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Reorientation in alkali-halide single crystals under mechanical stress in an initial stage of high-temperature creep

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Structural changes in KCl and NaCl single crystals were investigated at the initial stage of the high-temperature creep during impeded motion of dislocation in easy-slip systems. The main features of the formation of dislocation structures were studied at the initial stage of rotational deformation, marked by the development of reorientation bands in single crystals. The subsequent process of rotational deformation was also analyzed, as the reorientation bands enlarge and merge and hence, single crystals become polycrystals.
Keywords: dislocation, rotational deformation, single crystal, polycrystal, reorientation band, kink band.

Досліджено структурні зміни в монокристалах KCl і NaCl на початковій стадії високотемпературної повзучості в умовах, коли в системі легкого ковзання рух дислокацій ускладнено. Вивчено особливості формування дислокаційних структур на самому початковому етапі ротаційної деформації, коли зароджуються смуги переорієнтації в окремих областях монокристала, зростання і злиття яких призводить до перетворення монокристалла в полікристал.
Ключові слова: дислокації, ротаційна деформація, монокристал, полікристал, смуги переорієнтації, смуга скиду.

Исследованы структурные изменения в монокристаллах KCl и NaCl на начальной стадии высокотемпературной ползучести в условиях, когда в системе легкого скольжения движение дислокаций затруднено. Изучены особенности формирования дислокационных структур на самом начальном этапе ротационной деформации, когда зарождаются полосы переориентации в отдельных областях монокристалла, рост и слияние которых приводит к превращению монокристалла в поликристалл.
Ключевые слова: дислокации, ротационная деформация, монокристалл, поликристалл, полосы переориентации, полоса сброса.

The transformation of single crystals to polycrystals due to reorientation of large areas during rotational deformation can occur at different load regimes in crystals with different bond types and unit cell types [1, 2].

What happens at the initial stage of reorientation band formation is unclear. Simple structure of reorientation band consists of two edge dislocation walls with antiparallel Burger's vectors [3, 4]. This structure indicates an already formed kink band, but not the process of its forming. The only explanation of such structure is a so-called "mechanical polygonisation," which sometimes occurs during the low-temperature deformation [3]. This model has a defect: the probability that such dislocations form a band is rather small.

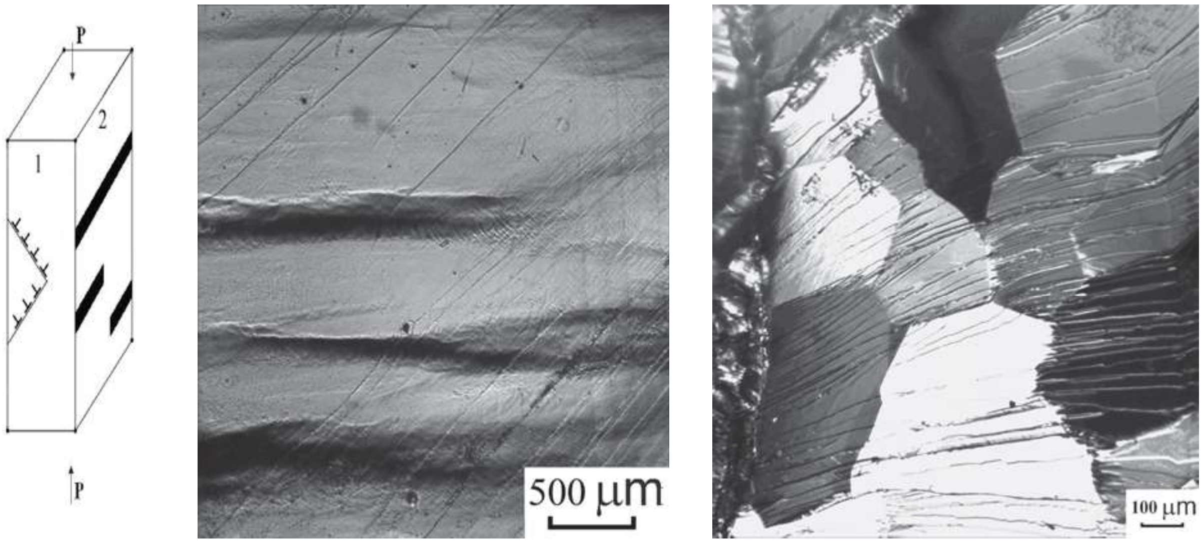
The reorientation of crystal areas causes the significant decrease of internal stresses. The formation of reorientation band effects a dip on strain hardening curve $\sigma(\varepsilon)$. However, the formation of reorientation bands at the initial stage of fragmentation during the rotational deformation is hardly studied [4]. The purpose of this investigation was to explore a surface relief forming of single crystals at an initial stage of high-temperature creep, forming of dislocation structure at these conditions and influence of such dislocation structures on the rotation deformation.

In this paper, the structural changes in single crystals with NaCl-type lattice are investigated at the initial stage of reorientation during high-temperature creep when dislocation glide (motion) is impeded.

Experimental technique

The performed experiments used alkali halide single crystals NaCl and KCl shaped as rectangular prisms with an initial dislocation density $\rho \sim 10^5\ \text{cm}^{-2}$ and average linear size of the blocks $l \cong 10^{-3}\ \text{m}$.

Single crystals were compressed uniaxially in the direction <111> at temperature range from 0.6 to 0.92 T_{melt} in the creep mode. Because of the orientation of the compression, the reduced shear stresses in all primary slip



a *b* *c*

Fig 1. a – scheme of deformation; b – the initial stage of the reorientation bands formation in NaCl. T=625°C, $\sigma = 0.6$MPa, t=5 min, c – KCl T=650°C, $\sigma = 0.8$MPa, t=30 min.

systems $\{110\} < 110 >$ were zero.

Substructure evolution

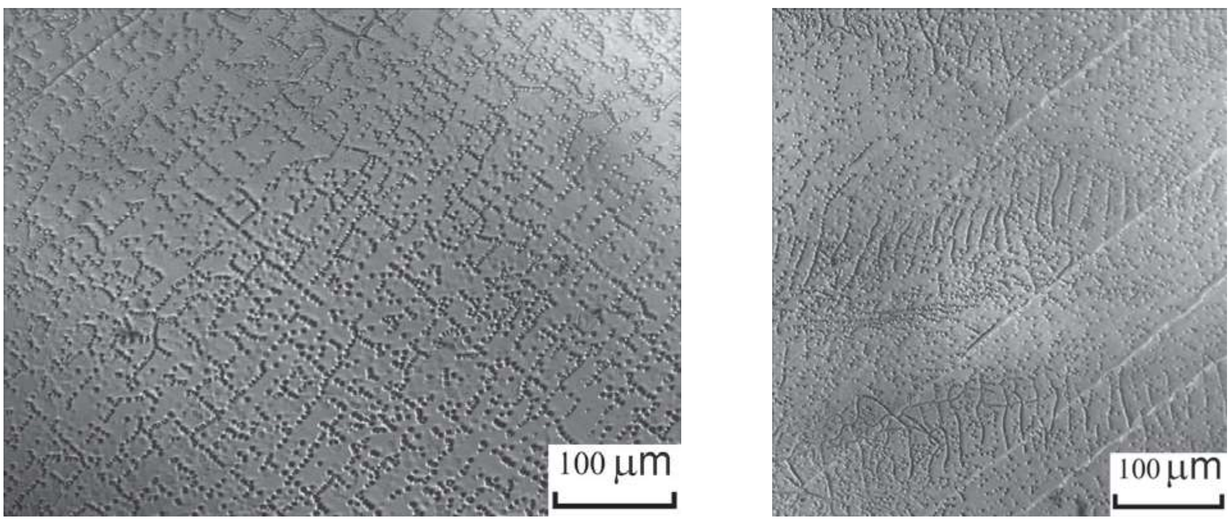
The dislocation structure was visualized by selective etching.

Single crystals became polycrystals at high temperature and high level of external stresses during creep at relative deformation $\varepsilon > 0.1$ due to the formation of sets of reorientation areas [5, 6]. The angles between these areas reach several degrees.

During the initial stage of deformation of single crystal prisms the reorientation bands started to form on the crystal sides which were parallel to the compression vector and have greater area (surface “2” on Fig 1a).

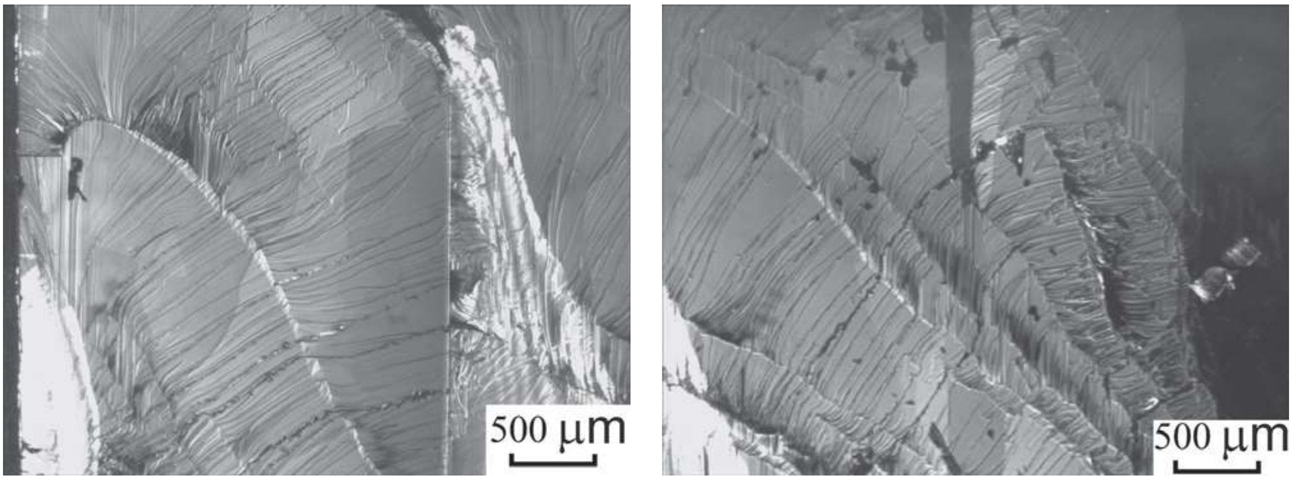
Initially the reorientation bands were perpendicular to the direction of external uniaxial compression. Before forming of the reorientation band, the surface relief became striped (“crumpled”). With the increase of deformation the reorientation bands became wider, merged together and changed their orientations (Fig 1c). As a result of deformation, the dislocation structures of single crystals on surfaces “1” and “2” were significantly altered (Fig. 1 a).

On surface 1, one can see the set of etching pits forming the rectangular cells (Fig 2a). The orientation of etch pits rows is <110>. Hence, they denote the formation of the low-angle boundaries composed of edge dislocations. Two sets of dislocation boundaries indicate that the deformation process is provided by dislocations of two perpendicular slip systems $\{110\}$. During deformation the dislocation structures transform into the typical for the high temperature creep block structures with big blocks and arbitrarily oriented block boundaries. The arbitrary orientation of boundaries indicates the presence of dislocations of two



a *b*

Fig. 2. Dislocation structures of NaCl single crystals, T=625°C, $\sigma = 0.6$MPa, t=5 min, a – surface “1”, b – surface “2”.



a *b*

Fig. 3. The cleavage steps on surface "2" in NaCl single crystal. T=600°C, $\sigma = 0.4$MPa, t=30 min..

slip systems in each boundary.

On the surface of type "2," the dislocation structure is quite different. Along with the chaotically distributed dislocations, there are periodic rows of etch pits in <100> direction. Such areas indicate reorientation bands beginning to form. These periodic rows of etch pits consist of screw dislocations. This fact is confirmed by three experimental evidences. The first of which is the direction of these short rows. Second, these rows disintegrated into chaotically distributed dislocations, as pile-ups of screw dislocations with the same Burger's vectors are unstable. Third, the analysis of cleavage steps on surface of deformed crystal confirms the presence of screw dislocations.

The alkali-halide crystals with NaCl-type lattice are such, that if we apply external concentrated force, the crystal cleaves out along the planes with minimum surface energy {100}. Since the splitting forms two free surfaces, it requires high energies. Thus the cleavage cannot instantly occur in the whole crystal. The cleavage spreads from one point to another in the form of crack, which starts in the place of the force application.

In a single crystal without dislocations, the cleavage surfaces have to be perfectly smooth on atom level. In real single crystals, the cleavage surface consists of the system of cleavage steps formed during the crack propagation through the rows of screw dislocations. If the crack crosses the twist boundary consisting of at least two screw dislocation systems with different Burgers vectors, numerous cleavage steps appear. Such cleavage steps can merge, thus forming either higher steps or merging creeks that spread in the direction of crack propagation.

If after the crack has crossed the boundary and only orientation of cleavage steps is changed, the nonappearance of new steps implies that this boundary is the tilt boundary, consisting of edge dislocations. An increased amount of cleavage steps indicates the twist boundary consisting of screw dislocations. In all crystals we can see both types of dislocations, particularly in the areas of reorientation band formation (Fig. 3).

Conclusions

Actively discussed in literature, simple dislocation structure of reorientation bands indicates the collective nature of evolution of dislocation structure during the formation and motion of such reorientation bands. It was shown before reorientation band forming, the surface relief becomes striped. The dislocation structures were completely different on surfaces "1" and "2". They depend on nucleation of dislocations in different slip systems.

In high temperature creep experiments under the condition of formation of new dislocations in crystal, a high amount of dipoles of partial disclinations develop. Thus, we can infer that partial disclinations carry the rotational deformation.

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