

**"EFFECT OF THE VARIATIONS OF THE MOBILE DISLOCATION DENSITY ON THE THERMALLY ACTIVATED CYCLIC DEFORMATION BEHAVIOUR"**

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**ABSTRACT**

The application of the transition state theory of rate processes to describe tension-tension, strain controlled cyclic deformation BEHAVIOUR was extended to describe the effect of the variations of the mobile dislocation density on the cyclic deformation BEHAVIOUR. It was shown from the derived constitutive relation that due to the net increase in the mobile dislocation density during strain controlled cyclic deformation the stress change per cycle (or in function of time) increases.

**INTRODUCTION**

The deformation and subsequent fracture of structural metals subjected to cyclic plastic loading is critical in the design of steam and gas turbines, jet engines, nuclear reactors, etc. The development of materials and subsequent design of the components for such applications is often a complex problem. The difficulty of the problem is primarily due to the fact that the cyclic stress often leads to complex sub-microscopical and microscopical changes which are of cumulative and irreversible type. Consequently, the yield stress, the resistance to plastic deformation (internal stress), and the material structural characteristics may vary in a complex manner, leading to complicated cyclic stress-strain BEHAVIOUR. The formulation of rational constitutive equations for cyclic plastic deformation is thence a formidable task.

The unity of identity of plastic flow and chemical reactions has long been established [1-3]. Both are transport processes and involve breaking and establishing of atomic bonds. These fundamental atomic events are rate dependent (hence they are time and temperature dependent). Thus, plastic flow was identified as a process of thermally activated dislocation (and/or vacancy) movements over energy barriers (or obstacles; Fig.1) under the drive of the applied shear stress. The observed macroscopic plastic strain is therefore the accumulation or summation of the atomic, stepwise motion of the mobile dislocations. Accordingly, the determination of plastic strain rate is based on the transition state theory of rate processes. The application of these concepts to describe plastic flow (of metals, polymers, etc.) during monotonic loading is now firmly established [1-3]. Recently, the author has extended the transition state theory to describe plastic deformation under tension-tension, strain and load controlled cyclic loading conditions [4]. The description of the cyclic plastic deformation, however, was based on the assumption (among others) that the material

structural characteristics are invariant. While this assumption is physically reasonable (for some materials), it is by no means necessary. Nonetheless, the description of the material structural characteristics (in function of time, stress, or strain) during plastic deformation has always been a difficult task. Several empirical phenomenological relations have been proposed [5-7] to describe the mobile dislocation density in function of time [5], stress [6] and strain [7].

The present paper describes a further extension of the previous work. In addition to reviewing the later, an attempt is made to incorporate into the constitutive equation the variation of the dislocation density during strain controlled, tension-tension cyclic deformation. Only a qualitative analysis of the material response (stress-time relation) is made to determine the effect of the variation of the dislocation density (in function of time) on the deformation BEHAVIOUR.

## 2. THERMALLY ACTIVATED PLASTIC FLOW

Plastic deformation is generally produced by the motion of dislocations under the drive of the applied shear stress. In most cases it is rate dependent (and, therefore, temperature dependent); that is, thermally activated. Over a specific stress and temperature range the rate of plastic flow may be controlled by activation over a single energy barrier. The plastic flow may be controlled by activation over a single energy barrier. the plastic strain rate,  $\dot{\epsilon}_p$ , that results from the thermally activated motion of dislocations over the energy barrier, as shown schematically in Fig. 1, is described by the relation [1-3]

$$\dot{\epsilon}_p = \frac{1}{M} b \rho_m \bar{v} = \frac{1}{M} b \rho_m l (k_f - k_b) \quad (1)$$

where  $M$  is the Taylor orientation factor relating the tensile stress and the tensile strain  $\epsilon$  to the shear stress  $\tau$  and to the shear strain  $\gamma (= M\epsilon)$  resolved into the rate controlling slip system,  $b$  is the Burger's vector,  $\rho_m$  is the mobile dislocation density,  $l$  is the distance travelled by the dislocation between obstacles,  $\bar{v}$  is the average dislocation velocity,  $k_f$  and  $k_b$  are the fundamental rate constants representing the number of activations in unit time; in the forward and backward directions, respectively over the energy barrier. The rate constants were derived from statistical mechanics (Fig. 1) as [1-3]

$$k_f = \kappa \frac{T}{h} \exp - \frac{\Delta G_f^* - W_f(\tau)}{\kappa T}$$

and

$$k_b = \kappa \frac{T}{h} \exp - \frac{\Delta G_b^* + W_b(\tau)}{\kappa T} \quad (2)$$



In Eqs. (2)  $k$  is the Boltzman constant,  $T$  is the absolute temperature,  $h$  is the Planck's constant,  $\Delta G^*$  is the free energy of activation and is equal to the chemical bond energy associated with the stems that take part in the dislocation movement, and the subscripts  $f$  and  $b$  refer to the forward and backward activations, respectively over a single energy barrier,  $W(\tau)$  is the work contributed by the shear stress which causes the plastic flow. The former is usually a linear function of the applied stress and is of the form [1]

$$W = V(\tau_a - \tau_i) \quad (3)$$

where  $\tau_a$  is the applied shear stress,  $\tau_i$  is the internal shear stress representing the resistance of the material to dislocation motion, and  $V$  is the activation volume or the product of the area swept out by the dislocation during a thermally activated movement and the Burger's vector  $b$  of the dislocation.

### 3. MOBILE DISLOCATION DENSITY

Specimens or machine components manufactured from engineering materials contain a large number of dislocations, vacancies, and other defects. During plastic deformation (caused by dislocation motion) the number of dislocations may remain fairly constant, as was assumed in previous studies [4, 8-13]. It was confirmed experimentally (and theoretically) that the assumption is indeed valid for the cyclic plastic deformation of a near eutectoid Zn-Al alloy. For other materials, however, the number of mobile dislocations changes in function of time, strain, and stress. Several empirical models have been proposed to describe the variation of the number of mobile dislocations during plastic deformation [5-7]. For the purpose of the present discussion, we use the relation proposed by Johnston and Gilman [5] describing the rate of change of the mobile dislocation as

$$\frac{d\rho_m}{dt} = \alpha\rho_m - \beta\rho_m^2 \quad (4)$$

where  $\alpha$  and  $\beta$  are multiplication and stalemating coefficients, respectively. According to Johnston and Gilman, the first term describes dislocation multiplication via breeding by Koehler multiple - cross - glide mechanism, while the second term describes the decrease in the mobile dislocation density caused by pairwise interactions through which the components of a pair are mutually stopped from moving or from existing. Integration of Eq. (4) leads to

$$\rho_m = \frac{\alpha\rho_0 \exp(\alpha t)}{\alpha + \beta\rho_0\{\exp(\alpha t) - 1\}} \quad (5)$$

where  $\rho_0$  is the number of mobile dislocations at  $t = 0$ . Equation (5) indicates that the dislocation density increases exponentially with time at first, because of the breeding process, and then the rate of change decreases to zero as  $\rho$  approaches the value  $\alpha/\beta$  asymptotically. Fig. 2 illustrates schematically the variation of the mobile dislocation density with time, based on Eq. (5).

#### 4. STRAIN CONTROLLED, TENSION-TENSION CYCLIC LOADING

##### 4.1 Constructive Equation

During cyclic deformation, the overall deformation rate of the specimen,  $\dot{\epsilon}$ , which can be measured experimentally is the sum of two components: the elastic strain rate,  $\dot{\epsilon}_e$ , and the plastic strain rate,  $\dot{\epsilon}_p$ . That is,

$$\dot{\epsilon} = \dot{\epsilon}_e + \dot{\epsilon}_p \quad (6)$$

The elastic strain rate is related to the shear stress rate as

$$\dot{\epsilon}_e = \frac{\dot{\sigma}}{E} = M \frac{\dot{\tau}}{E} \quad (7)$$

where  $E$  is the combined elastic modulus describing the net elastic response of the test specimen and grip assembly.

In the simplest deformation kinetics where thermally activated plastic flow in strain controlled cyclic deformation can be approximated with activation over a single energy barrier, the plastic strain rate is

$$\dot{\epsilon}_p = \rho_m A_f \exp V_f \frac{(\tau_a - \tau_i)}{kT} \quad (8)$$

where

$$A_f = \frac{b kT}{M h} \exp -\Delta \frac{G_f^*}{kT}$$

Consider that during cyclic deformation the material undergo work hardening. Within the low temperature range where annealing effects are negligibly small, the internal stress increases with the plastic strain (absolute value) as

$$\tau_i = \tau_i^0 + \frac{H}{M} \epsilon_p \quad (9)$$

where  $\tau_i^0$  is the internal stress at the beginning of the experiment and  $H$  is the work hardening coefficient. The applied shear stress is then expressed in function of the plastic strain rate (from Eq.(8)) by the relation



$$\tau_a = \frac{kT}{V_f} \ln \left( \frac{\dot{\epsilon}_p}{\rho_m A_f} \right) + \tau_i + \frac{H}{M} \epsilon_p \quad (10)$$

The applied shear stress rate at constant temperature then is

$$\dot{\tau}_a = \frac{kT}{V_f} \frac{1}{\dot{\epsilon}_p} \frac{d\dot{\epsilon}_p}{dt} - \frac{\tau_{eff}}{V_f} \frac{dV_f}{dt} - \frac{kT}{V_f} \frac{\dot{\rho}_m}{\rho_m} + \frac{H}{M} \dot{\epsilon}_p \quad (11)$$

where  $\tau_{eff} = \tau_a - \tau_i$  is the effective shear stress. However, it was established by Krausz and Eyring [1] that within the high stress and low temperature range, the activation volume is independent of stress and time.

Consequently, the applied shear stress rate within this range can be approximately as

$$\dot{\tau}_a / T \sim \frac{kT}{V_f} \frac{1}{\dot{\epsilon}_p} \frac{d\dot{\epsilon}_p}{dt} - \frac{kT}{V_f} \frac{\dot{\rho}_m}{\rho_m} + \frac{H}{M} \dot{\epsilon}_p \quad (12)$$

The combination of Eqs. (4), (6), (7) and (12) results in

$$\frac{MkT}{EV_f} \frac{1}{\dot{\epsilon}_p} \frac{d\dot{\epsilon}_p}{dt} + \left( 1 + \frac{H}{E} \right) \dot{\epsilon}_p = \dot{\epsilon}_p + \frac{MkT}{EV_f} (\alpha - \beta \rho_m) \quad (13)$$

The non-linear differential equation is similar to that derived previously [12] with  $\dot{\rho}_m = 0$ . The last term on the RHS of Eq. (13) represents the effect of the variations in the mobile dislocation density with time during strain controlled, tension-tension cyclic deformation. Following the procedure described before [11, 12], the solution of Eq. (13) is

$$\epsilon_p = \rho_0 A_f \exp \frac{\left\{ f(t) + \frac{V_f \dot{\epsilon}_p}{MkT} \right\}}{\rho_0 E A_f \frac{(1-\frac{n}{2})}{MkT} \int_0^t \exp \left\{ f(t) + V E \frac{\epsilon}{MkT} \right\}} dt + \dots$$

$$\dots \exp V_f \frac{(E \epsilon_0 - M(\tau_0 - \tau_i))}{MkT} \quad (14)$$

where  $f(t) = \int_0^t (\alpha - \beta \rho_m) dt$ ,  $\epsilon_0$  and  $\tau_0$  are the initial strain and stress, respectively at  $t = 0$ . The total strain  $\epsilon = \epsilon(t)$ , depending on the waveform (random, sinusoidal, triangular etc.) From Eq.(5),  $\rho_m = \rho_m(t)$ . Equation (14) therefore describes fully the plastic strain rate in function of time, temperature, material properties, and structural characteristics. It is emphasized that the equation is valid only within the temperature and stress range where thermally activated plastic flow can be approximated by activation of the applied shear stress during strain controlled cyclic loading follows from Eqs. (6), (7) and (14), thus

$$\tau_o = \tau_v + \frac{E(\epsilon - \epsilon_o)}{M} - \frac{kT}{V_f \left(1 + \frac{H}{E}\right)} \ln \left\{ \frac{V_f E A_f \left(1 + \frac{H}{E}\right)}{MkT} \exp V_f \frac{(\tau_o - \tau_i)}{kT} \rho_o \int_0^t \exp \left\{ f(t) + \frac{V_f E (\epsilon - \epsilon_o)}{MkT} \right\} dt + 1 \right\} \quad (15)$$

Stress relaxation is considered as a special case of strain controlled cyclic deformation where  $\epsilon = \epsilon_o = \text{Constant}$ . Because the total strain remain constant during stress relaxation, plastic deformation takes places without significant structural change. This means that the mobile dislocation density;  $\rho_m$  Constant and  $\dot{\rho}_m = 0$ . Consequently, Equation (15) reduces to

$$\tau_s = \tau_o - \frac{kT}{V_f \left(1 + \frac{H}{E}\right)} \ln \left\{ E A_f V_f \left(1 + \frac{H}{E}\right) \frac{\rho_o}{MkT} t \exp V_f \frac{(\tau_o - T_i)}{kT} + 1 \right\} \quad (16)$$

Eq. (16) is formally identical to that derived by Wielke and Shock [14], Krausz and Eyring [1], and also by Mshana and Krausz [11, 12]. It was widely utilized to describe stress relaxation in many materials (Fe, Cu, Zn, AL, steels, Pb, many polymers, graphite, etc.). The conclusion that follows from Eqs. (15) and (16) is an important one: stress relaxation is a special case of strain-controlled, tension-tension cyclic deformation. Consequently, stress relaxation experiments can be used to measure the constitutive parameters  $V_f$  and  $A_f$  that represent the microstructure; these can then be used in the development of the constitutive equations of the more complicated strain controlled cyclic deformation. However, the later requires the determination of the empirical parameters  $\alpha$  and  $\beta$  which characterize, define the variation of the mobile dislocation density with time.

#### 4.2 Evaluation of Stress Response

In a strain controlled cyclic loading experiment the stress response of the material BEHAVIOUR is determined. Within the stress, time and temperature range where the rate of plastic deformation can be approximated by activation over a single energy barrier, the stress response is evaluated using Eq. (15). It was shown before [1, 8-13] that (in the case of constant mobile dislocation density) when the first term in the argument of the exponent is much greater than unity, the stress change (or decrease in the load or stress) is propotional to the natural logarithm of time. Figure (3) shows typical material BEHAVIOUR or response during strain controlled cyclic loading. The material under investigation was a near entectoid Zn-Al alloy. The experimental details are presented elsewhere [4].

It is evident from Eq. (15) and from Fig.(2) that after sufficiently long time, the mobile dislocation density,  $\rho_m$ , approaches assymptotically an infinity value  $\alpha/\beta$ . The function  $f(t)$  in Eq. (15) (represented by the shaded are in Fig. (2)) then is approximately constant,

$$\text{i.e. } f(t) \Rightarrow \bar{f}(t) = \text{constant}$$



Subsequently, the stress change is evaluated as before; that is, the stress decrease during strain controlled cyclic loading is proportional to the natural logarithm of time. Fig. (4) shows qualitatively the effect of the variations in the mobile dislocation density on the stress change during strain controlled cyclic deformation. Curve A presents schematically the deformation during stress relaxation experiment where the total strain is kept constant (strain range  $\epsilon_r = 0$ ) and the mobile dislocation density is constant. The latter is indeed a valid assumption because there is very little plastic deformation during stress relaxation. The deformation BEHAVIOUR during tension-tension strain controlled cyclic deformation (for the same strain range,  $\epsilon_r$ ) is represented schematically by curves B and C. For curve B, it was assumed that the mobile dislocation density remains constant (hence  $\dot{\rho}_m = 0$ ) while for curve C the mobile dislocation density varies with time ( $\dot{\rho}_m \neq 0$ ). The change in dislocation density leads to a higher stress change. Because the mobile dislocation density increases, the plastic strain and strain rate increases as well. Consequently, according to Eq. (15), the stress change (or decrease) increases.

## 5. DISCUSSIONS AND CONCLUSIONS

The mathematical description of the variations of the material structural characteristics during plastic deformation has never been clearly established. There are several factors that make the formulation of the mathematical relations extremely difficult. Among them is the complexity due to the three (or sometimes multi) dimensionality of the problem. Usually the plastic strain rate as well as the material structural characteristics are represented by tensors [15]. In addition, manufacturing processes, such as rolling, forging, extrusion, etc. lead to anisotropy and hence the material properties (such as Young's Modulus, internal stress, etc.) and the material structural characteristics (activation energy, activation volume, mobile dislocation density etc.) vary with orientation. Furthermore, temperature variations cannot be predicted in real working conditions, yet this is an important service and manufacturing parameter. These are but only a few of the important factors that make the mathematical formulation of rational constitutive relations for cyclic plastic deformation of formidable task.

It is therefore evident that the exact mathematical description of the deformation BEHAVIOUR is not possible because of the unpredictability of the material structural characteristics. One can only incorporate empirical, phenomenological models for the former into the constitutive equation. The associated empirical parameters have then to be determined from experimental results: to be obtained from carefully designed experiments. This approach was illustrated in previous publications by the author [4, 8-13] using the simplest deformation kinetics or model. While the constitutive equation was vigorously derived, the associated material structural characteristics, that is, the activation volume, activation energy, and the mobile dislocation density were assumed to remain constant during plastic deformation. It was evident from the study that this assumption is only valid for certain materials and for specific temperature and stress range.

In the present paper, an empirical, phenomenological model for the mobile dislocation density was incorporated into the constitutive equation describing the plastic deformation during strain controlled cyclic loading. The qualitative analysis showed that due to the net increase in the number of mobile dislocations, the plastic and strain rate increases. Consequently, the stress change (or stress decrease) per cycle or in function of time during strain controlled cyclic deformation increases. However, the validity of the constitutive equation is limited to the stress and temperature range where the rate of plastic flow is controlled by activation over a single energy barrier. Needless to say, more work is yet to be carried out to collaborate the analysis above: both quantitative evaluation and experimental verification of the theory. The author is actively involved in the later.



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### Figure Captions

Figure 1 Schematic representation of the effect of the shear stress on the energy barrier associated with the plastic flow,  $w(r) \wedge \Delta G^*$  are the same, both for forward and backward activation. \* represents the activated state of the atoms during the usual random atomic vibrations.

Figure 2 Schematic representation the mobile dislocation density in function of time following Eq. (5). The shaded area represents the integral

$$f(t) = \int_0^t (\alpha - B\rho_m) dt.$$

Figure 3 Strain controlled cyclic loading and stress relaxation mean shear stress change represented in the shear stress change versus natural logarithm of time coordinate system for evaluation of the activation volume,  $V_f$ , and the activation parameter,  $S_f$ . The experiments were carried out on a near eutectoid Zn-Al alloy. The experimental details are presented elsewhere [4].

Figure 4 Schematic representation of the effect of the variation of the mobile dislocation density on the strain controlled cyclic deformation BEHAVIOUR.

Curve A represents stress relaxation while curve B and C represents the cyclic deformation BEHAVIOUR, for strain range,  $\sigma_c - \sigma_c'$ . The BEHAVIOUR represented by curve B assumes that  $\rho_m = \text{constant}$  while that of curve C considered that  $\rho_m \neq \text{constant}$ .

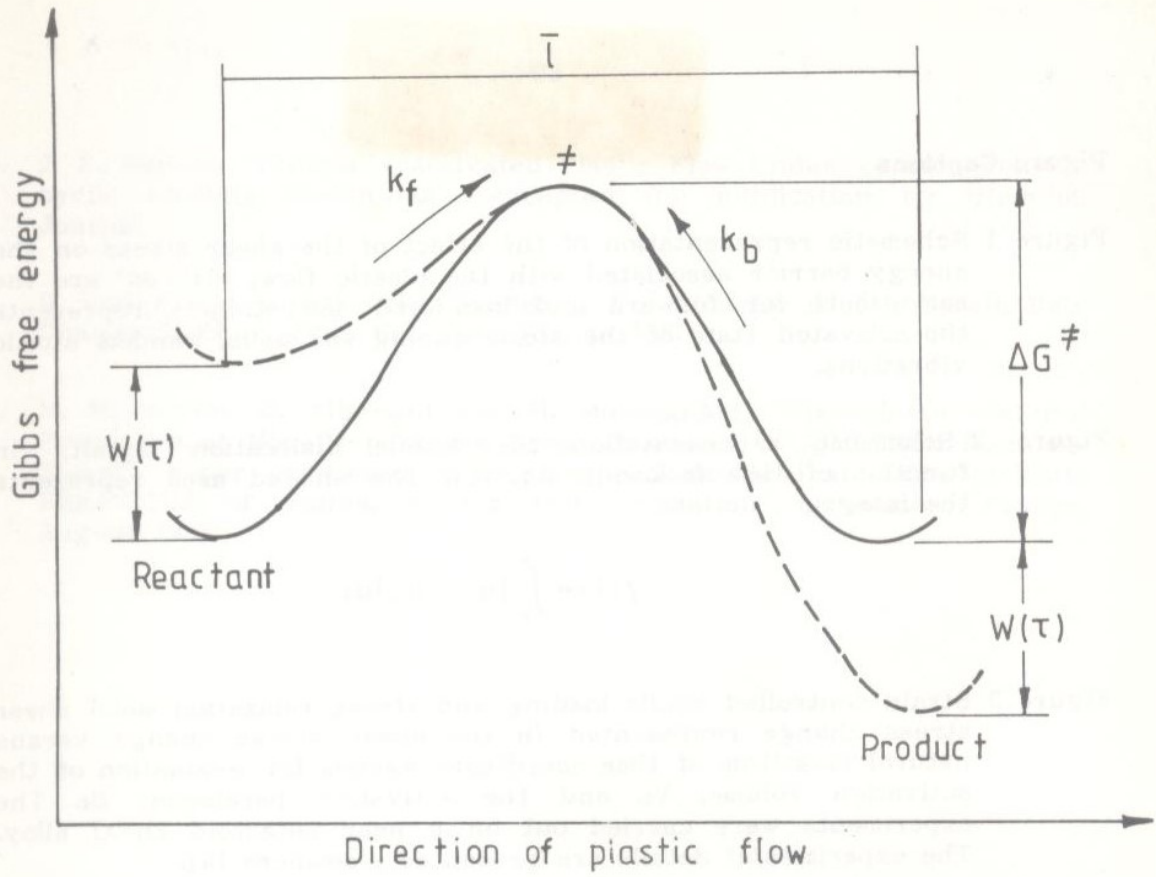


Figure. 1.

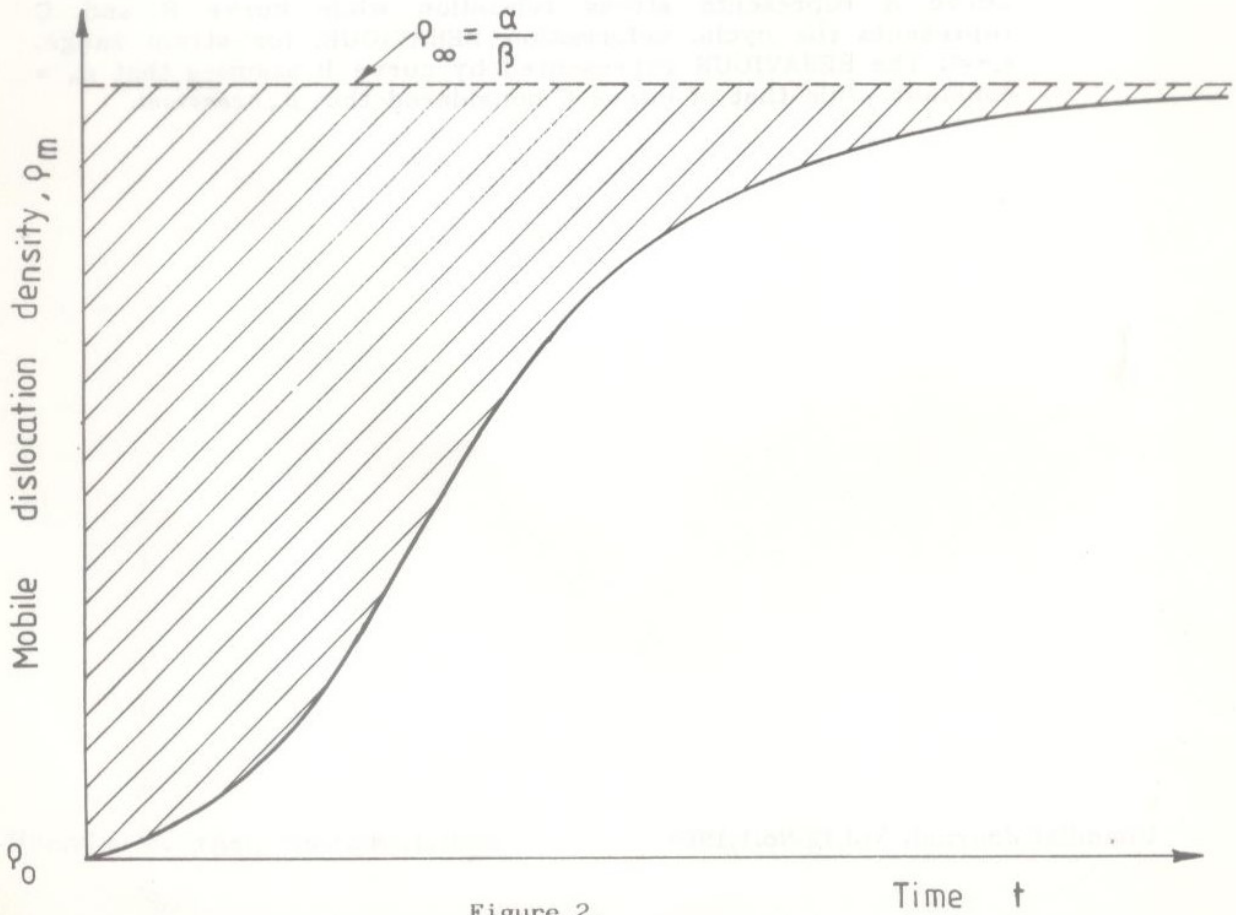


Figure.2.



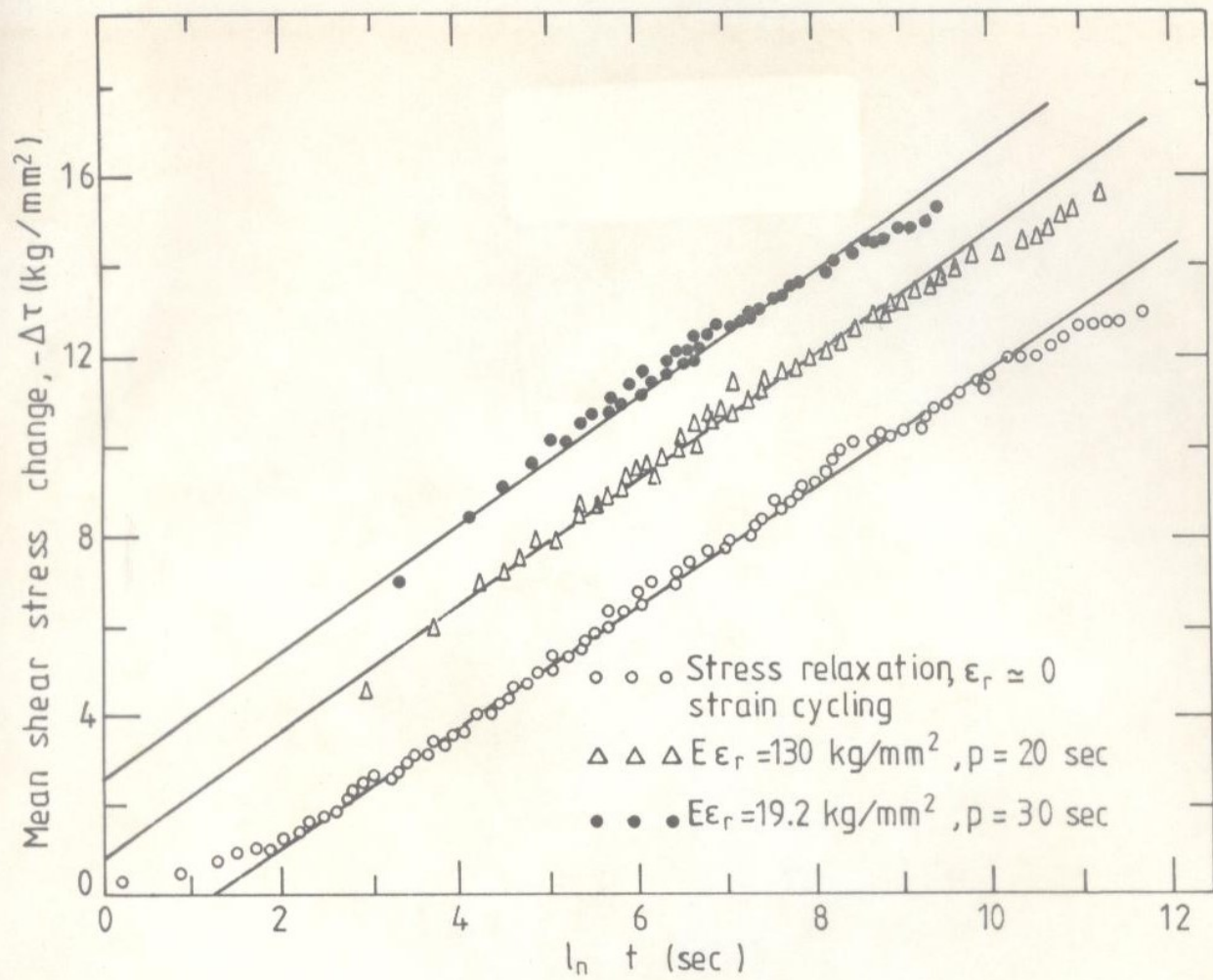


Figure. 3.

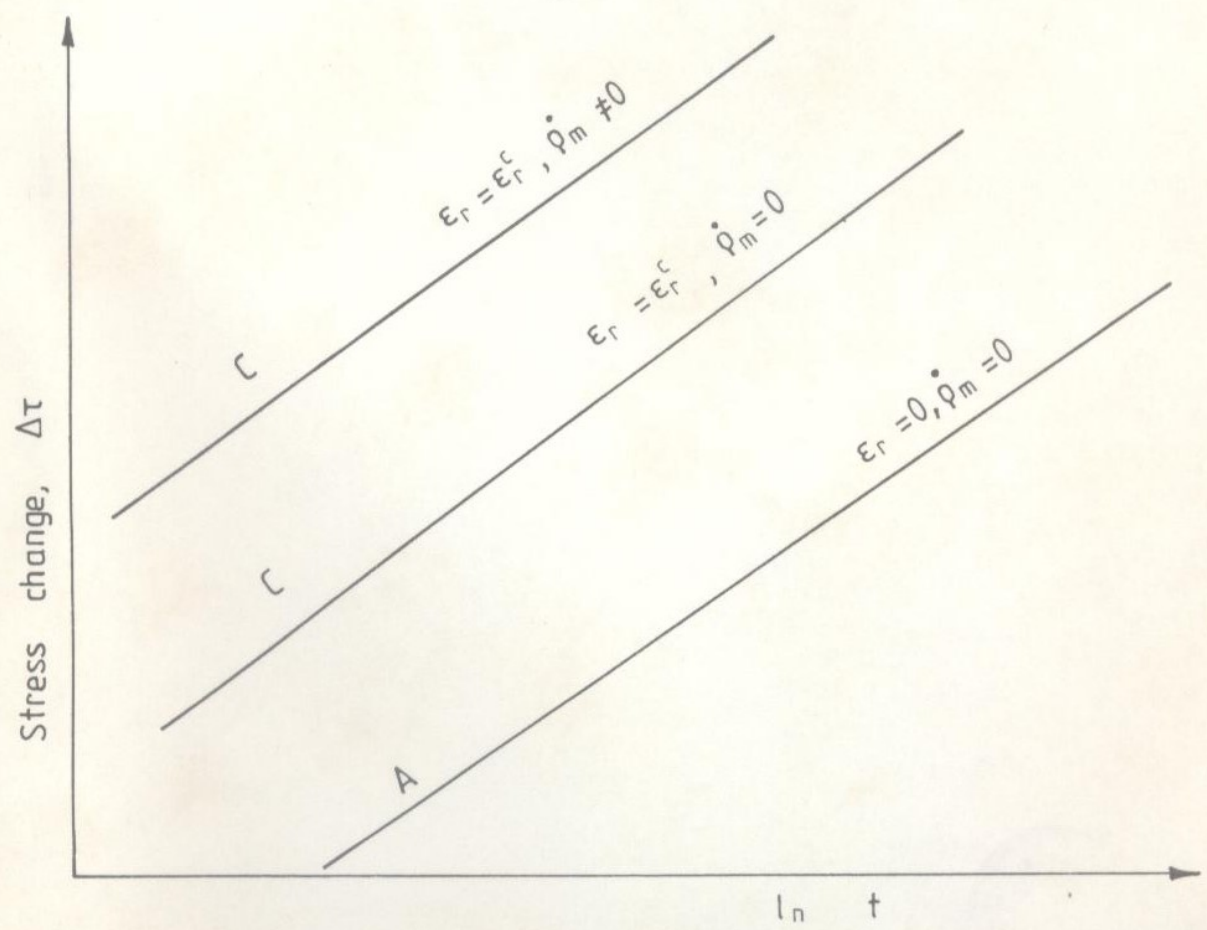


Figure. 4.