values at a given time. Therefore, in order for the Clausius-Duhem inequality to be satisfied by all thermodynamic processes compatible with the balance laws, it is necessary that the co-factors of $\dot{\mathbf{A}}$ and $\dot{\theta}$ in the above inequality vanish, whence

$$\mathbf{T}=\rho\frac{\partial\tilde{\psi}(\mathbf{A}, \theta)}{\partial\mathbf{A}}\mathbf{A}^{T}, \qquad \eta=-\frac{\partial\hat{\psi}(\mathbf{A}, \theta, \boldsymbol{\alpha}, \mathbf{c})}{\partial\theta}. \tag{5.9}$$

The possible form of the constitutive equations $(5.6)_1$, $(5.6)_4$, and (5.9) may be further restricted by requiring their form invariance under superimposed rigid-body motions. It results that:

$$\begin{gathered}\psi=\hat{\psi}(\mathbf{E}, \theta, \boldsymbol{\alpha}, \mathbf{c})=\tilde{\psi}(\mathbf{E}, \theta)+\bar{\psi}(\theta, \boldsymbol{\alpha}, \mathbf{c}),\\ \mathbf{T}=\rho\mathbf{A}\frac{\partial\tilde{\psi}(\mathbf{E}, \theta)}{\partial\mathbf{E}}\mathbf{A}^{T}, \qquad \eta=-\frac{\partial\hat{\psi}(\mathbf{E}, \theta, \boldsymbol{\alpha}, \mathbf{c})}{\partial\theta},\\ \mathbf{q}=\mathbf{A}\tilde{\mathbf{q}}(\mathbf{E}, \theta, \mathbf{A}^{T}\operatorname{grad}\theta, \boldsymbol{\alpha}, \mathbf{c}),\end{gathered} \tag{5.10}$$

where

$$\mathbf{E}=(1/2)(\mathbf{A}^{T}\mathbf{A}-\mathbf{1}), \tag{5.11}$$

is the elastic strain tensor, and where, for simplicity, the same notations were preserved for the functions $\hat{\psi}$, $\tilde{\psi}$, and $\bar{\psi}$, after replacing $\mathbf{A}$ by $\mathbf{E}$.

The equation (4.8) suggests that the term $(\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1})\cdot\mathbf{T}$ in (5.5) is connected with the mechanical power expended in viscoplastic flow. Indeed, by using (4.9), it follows that

$$(5.12)\qquad (\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1})\cdot\mathbf{T}=(\rho/\tilde{\rho})(\dot{\mathbf{P}}\mathbf{P}^{-1})\cdot\mathbf{\Sigma}=(\rho/\tilde{\rho})\sum_{s}\dot{a}^{(s)}\tau^{(s)},$$

where $\tilde{\rho}$ is the mass density in the configuration $(\tilde{k})$, $\mathbf{\Sigma}$ is a stress tensor related to the Cauchy stress tensor $\mathbf{T}$ by [97]

$$(5.13)\qquad \mathbf{\Sigma}=(\tilde{\rho}/\rho)\mathbf{A}^{T}\mathbf{T}(\mathbf{A}^{T})^{-1},$$

and $\tau^{(s)}$ is the resolved shear stress(¹²) corresponding to $\mathbf{\Sigma}$ in the glide system (s), i.e.,

$$(5.14)\qquad \tau^{(s)}=(\mathbf{g}^{(s)}\otimes\mathbf{n}^{(s)})\cdot\mathbf{\Sigma}=(\mathbf{\Sigma}\mathbf{n}^{(s)})\cdot\mathbf{g}^{(s)}.$$

Taking into account (5.4), (5.11), and (5.12), the balance equation of energy (5.2) and the Clausius-Duhem inequality (5.8) become

$$(5.15)\qquad \tilde{\rho}\left(\theta\dot{\eta}+\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}}+\frac{\partial\psi}{\partial\mathbf{c}}\cdot\dot{\mathbf{c}}\right)=\sum_{s}\dot{a}^{(s)}\tau^{(s)}-(\tilde{\rho}/\rho)\operatorname{div}\mathbf{q}+\tilde{\rho}r,$$

$$(5.16)\qquad -\tilde{\rho}\left(\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}}+\frac{\partial\psi}{\partial\mathbf{c}}\cdot\dot{\mathbf{c}}\right)+\sum_{s}\dot{a}^{(s)}\tau^{(s)}-(\tilde{\rho}/\rho\theta)\mathbf{q}\cdot\operatorname{grad}\theta\geqslant 0.$$

When no plastic deformation takes place ($\dot{\boldsymbol{\alpha}}=\dot{\mathbf{c}}=\mathbf{0}$, $\dot{a}^{(s)}=0$ for any $s=1,\ldots,n$), these relations reduce to the familiar forms corresponding to the purely thermoelastic deformation:

$$(5.17)\qquad \rho\theta\dot{\eta}=-\operatorname{div}\mathbf{q}+\rho r,$$

$$(5.18)\qquad \mathbf{q}\cdot\operatorname{grad}\theta\leqslant 0.$$

Inspection of the Eqs. (4.10), (5.16), and (5.18) reveals that the nonthermal part of the dissipation is entirely due to the motion of crystal defects.

In the subsequent two sections, the thermoelastic constitutive equations (5.11) will be completed by evolution equations for the structural variables.

6. RATE-INDEPENDENT PLASTICITY

It is worth noting that for sufficiently high temperatures ($\theta>\theta_{\mathrm{cr}}$) at a prescribed strain rate, or for sufficiently low strain rates ($\dot{a}<\dot{a}_{\mathrm{cr}}$) at a given temperature, the necessary effective stress for overcoming the local obstacles is negligibly small, and the glide proceeds by a thermal mechanism. The critical values of $\dot{a}$ and θ corresponding to the boundary between thermal and thermally activated glide can be

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(¹²) It can be proved [3] that in the case of a finite elastic deformation, this resolved shear stress coincides with the one used for analyzing the dislocation glide in Sec. 2. For infinitesimal elastic deformations, the resolved shear stresses corresponding to $\mathbf{T}$ and $\mathbf{\Sigma}$ are equal to each other.

obtained by setting $\tau^* = 0$ in the relation (3.18), which neglects terms accounting for back fluctuations and drag dissipation. It results that(¹³)

$$(6.1) \qquad \dot{a}_{\mathrm{cr}} = b^2 \alpha_M \nu_D \exp(-\Delta F_i / k\theta), \qquad \theta_{\mathrm{cr}} = \Delta F_i \, [k \log (b^2 \nu_D \alpha_M / \dot{a})]^{-1}.$$

Considering also (3.20), we deduce that for $\theta = \mathrm{const}$, the strain-rate range of the thermally activated glide is given by

$$(6.2) \qquad \dot{a}_{\mathrm{cr}} < \dot{a} < b^2 \alpha_M \overset{*}{\tau_0} / B.$$

Alternatively, to point out the critical temperature in a constant-strain-rate test, the *flow stress*, τ_f, is commonly written, by considering (1.1), as

$$(6.3) \qquad \tau_f = \tau^* (\dot{a}, \theta) + \tau_\mu .$$

The variation of the flow stress with θ for $\dot{a} = \mathrm{const}$ is schematically shown in Fig. 8. Such a diagram is in agreement with many experimental observations and in fact also with the Eq. (3.16). According to the considerations above, thermal fluctuations can provide for $\theta > \theta_{\mathrm{cr}}$ the entire energy necessary for overcoming short-range obstacles. As shown in Fig. 8, θ_{cr} increases with $\dot{a}$ in agreement with the Eq. $(6.1)_2$. For $\theta > \theta_{\mathrm{cr}}$, practically $\tau^* = 0$, and the flow stress slowly decreases with increasing temperature due to the temperature dependence of the elastic constants intervening in τ_μ. If θ_{cr} lies above the melting temperature, the flow stress vs. temperature diagram in Fig. 8 has no longer a flat portion. Also, more than one flat region may occur for the entire temperature range from 0°K to the melting temperature, for a short-range obstacle at some lower temperature may become ineffective at a higher one [6].

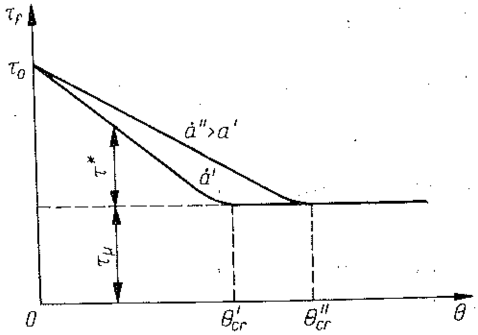

Fig. 8. Flow stress vs. temperature at a prescribed strain rate

Suppose now that an *isothermal* elastic-plastic deformation proceeds at sufficiently small plastic shear rates that $\dot{a}^{(s)} < \dot{a}^{(s)}_{\mathrm{sr}}$ for any $s = 1, \ldots, n$. Then, since $\tau^{*(s)} \approx 0$ for any s, in order for the glide system (s) to be active, it is necessary that the corresponding resolved shear stress satisfies the *activation condition*(¹⁴)

$$(6.4) \qquad \tau^{(s)} = \tau^{(s)}_\mu (\boldsymbol{\alpha}).$$

If plastic flow takes place, say in the first p glide systems, then the Eq. (6.4) is identically satisfied for $s = 1, \ldots, p$. Differentiating the corresponding equations with respect to t yields

$$(6.5) \qquad \dot{\tau}^{(s)} = \sum_{i=1}^{p} \frac{\partial \tau^{(s)}_\mu (\boldsymbol{\alpha})}{\partial \alpha^{(i)}} \dot{\alpha}^{(i)}, \qquad s = 1, \ldots, p.$$

(¹³) For $\tau^* = 0$, obviously, $\Delta g = \Delta G = \Delta F_i$ (cf. also Sec. 2).

(¹⁴) We assume that point defects give no contribution to the long-range stress field and to the mean free path of the gliding dislocations, L.

By solving this system with respect to $\dot{\alpha}^{(1)}, \ldots, \dot{\alpha}^{(p)}$, we obtain the *evolution equations*

$$\dot{\alpha}^{(s)} = \sum_{s=1}^{p} A^{(st)}(\boldsymbol{\alpha})\,\dot{\tau}^{(t)}, \qquad s=1,\ldots,p, \tag{6.6}$$

where $A^{(st)}$ are known functions of their arguments.

Since the deformation is assumed to proceed slowly, the dislocation glide is certainly stationary (cf. Sec. 3). Hence, we can apply (3.14) for each active glide system, thus obtaining

$$\dot{a}^{(s)} = b^{(s)} L^{(s)}(\boldsymbol{\alpha}) \sum_{s=1}^{p} A^{(st)}(\boldsymbol{\alpha})\,\dot{\tau}^{(t)}, \tag{6.7}$$

where $L^{(s)}(\boldsymbol{\alpha})$ denotes the mean free path of the dislocations gliding in the system (s). Finally, substituting (6.7) into (4.9) gives

$$\dot{\mathbf{P}}\mathbf{P}^{-1} = \sum_{s,t=1}^{p} A^{(st)}(\boldsymbol{\alpha}) L^{(s)}(\boldsymbol{\alpha})\,\dot{\tau}^{(t)}\,\mathbf{b}^{(s)} \otimes \mathbf{n}^{(s)}. \tag{6.8}$$

This equation(¹⁵) is valid if at least one glide system is active. If $\tau^{(s)} < \tau_{\mu}^{(s)}(\boldsymbol{\alpha})$ for any s, then all rates $\dot{\alpha}^{(s)}$, $\dot{a}^{(s)}$ vanish by virtue of (3.15), and hence $\dot{\mathbf{P}}\mathbf{P}^{-1}=0$, i.e., the deformation proceeds elastically.

Equation (6.8) is obviously invariant to a change of the time scale and hence it characterizes a rate-independent plasticity.

7. RATE-DEPENDENT PLASTICITY (VISCOPLASTICITY)

Let us consider now the more general case when rate effects cannot be disregarded and transitory phenomena corresponding to rapid changes in temperature and/or strain-rate regime must be also taken into account.

The *activation condition* for the glide system (s) reads now

$$\tau^{*(s)} = \tau^{(s)} - \tau_{\mu}^{(s)}(\boldsymbol{\alpha}) > 0. \tag{7.1}$$

Suppose again that this condition is fulfilled for the first p glide systems. By virtue of (4.9) and (4.10), we have

$$\mathbf{P}\dot{\mathbf{P}}^{-1} = \sum_{s=1}^{p} \alpha_M^{(s)} v^{(s)}\,\mathbf{b}^{(s)} \otimes \mathbf{n}^{(s)}. \tag{7.2}$$

The microscopic analysis done in Sec. 3 suggests the adoption of the following *evolution equations*:

$$v^{(s)} = \begin{cases} \hat{v}^{(s)}(\tau^{(s)} - \tau_{\mu}^{(s)}(\boldsymbol{\alpha}), \theta, \boldsymbol{\alpha}, \mathbf{c}) & \text{for} \quad s=1,\ldots,p, \\ 0 & \text{for} \quad s=p+1,\ldots,n, \end{cases} \tag{7.3}$$

$$\dot{\alpha}^{(s)} = \begin{cases} \hat{\alpha}^{(s)}(\tau^{(s)} - \tau_{\mu}^{(s)}(\boldsymbol{\alpha}), \theta, \boldsymbol{\alpha}, \mathbf{c}) & \text{for} \quad s=1,\ldots,p, \\ 0 & \text{for} \quad s=p+1,\ldots,n, \end{cases} \tag{7.4}$$

$$\dot{\alpha}_M^{(s)} = \dot{\alpha}^{(s)} - \alpha_M^{(s)} v^{(s)} / L^{(s)}(\boldsymbol{\alpha}), \tag{7.5}$$

(¹⁵) The linear form of the Eq. (6.8) has been discussed by ZARKA [88, 94] for a special choice of the functions $L^{(s)}(\boldsymbol{\alpha})$. The present form has been independetly derived by TEODOSIU [89].

where the functions $\tau_\mu^{(s)}$, $L^{(s)}$, $\hat{v}^{(s)}$, and $\hat{\alpha}^{(s)}$ are characteristic for the given crystal. Their form can be deduced theoretically, by using microscopic models, as has been done under certain simplifying hypotheses by ZARKA [88], or can be determined experimentally.

We complete the system (7.3) – (7.5) by adopting for $\mathbf{c}$ an evolution equation of the type

$$\dot{\mathbf{c}}=\hat{\mathbf{c}}\,(\theta,\boldsymbol{\alpha},\mathbf{c})\,. \tag{7.6}$$

We recall that the viscoelastic behaviour produced by the migration of point defects when no disloaction glide takes place is not taken into consideration. The equation (7.6) is primarily intended to take into account the influence of the temperature and of the dislocation glide on the concentration of point defects, in particular the generation of point defects during glide (^{16}).

The influence of the stress tensor on $\mathbf{c}$ is rather complicated, for it depends on whether the symmetry of the point defects is the same or lower than that of the lattice. A complete description of the evolution of point defects would also require considering diffusion equations for various species of point defects. All these complex phenomena are not included in the present theory. For recent progress in achieving a more complete description of the viscoelastic-viscoplastic behaviour of single crystals, we refer to [3].

8. DISCUSSION OF THE THEORY PROPOSED

We collect here for convenience the basic field equations, namely the *kinematic equations*

$$\mathbf{F}=\mathbf{A}\mathbf{P}\mathbf{A}_0^{-1}\,,\qquad \mathbf{E}=(1/2)(\mathbf{A}^T\mathbf{A}-\mathbf{1})\,, \tag{8.1}$$

$$\operatorname{grad}\dot{\mathbf{x}}=\dot{\mathbf{A}}\mathbf{A}^{-1}+\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1}\,,\qquad \dot{\mathbf{P}}\mathbf{P}^{-1}=\sum_{s=1}^{p}\dot{a}^{(s)}\,\mathbf{g}^{(s)}\otimes\mathbf{n}^{(s)}\,, \tag{8.2}$$

the *balance laws*

$$\operatorname{div}\mathbf{T}+\rho\mathbf{f}=\rho\ddot{\mathbf{x}}\,,\qquad \mathbf{T}=\mathbf{T}^T\,, \tag{8.3}$$

$$\rho\left(\theta\dot{\eta}+\frac{\partial\bar{\psi}}{\partial\boldsymbol{\alpha}}\cdot\dot{\boldsymbol{\alpha}}+\frac{\partial\bar{\psi}}{\partial\mathbf{c}}\cdot\dot{\mathbf{c}}\right)=(\mathbf{A}\dot{\mathbf{P}}\mathbf{P}^{-1}\mathbf{A}^{-1})\cdot\mathbf{T}-\operatorname{div}\mathbf{q}+\rho r\,, \tag{8.4}$$

the *thermoelastic constitutive equations*

$$\psi=\hat{\psi}\,(\mathbf{E},\theta,\boldsymbol{\alpha},\mathbf{c})=\tilde{\psi}\,(\mathbf{E},\theta)+\bar{\psi}\,(\theta,\boldsymbol{\alpha},\mathbf{c})\,, \tag{8.5}$$

$$\mathbf{T}=\rho\mathbf{A}\frac{\partial\tilde{\psi}\,(\mathbf{E},\theta)}{\partial\mathbf{E}}\mathbf{A}^T,\qquad \eta=-\frac{\partial\hat{\psi}\,(\mathbf{E},\theta,\boldsymbol{\alpha},\mathbf{c})}{\partial\theta}\,, \tag{8.6}$$

$$\mathbf{q}=\mathbf{A}\tilde{\mathbf{q}}\,(\mathbf{E},\theta,\mathbf{A}^T\operatorname{grad}\theta,\boldsymbol{\alpha},\mathbf{c})\,, \tag{8.7}$$

(^{16}) For a description of this phenomenon in NaCl see FRANK [100].

which have to be associated with the *condition of activation* and the *evolution equations*, i.e., (6.4) and (6.6) for the rate-independent plastic deformation and (7.1), (7.3) – (7.6) for the viscoplastic deformation. To complete the formulation of the boundary-value problem, we have to add to the above field equtions the thermomechanical boundary conditions.

Let us test now the completeness of the above system of equations by using a time discretization. Assume that we know at a given time t the configuration (k), and the state of the material, i.e., all thermoelastic and structural variables. The evolution equations permit to calculate the rates $\dot{\alpha}^{(s)}$, $\dot{\alpha}_M^{(s)}$, and $\dot{\mathbf{c}}$, as well as the quantities $L^{(s)}$ and $v^{(s)}$, and hence the term $\dot{\mathbf{P}}\mathbf{P}^{-1}$ is determined by the Eqs. (6.8) or (7.2). Then, the determination of $\dot{\mathbf{x}}$ and $\dot{\theta}$ from system (8.1) – (8.7) becomes a generalized thermoelastic boundary-value problem. By considering that the solution of this problem is valid during the time interval $(t, t+\Delta t)$, where Δt is small enough, we can determine the configuration and the state of the body at time $t+\Delta t$, and then continue the solving procedure in the same way.

We conclude that the theory proposed provides a sufficiently general framework for the macroscopic analysis of the elastic-viscoplastic deformation of single crystals.

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STRESZCZENIE

FIZYCZNA TEORIA ZACHOWANIA SIĘ MONOKRYSZTAŁÓW PRZY SKOŃCZONYCH SPRĘŻYSTO-PLASTYCZNYCH ODKSZTAŁCENIACH

Celem niniejszej pracy jest przegląd niektórych podstawowych rezultatów dotyczących mikrodynamiki ruchu dyslokacji w monokryształach i na ich podstawie zbudowanie fenomenologicznej teorii sprężysto-plastycznego zachowania się monokryształów w zakresie odkształceń skończonych.

Przeprowadzone w ostatnich czterdziestu latach badania fizykalne wykazały, że plastyczność i lepkosplastyczność są typowymi cechami materiałów krystalicznych i że ruch defektów kryształów (dyslokacje, defekty punktowe, granice ziaren i faz) jest podstawowym elementarnym procesem obserwowanym w skali makroskopowej jako deformacja lepkoplastyczna. Jednakże rzeczywisty fizyczny proces makroskopowy jest tak złożony, że każda teoria makroskopowa wyprowadzona przy użyciu niektórych procedur uśredniających musi skupić się jedynie na głównych aspektach procesu w nadziei wyjaśnienia ich względnego znaczenia w różnych zakresach obciążenia, temperatury i warunków krystalicznych.

Zamierzeniem niniejszej pracy jest podanie wystarczająco ogólnego opisu sprężysto-plastycznego zachowania się pojedynczych kryształów. Nie zostały jednakże uwzględnione w rozważaniach odkształcenia niesprężyste, odkształcenia lepkosprężyste wywołane ruchem defektów punktowych jak również procesy nawrotu, a odciążenie przyjęto jako czysto sprężyste.

Pierwsze trzy rozdziały zawierają przegląd podstawowej aktualnej wiedzy dotyczącej mikrodynamiki lepkoplastycznego płynięcia celem dostarczenia pewnych wskazówek dla teorii makroskopowej rozwijanej w pięciu końcowych rozdziałach pracy, a bazującej na poprzednich pracach Krönera i Teodosiu [4] i Teodosiu [5].

Резюме

ФИЗИЧЕСКАЯ ТЕОРИЯ ПОВЕДЕНИЯ МОНОКРИСТАЛЛОВ ПРИ КОНЕЧНЫХ УПРУГО-ПЛАСТИЧЕСКИХ ДЕФОРМАЦИЯХ

Целью настоящей работы является обозрение основных результатов касающихся микродинамики движения дислокации в монокристаллах и на их основе построение феноменологической теории упруго-пластического поведения монокристаллов в области конечных деформаций.

Проведенные в последний сорок лет физические исследования показали, что пластичность и вязкопластичность являются типичными свойствами кристаллических материалов и что движение дефектов кристаллов (дислокации, точечные дефекты, границы зерен и фаз) является основным элементарным процессом, наблюдаемом в макроскопическом масштабе как вязкопластическая деформация. Однако реальный физический макроспопический процесс так сложен, что всякая макроскопическая теория, выведенная при использовании некоторых усредняющих процедур, должна сосредоточиться только на главных аспектах процесса в надежде выяснения их относительного значения в разных интервалах нагрузки, температуры и кристаллических условий.

Намерением ностоящей работы является приведение достаточно общего описания упругопластического поведения отдельных кристаллов. Однако в рассуждениях не учтены неупругие деформации, вязкоупругие деформации вызванные движением точечных дефектов, как тоже процессы возврата; разгрузка же принята как чисто упругая.

Первые три главы содержат обзор основных актуальных знаний, касающихся микродинамики вязкопластилеского течения с целью приведения некоторых указаний для макроскопической теории развиваемой в пяти заключительных главах работы и базирующих на предыдущих работах Кренера и Теодосиу [4] и Теодосиу [5].