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## Temperature Dependence of the Effective and Internal Stresses at the Initial Stages of Plastic Deformation of the LiF Single Crystals. Macrodeformation and Dislocation Mobility Data

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An important feature of temperature dependences of the macroscopic parameters of plastic deformation — critical resolved shear stress (CRSS) and strain rate sensitivity of flow stress — is their uncorrelated change in the temperature range of 4.2 — 300 K. This seems to be due to a large contribution of the athermal component  $\tau_i$  to CRSS. The magnitude of  $\tau_i$  and its temperature dependence are determined mainly by the dislocation line structure, i.e. by the presence of high athermal jogs on dislocation.

### 1. Introduction

One of the most complicated problems in the thermoactivation analysis of plastic deformation is the separation of the applied stress  $\tau$  into the athermal  $\tau_i$  and thermal  $\tau^*$  components, which characterize the fields of the long-range and short-range potential barriers [1].

Widely described in the literature is a simple method of determining  $\tau_i$  which uses the temperature dependence of critical resolved shear stress (CRSS) [2], and is therefore suitable only for the initial stage of deformation. It is assumed that the ratio  $\tau_i/\mu$  ( $\mu$  is the shear modulus) is independent of the strain rate and temperature and is equal to a corresponding value in the region where the plastic flow is athermal. The condition that  $\tau_i/\mu(T) = \text{const.}$  seems not always be fulfilled [3–8].

This paper deals with the investigation of results of the temperature dependencies of CRSS, stress relaxation parameters at the initial stage of plastic flow and of mobility data of single screw dislocations in LiF crystals in the temperature range 1.6–300 K. It is shown that these data can be consistently using the concept of a decisive role of dynamic properties of individual dislocations in the plastic deformation. The thermal and athermal components of CRSS and stress required for the motion of dislocations are comparable in magnitude over the entire temperature range.

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## 2. Results and discussion

The experimental results discussed below have been obtained on LiF-2 crystals [9]. Figures 1 and 2 show the temperature dependencies of CRRS  $\tau_0(T)$  and the magnitude of the stress increment  $\Delta\tau(T)$  describing the amount of stress relaxation for getting a tenfold lower relaxation rate (the stress relaxation depth). The vertical bars in Fig. 1

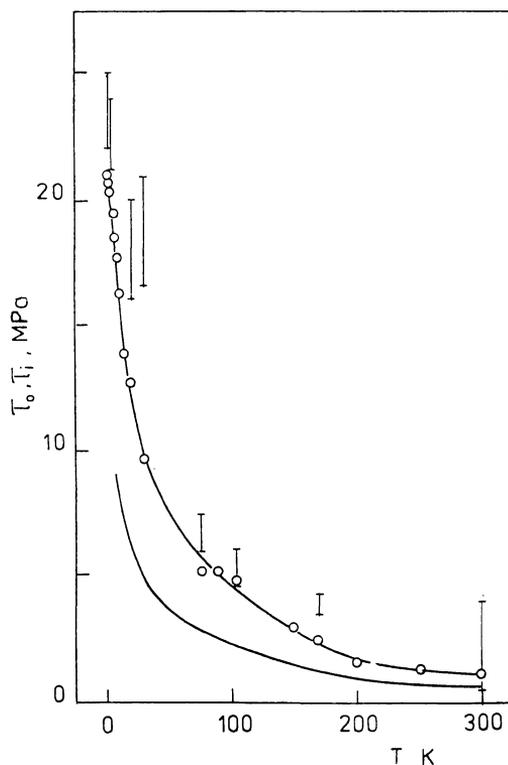


Fig. 1. Temperature dependences of the CRSS  $\tau_0(T)$  and of the athermal component  $\tau_i(T)$ . Vertical bars indicate the stress ranges at which the velocities of individual screw dislocations at corresponding temperatures were measured.

indicate the stress intervals in which the mobility of single screw dislocations was measured at the corresponding temperatures. In these cases the dislocation velocities were in the range of  $10^{-6}$  cm/s  $< v < 10^{-2}$  cm/s. Some  $v(\tau)$  dependence covering the widest range of velocities and stresses are given in [9]. In the  $\log v - \tau$  coordinates they become rectilinear with the slope being decreasing with the decreasing temperature.

An important feature of the  $\tau_0(T)$  and  $\Delta\tau(T)$  curves shown in Fig. 1 and 2 is their uncorrelated change in the temperature range studied, which disagrees with

the concept of thermal character of the deformation. Indeed, the exponent  $m = H/kT$  of the Arrhenius equation, should be temperature-independent provided that the preexponential factor  $\dot{\gamma}(\tau T) = \text{const.}$ . Its value is acceptable if it is within  $m = 20$  to 30. However, as is seen from Fig. 2, the value of  $m'$  calculated from the  $\tau_0(T)$  and  $\Delta\tau(T)$  data by the formula

$$m' = -T(\Delta \ln |\dot{\epsilon}|/\Delta\tau)_T(\Delta\tau_0/\Delta T)_{\dot{\gamma}} \quad (1)$$

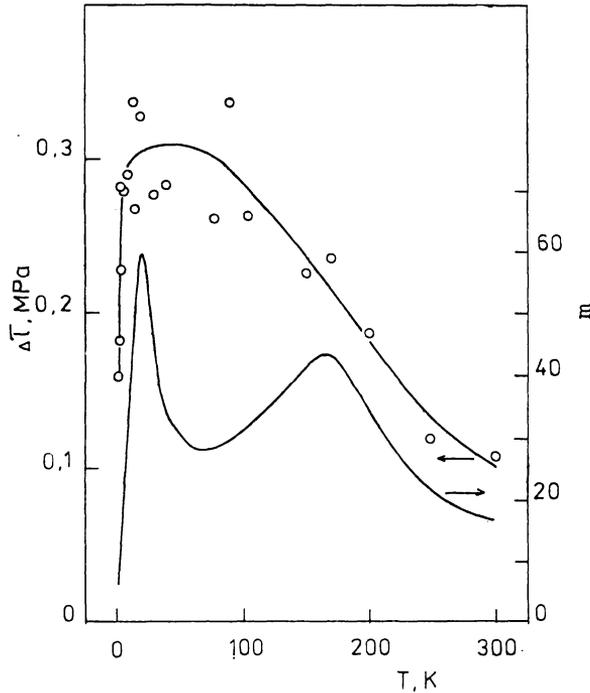


Fig. 2. Temperature dependences of the stress relaxation depth  $\Delta\tau$  and  $m' = -T(\Delta \ln |\dot{\epsilon}|/\Delta\tau)_T \cdot (\Delta\tau_0/\Delta T)_{\dot{\gamma}}$ .

( $\dot{\epsilon}$  is stress relaxation rate and  $\dot{\gamma}$  is shear strain rate) is not only strongly temperature-dependent, but also assumes unreasonably high values of the order of 60.

It seems reasonable to assume that this discrepancy can be principally caused by the fact that the temperature dependence of the CRRS is determined by the both stress components. Then the  $\Delta\tau_0/\Delta T$  value determined by graphical differentiation of the  $\tau_0(T)$  curve consists of two terms and Eq. (1) read as

$$m' = -T(\Delta \ln |\dot{\epsilon}|/\Delta\tau)_T(\Delta\tau^*/\Delta T)_{\dot{\gamma}} - T(\Delta \ln |\dot{\epsilon}|/\Delta\tau)_T(\Delta\tau_i/\Delta T)_{\dot{\gamma}} \quad (2)$$

Since the stress relaxation at low-temperature deformation in most materials is due to the decrease of the effective stresses  $\tau^*$  [7], one can assume that the first term in (2)  $m = -T(\Delta \ln |\dot{\epsilon}|/\Delta\tau)_T(\Delta\tau^*/\Delta T)_{\dot{\gamma}}$  characterizes the thermally activated

processes and  $m(T) \cong \text{const}$ . In this case the second term should be responsible for the anomalous behavior of the experimental value of  $H/kT$ .

Let us estimate the relative contribution of  $\tau^*$  and  $\tau_i$  to  $\tau_0$ . We will calculate the effective stress using the  $\Delta\tau(T)$  data shown in Fig. 2 by graphical integration using the formula

$$\tau^*(T) = - \frac{m}{\Delta \ln |\dot{\epsilon}|} \int_{T_1}^T \frac{\Delta\tau}{T} dT, \Delta \ln |\dot{\epsilon}| = 2.3 \quad (3)$$

At  $T_1 = 300$  K we took the value of  $\tau^* = 0.5$  MPa, which is equal to the difference between CRSS and the breakaway stress of the screw dislocation motion. The  $\tau_i(T)$  dependence shown in Fig. 1 has been obtained for  $m = 20$  as the difference between curves  $\tau_0(T)$  and  $\tau^*(T)$ .

The analysis made indicates that the athermal component contribution to  $\tau_0$  can be large and comparable in magnitude with  $\tau^*$  in the whole temperature range studied.

The question of microscopic dislocation mechanisms which provide a strong temperature dependence of both CRSS components is not quite clear. The situation concerning the nature of thermally activated process is comparatively simple. The model of dislocation drag by impurity-vacancy dipoles proposed by FLEISCHER [10] successfully explained the solid-solution hardening of alkali halide is described by

$$\frac{\Delta\tau}{T^{1/2}} = \frac{\tau_c^*}{T_c^{1/2}} \frac{\Delta \ln \dot{\gamma}}{\ln(\dot{\gamma}_0/\dot{\gamma})} \left( 1 - \left( \frac{T}{T_c} \right)^{1/2} \right) \quad (4)$$

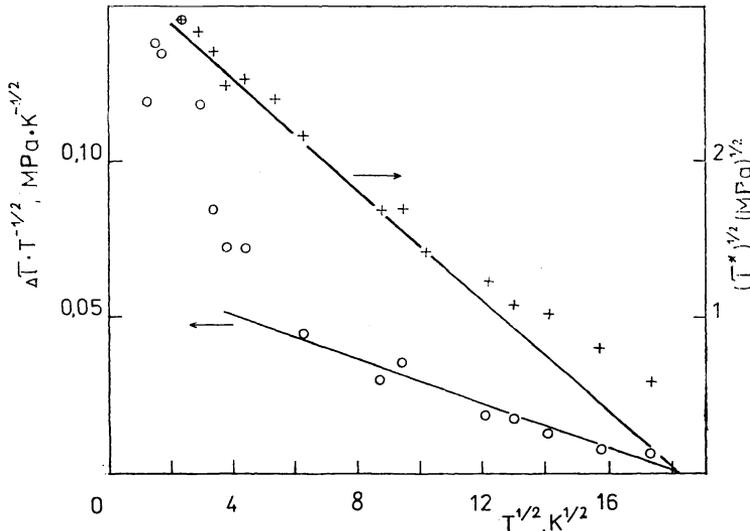


Fig. 3. Temperature dependence of the stress relaxation depth  $\Delta\tau$  and the effective stress  $\tau^*$  in coordinates of  $\Delta\tau/T^{1/2} - T^{1/2}$  according to FLEISCHER's theory.

where  $\tau_c^* = \tau_0^* (0 \text{ K}) = 0.55 H_0 c^{1/2} / b^3$ ,  $T_c = H_0 / k \ln(\dot{\gamma}_0 / \dot{\gamma})$ ,  $H_0 = \mu b^3 \Delta \varepsilon / 3.86$  is the potential barrier height,  $b$  is the Burgers vector modulus,  $\Delta \varepsilon$  is the tetragonality of local impurity-vacancy defect,  $c$  is the concentration of these defects. Figure 3 shows that for LiF-2 crystals the relation (4) holds fairly well up to  $T \sim 20 \text{ K}$ . The deviation from this dependence at lower temperatures can be attributed to a new dislocation drag mechanism connected with the Peierls relief [11]. The theoretical parameters [10] are quite reasonable:  $T_c = 342 \text{ K}$ ,  $H_0 = 0.6 \text{ eV}$  (at  $m = 20$ ),  $\Delta \varepsilon = 0.38$ ,  $\tau_c^* = 10.3 \text{ MPa}$ ,  $c = 20 \cdot 10^{-6}$  (the impurity concentration measured by LUBENETS et al. [9] is equal  $11 \cdot 10^{-6}$ ). The  $\tau_c^*$  value is about half that of the CRSS measured at  $T = 1.6 \text{ K}$ . Thus, the dependence  $\tau(T)$  (and hence  $\tau^*(T)$ ) can be explained in terms of the theory of thermally activated overcoming of local barriers by dislocations.

Before discussing the question of the origin of athermal component  $\tau_i$  and its temperature dependence we should consider Fig. 1. One can see an approximate equality and qualitative agreement in the behavior, within the temperature range studied, of two values: CRSS and stress required for the motion of individual dislocations. For this reason, it can be supposed that the dislocation ensembles formed at the beginning of deformation do not significantly influence the dislocation mobility, so that the kinetics of deformation in the CRSS region is, probably, mainly determined by the behavior of individual dislocations in the initial crystal.

In ionic crystals screw dislocation can easily cross slip. Due to the repetition of double cross slip events, a system of differently high jogs acting as additional pinning points may be formed. From these jogs superjogs can be generated by coalescence. Due to this structure changes of the dislocations the shear stress to move them probably increases.

The hypothesis of structure change of the dislocation line in the process of its motion was proposed when discussing the experimentally obtained unusual dependences of screw dislocation velocity on the stress and temperature  $v(\tau, T)$  in KCl crystals within the temperature range  $77-300 \text{ K}$  [12]. These dependences are qualitatively similar to those observed in LiF crystals up to  $T = 4.2 \text{ K}$ . The level of opposing stresses is determined by the stationary state of dislocation which should probably depend both on the initial defect structure of a crystal dictating the initial distribution of internal stresses and on the ambient conditions: the temperature and the applied stress. This means that the  $\tau_i$  value under discussion is not obligatorily a direct characteristic of microinhomogeneous elastic field really existing in a crystal.

Assuming that the athermal stresses shown in Fig. 1 are completely due to the presence of superjogs on the dislocations, their density calculated by the formula  $n_j = \tau_i / \mu b$  varies from  $n_j = 5 \cdot 10^2 \text{ cm}^{-1}$  at  $T = 300 \text{ K}$  to  $n_j = 10^4 \text{ cm}^{-1}$  at  $T = 4.2 \text{ K}$ , i.e. increases by a factor of 20 when decreasing the temperature from room to  $4.2 \text{ K}$ . A comparison with the estimation of the total density of jogs [13-14], indicates that athermal jogs can amount to only a small portion of their total number on a dislocation.

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