### Материаловедение. Нанотехнологии

УДК 539.3

## ELECTRIC EFFECTS UNDER PLASTIC DEFORMATION AT THE CRACK TOP IN CRYSTALS WITH CHARGED DISLOCATIONS

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Key words and phrases: charged dislocation; crack; electric field; modeling.

**Abstract:** Static and dynamic of a sliding line formation at the crack top were carried out. The number, equilibrium positions and kinetics of dislocations in a plastic zone were determined. An electric field, dipole moment and dislocation current, connected with the movement of dislocations in the plastic zone, for crystals with charged dislocations were calculated.

#### Introduction

In many dielectric and semiconductor crystals dislocations are charged. The electric charge of a dislocation can be sufficiently great and amounts to a value of one elementary charge *e* falling on a lattice parameter. In this case additional electrostatic interaction of dislocation is nearly equal to elastic and also can essentially influence their equilibrium positions in pile-ups. Besides, charged dislocation pile-ups create not only elastic, but also electric fields in a crystal. The fields can be stationary fields of motionless charged dislocation pile-ups and low-frequency variable electric fields connected with movement and reorganization of dislocation pile-ups. For the first time attention to some peculiarities of manifestations of such effects was paid in work [1].

In the present paper the electric fields created by a plastic zone at the top of a crack in LiF crystals are considered. Similar results for the planar stopped pile-up extending after load removal are given for comparison.

### A Method of Calculation

Let's consider a dislocation to be charged uniformly with linear density of a charge  $\lambda$ . We shall introduce function [2]

$$E(z) = E_x(z) + iE_v(z),$$

real and imaginary parts of this function represent intensity components of an electric field in the decart system of coordinates with the center on the dislocation line, and z = x + iy is a point of a complex plane. Then the field of the charged edge dislocation is determined by expression

$$\overline{E}(z) = \frac{2\lambda}{\varepsilon} \frac{1}{z},\tag{1}$$

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where in the left part there is a function which is complex-conjugate to E(z),  $\varepsilon$  is the dielectric constant.

For definition of an electric field dislocation pile-up it is necessary to summation (1) on number of dislocations in the pile-up

$$\overline{E}(z) = \frac{2\lambda}{\varepsilon} \sum_{i=1}^{n} \frac{1}{z - x_i},$$

where  $x_i$  are the coordinates of pile-up dislocation, n is the dislocation number in it.

The procedure of calculation of a static configuration of dislocations in the sliding line at the top of a crack is described [2]. Two stages of formation of the dislocation structure at the top of a crack are considered: formation of sliding lines at the moment of a crack stop (the sample remains loaded) and their evolution after unloading of the sample.

In the dynamic approach the equations of the dislocation movement are solved

$$\frac{dx_i}{dt} = \begin{cases} b\sigma(x_i)/B, \ \sigma(x_i) \ge \tau_s; \\ 0, \ \sigma(x_i) < \tau_s, \end{cases}$$
(2)

where  $\sigma(x_i)$  are stresses working on a dislocation, *B* is the constant of braking,  $\tau_s$  is the friction stress of the lattice, equal to a starting stress of dislocation movement. The value  $\sigma(x_i)$  is defined the same way as in [2]. The equations (2) were solved numerically.

#### **Results and Discussion**

Results of one variant of calculation for the loaded crack and after removal of loading are shown in Fig. 1.

It is seen, that the values of the field intensity E can be sufficiently great. At a distance of ~20 µm from the pile-up boundary it can achieve values of the order  $3 \cdot 10^5$  V/m. In the area adjoining the pile-up boundary the field intensity increases inversely proportional to the distance from the last dislocation. Therefore on smaller distances its value can be equal to the intensity of an ambient air voltage failure.



a – the loaded sample; b – after unloading; l – on continuation of the pile-up; 2 – in the tail part of the pile-up



After the sample is unloaded the values of the field intensity slightly decrease due to the fact that a part of dislocations come out onto the surface of a crack (Fig. 1, b).

If the amount of dislocations in the pile-up is changed the electric dipole moment *P* connected with the pile-up will vary as well. The electric moment of the pile-up related to the unit of length of a dislocation is as follows

$$P(t) = \lambda \sum_{i=1}^{n} x_i(t).$$
(3)

The derivative of (3) will determine the dislocation current

$$I(t) = \lambda \sum_{i=1}^{n} \frac{dx_i}{dt} = \lambda \sum_{i=1}^{n} v_i.$$

Change of the value P depending on time is shown on Fig. 2. It is seen, that the value P grows at the stage of dislocation emission up to the upper bound. Then at the second stage of the process it slightly decreases as a result of coming out of a part of dislocations onto the surface of a crack. Each stage takes  $\sim 50 \ \mu s$ . The total time of formation of the sliding line is approximately twice more. It will vary a little depending

on conditions of the crack stop and characteristics of a crystal. Thus the majority of the electric signals, connected with formation of the sliding line at the top of a crack, will have average frequency  $\sim 5 \cdot 10^4 \text{ s}^{-1}$ .

It was thought to be interesting to compare results received for a crack with the data relating to movement of the isolated sliding bonds in crystals. Calculations have been made for the stopped pile-up extending after it's fast unloading. The pile-up electric moment is the increasing function of time during the whole process of dislocation movement (Fig. 3). The dislocation current connected with the pile-up movement has the form of a sharp spike quickly descending later to a zero level at the end of movement. Dependencies P(t) and I(t)



Fig. 3. Time-dependent electric moment (1, 2, 3) and dislocation current (4, 5, 6) of the extending pile-up, initially locked on both sides:  $1, 6 - \alpha = 2; 2, 5 - \alpha = 3; 3, 4 - \alpha = 8$ 

are more slightly sloping at small  $\alpha$ . Here coefficient  $\alpha$  is equals the ratio of final pileup length and the initial one, i.e. it characterizes the level of initial loading.

Within the limits of sufficiently great  $\alpha$  we have pile-up expansion, all dislocations of the pile-up at t=0 are in a point x=0. Relaxation time can be estimated as the time during which the head dislocation moves off on the final distance  $l_k$ . We shall make the necessary estimations.

Using results [3], for an extreme case the pile-up length can be written down as follows

$$l = \left(\frac{8bAn}{3B}\right)^{1/2} \sqrt{2t},\tag{4}$$

where  $A = Gb/2\pi(1-\nu)$ , G is the shear modulus, v is Poisson's ratio. We shall receive relaxation time from equality  $l = l_k$ 

$$t = \frac{3BnA}{4b\tau_s^2},$$

where  $\tau_s$  are friction stresses. For LiF crystals  $t = 14, 4 \cdot 10^{-6}$  s. From the solution of equations (2) we receive  $t = 13, 2 \cdot 10^{-6}$  s.

At greater  $\boldsymbol{\alpha}$  it is possible to receive the following expressions for the dipole moment

$$P(t) = \frac{\lambda B l^3}{8bA} (2t)^{1/2},$$
(5)

and for the dislocation current of a moving pile-up

$$I(t) = \frac{\lambda B l^3}{8bA} (2t)^{-1/2}.$$
 (6)

Expressions (5) and (6) make a satisfactory approximation of real dependencies of the moment and the current on time at high levels of initial loading on the sample or small friction stresses  $\tau_s$  accordingly.

Asymptotic root dependence of the pile-up length on time (4) can be also used for estimation of time parameters of formation of the sliding line at the top of a crack.

#### Conclusions

The electric field intensity connected with the dislocation emission from the top of a crack in LiF crystals was calculated. Time parameter of the formation of the electric signal is estimated. Results can be used for interpretation mechanoelectrical phenomena in crystals with charged dislocations.

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# Электрические эффекты при пластической деформации в вершине трещины в кристаллах с заряженными дислокациями

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**Ключевые слова и фразы:** заряженная дислокация; моделирование; трещина; электрическое поле.

Аннотация: Выполнено статическое и динамическое моделирование формирования линии скольжения в вершине трещины. Определены число, равновесные положения и кинетика дислокаций в пластической зоне. Для кристаллов с заряженными дислокациями рассчитаны электрическое поле, дипольный момент и дислокационный ток, связанный с движением дислокаций в пластической зоне.

## Elektrische Effekte bei der plastischen Deformation im Gipfel des Risses in den Kristallen mit den geladenen Versetzungen

**Zusammenfassung:** Es ist die statische und dynamische Modellierung der Formierung der Linie des Gleitens im Gipfel des Risses erfüllt. Es sind die Zahl, die gleichschweren Lagen und die Kinetik der Versetzungen in der plastischen Zone bestimmt. Für die Kristalle mit den geladenen Versetzungen sind das elektrische Feld, das Dipolmoment und der Versetzungsstrom, der mit der Bewegung der Versetzungen in der plastischen Zone verbunden ist, berechnet.

# Effets électriques lors de la déformation plastique au sommet de la fissure dans les cristaux avec les dislocations chargées

**Résumé:** Est effectué le modélage dynamique et statistique de la formation de la ligne du glissement au sommet de la fissure. Sont déterminés le nombre, les positions d'équilibre et la cinétique des dislocations dans la zone plastique. Pour les cristaux avec les dislocations chargées sont calculés le champ électrique, le moment dipolaire et le courant de dislocation lié au mouvement des dislocations dans la zone plastique.

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