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The internal stress relaxation modeling in the polygonization in alkali halide single crystals

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The evolution of the dislocation system during annealing in the absence of external loading after the three-point bending of a single crystal with a NaCl-type lattice, pricked out along the cleavage planes is modeled with the discrete dislocation dynamics method. The change of the average shear stresses value produced by the dislocation structure in the surrounding crystal and stresses acting on the dislocation ensemble themselves are obtained.

Keywords: dislocation dynamics, internal stress, polygonization.

Методом дискретної дислокаційної динаміки промодельовано еволюцію дислокаційної системи при вільному відпалі після триточкового згину монокристала з граткою типу NaCl, що був виколотий по площинах спайності. Визначено зміну величини середніх зсувних напружень, які утворює дислокаційний ансамбль в оточуючому кристалі, та локальних напружень, що діють на самі дислокації ансамблю.

Ключові слова: динаміка дислокацій, внутрішні напруження, полігонізація.

Методом дискретной дислокационной динамики промоделирована эволюция дислокационной системы при свободном отжиге после трехточечного изгиба монокристалла с решеткой типа NaCl, выколотого по плоскостям спайности. Определено изменение величины средних сдвиговых напряжений, создаваемых дислокационным ансамблем в окружающем кристалле, и локальных напряжений, действующих на сами дислокации ансамбля.

Ключевые слова: динамика дислокаций, внутренние напряжения, полигонизация.

Introduction

It is well known that the plastic deformation of single crystals is largely determined by the movement of dislocations. The plastic deformation velocity provided by the motion of dislocations is defined by Orovan:

$$\dot{\varepsilon} = \rho b \upsilon ,$$

where ρ – density of the moving dislocations, b – the Burgers vector value, υ – the average velocity of dislocations.

In turn, the velocity of dislocations motion depends on the applying stress and the dislocation mobility. Effective stress applied to the dislocation is the sum of the external applying stress to the sample, and the stress from all sources within the crystal (internal stresses). In a fairly pure crystals main source of stress is the dislocation ensemble.

Thus, the factors that determine the rate of the crystal deformation are: external stresses (σ_{ext}); dislocation density; dislocation mobility which depends on the temperature and relative position of dislocations (dislocation configuration); the value of the internal stress (σ_{int}), which depends on their relative position at a constant dislocation density. If the external stresses we can change (we could put a define level of the external stresses), the internal stresses are determined mainly by the prehistory of the sample (so we could not influence on a level of internal stresses).

The internal stresses for creep or active loading tend to hinder the movement of dislocations and $\sigma_{eff} = \sigma_{ext} - \sigma_{int}$. Whereas in the absence of the external influence $\sigma_{eff} = \sigma_{int}$.

The field of elastic stresses generated by dislocations is inhomogeneous. We can use superposition principle to the stress. Then the level of stress will substantially depends on the point within the crystal. Therefore, we considered it in terms of the average value of the internal stresses σ_{int}. If the value of the external stresses is insufficient for the new dislocations multiplication, it makes sense to talk about internal stresses only as a consequence of the dislocations interaction themselves.

In considering the dislocation subsystem evolution of the crystal in the absence of external stress (for example, with the annealing in the absence of external loading) the relaxation of the internal stresses will be, mainly by reducing the number of dislocations (annihilation or following dislocation to the surface). The dislocations

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ensemble will change it's configuration at a sufficient temperature and time. The question arises, how the rebuilt dislocations change the internal stress?

In the literature there are conflicting data regarding this. From the fact that the internal stresses do not change till they reduce several times [1 - 3].

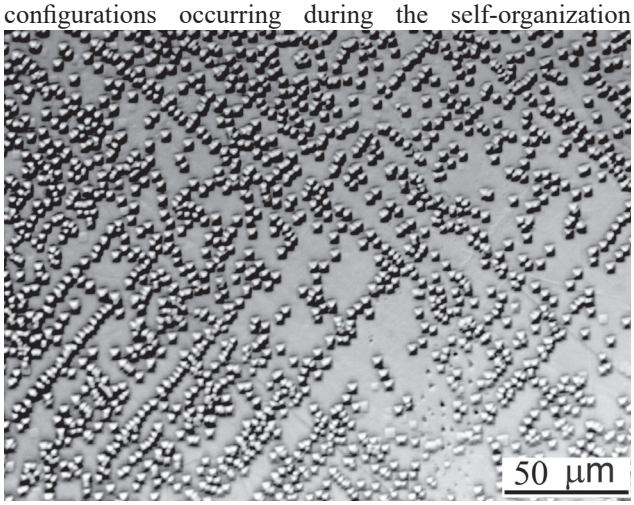
The internal shear stresses in the equilibrium position can be extremely small for dislocations forming a stable dislocation structure. Therefore such a dislocation can move even by applying slight external stress. However, in order to finally leave the stable structure (and contribute to plastic deformation) dislocation should overcome the potential barrier, much greater stress must be applied (for example, when the dislocation leaves the infinite symmetric tilt boundaries [4, 5]).

The problem of calculation of the field of elastic stresses generated by the dislocation ensemble has been theoretically solved in a few simple cases. For example, it was solved for an infinite symmetrical low-angle boundaries and slip bands with equidistant dislocations [4]. It is difficult to solve for intermediate dislocation configurations occurring during the self-organization process (in particular, in the polygonization) because of cumbersome calculations. Our goal was to determine by computer simulation the average shear stress value in the polygonization process. Furthermore, since the dislocation mobility is determined by elastic stress acting on them values of shear stress acting on a dislocation during polygonization are calculated.

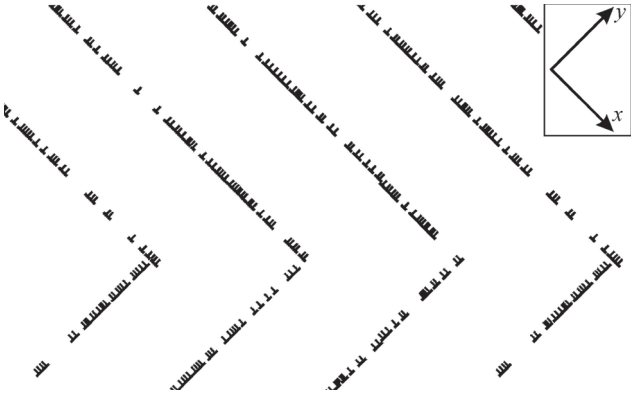
Model description

Using discrete dislocation dynamics method we can make a forecast of dislocation ensemble evolution and estimate the share stresses values which affect on dislocation mobility.

In this paper, by the discrete dislocation dynamics modeling (detailed simulation procedure is described in [6]) the internal average shear stress relaxation in the polygonization process in alkali halide single crystals with the NaCl type lattice is considered. The crystal was pricked out along the cleavage planes and deformed under three-point bending scheme. Such a deformation scheme is convenient because in the central part of crystal basically only edge dislocations with mutually perpendicular Burgers



a



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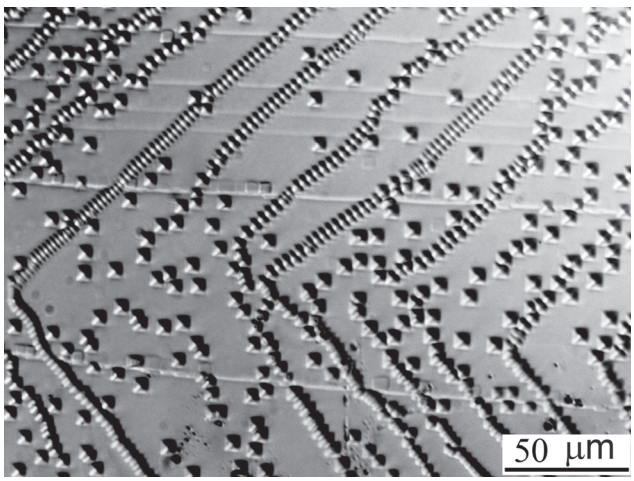

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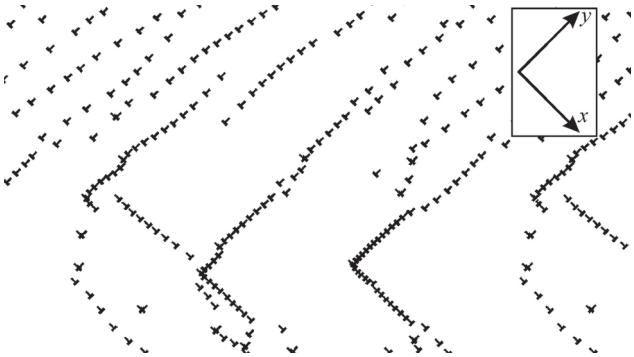

d

Fig.1. Dislocation configuration. a, b – initial distribution; c, d – $t = 200$ min, T = 550°C. NaCl.

vectors are formed. The dislocation lines are parallel to the bending axis. Then the problem of the distribution of dislocations and their movement actually becomes two-dimensional.

In this model, internal stresses are caused by the dislocations. Each dislocation produces around itself an elastic stress field. This field acts on the rest of the ensemble of dislocations. We assume that the velocity of movement of the dislocation line elements at each point is determined only by the total force acting on the element [6]. This model can be used when the radius of the dislocation line curvature greatly exceeds the average distance between dislocations.

The values of elastic moduli and the Burgers vector and parameters combining the dislocation velocity with the value of the applied stress were taken for NaCl crystals. There is easy slip system {110} <110> in crystals with the NaCl type lattice. We choose the coordinate axes so that the x and y axes are oriented along the {110}, the z axis is directed along the banding axis [001].

A system consisting of a straight edge dislocations with mutually perpendicular Burgers vectors («A» – $\vec{b}_A = (b,0,0)$ и «B» – $\vec{b}_B = (0,b,0,)$) is considered. The dislocation lines directed along the z axis. Such type of dislocations are formed in pricked out along the cleavage planes <100> crystals during three-point bending with respect to an axis parallel to the {100}.

Periodic boundary conditions were used to avoid dealing with features associated with the crystal surface. There is the rectangular area of the size $L_x \times L_y$ of the sides parallel to the Burgers vectors direction (it was determined that an arbitrary orientation of the rectangle sides in the xy plane does not change the results, if the size of the area is much larger than the average distance in the range dislocations). There are qualitatively the same results when selecting L_x and L_y in range 100 – 500 μm.

The initial dislocations distribution in the crystal deformed by three-point bending is shown (fig.1 a, b). The dislocations are located in two mutually perpendicular sliding bands. The initial dislocations positions within the area (x_i, y_i) have been set. The contents of this area was repeated 8 times in the surrounding (on the sides and corners) rectangular areas:

$$x_j = x_i + mL_x, \quad m = 0, \pm 1;$$

$$y_j = y_i + nL_y, \quad n = 0, \pm 1;$$

m and n are not simultaneously zero. The dislocation interaction with each other and with all the «clones» in neighboring areas is considered. If the dislocation leaves the selected area, such as a dislocation enters the area from the opposite side.

The first we settle the define initial dislocation arrangement by three point bending plastic deformation. After bending plastic deformation there is no external stresses, and the temperature is sufficient for the active dislocation creep. The number of dislocations is constant.

Results

In the process of modeling the average shear stress value created by the dislocation ensemble in the crystal is calculated. In order to reduce the effect of point observation location the stresses is calculated in 200 points uniformly distributed around the circumference whose radius is greater than tenfold L_x. The results are averaged.

In addition the total shear stress (normalized to the dislocation number) acting on the dislocation ensemble themselves is calculated.

The dependence of the average shear stress from time is shown in fig. 2. σ_{xy}^0 is shear stress at the initial time. It would seem that this average shear stress should be reduced

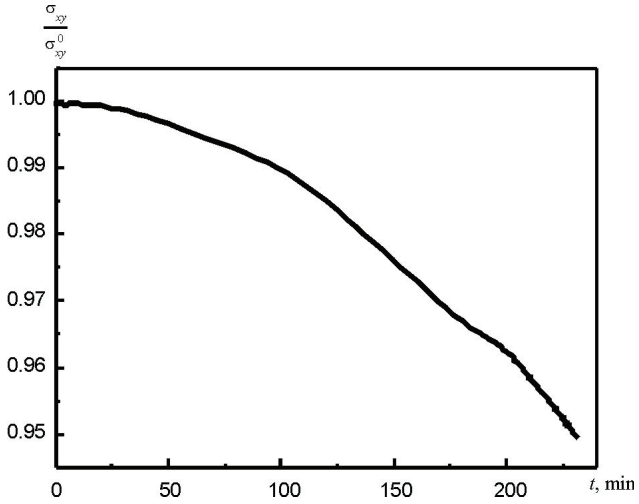

Fig. 2. The average shear stress value created by the dislocation ensemble in the surrounding crystal vs. time. T = 550°C. NaCl.

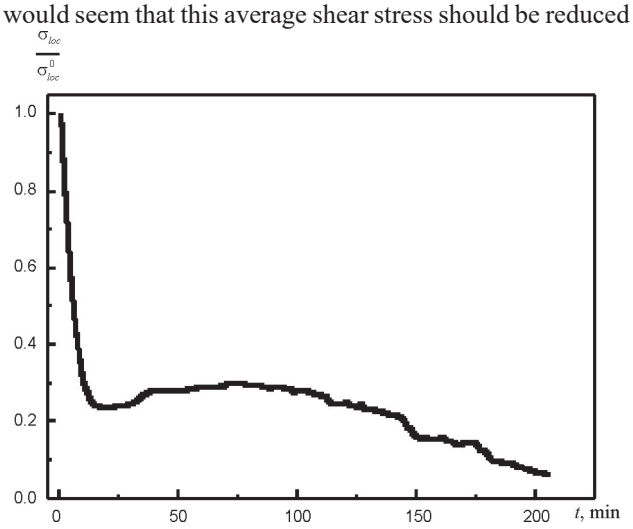

Fig. 3. The local average shear stress value created by the dislocation ensemble vs. time. T = 550°C. NaCl.

during dislocation self-organization process (from the placement of the dislocations in the slip bands to build dislocation boundaries) but average shear stress has changed near 5%. This suggests that if we considered the dislocation density reducing by annihilation process or dislocations leaving by crystal surface, then the effect we have obtained would not put evident contribution to the average shear stress reducing.

The simulation result agrees qualitatively with the conclusion reached by in [7]. Where it is stated that the dislocation self-organization in a condition of forbidden climb, the average shear stress is not changed. In our case, there are the two types of dislocation motion (sliding and climb) thus the average shear stress is reduced, although not so essential.

The internal local shear stress acting on the dislocation ensemble decreases during polygonization 5-10 times (depending on the dislocation density and the initial configuration) (fig. 3). The internal stresses relaxation must be experimentally tangible and will lead to the fact that dislocations are easier to respond to small external influences.

The simulations presented above indicate that the dislocation ensemble configuration affects significantly the level of local shear stresses acting on the individual dislocations, and has virtually no effect on the average shear stresses value produced according to the ensemble in the surrounding crystal.

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