MICROMECHANISMS AND MACRO-FRACTURE PARAMETERS OF LiF BICRYSTALS

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ABSTRACT

Peculiarities of plastic deformation and crack initiation within a tilt boundary being "attacked" by screw or edge dislocations in isoaxial LiF bicrystals with various misorientation angles $\alpha = 2-15^\circ$ at 293 and 77 K were studied by the single slip method. Cracks proved to appear at shear strain inversely proportional to the angle α in the first case, and not depending on α in the second case. Based on dislocation structure of deformed specimens, pattern and shape of cracks the conclusion is drawn, that crack formation occurs due to accumulation of grain boundary dislocations with differential Burgers vector, or due to opposite pile-ups arising at the boundary as a result of plastic deformation.

KEYWORDS

LiF bicrystals; tilt boundary; fracture; screw, edge dislocations; dislocation pile-ups; dislocation wall.

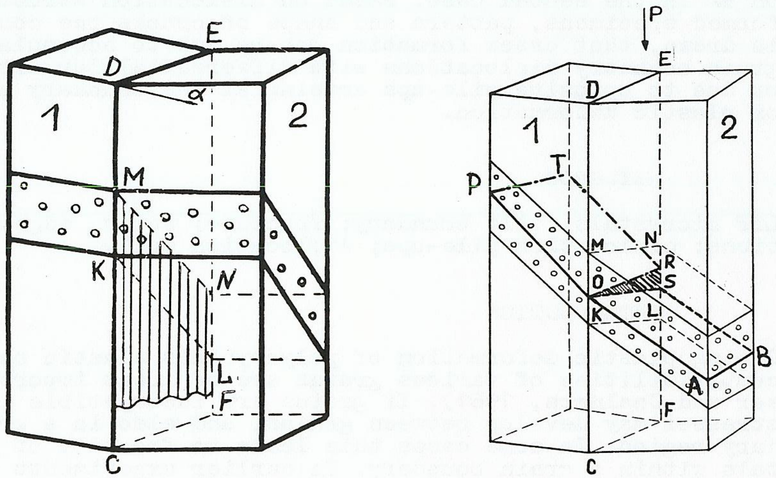
INTRODUCTION

During plastic deformation of polycrystals elastic and plastic compatibilities of various grains are of great importance (Hauser and Chalmers, 1961). If grains are incompatible interior stresses may develop between grains, and also in a grain boundary region. In some cases this leads to fracture of polycrystals within a grain boundary. In earlier experiments the model of retarded shear (Strow, 1957) was suggested to explain crack initiation within the boundary. Later (Indenbom, 1961; Das and Marcinkovski, J. Appl. Phys. and Acta Metallurgica, 1972; Likhachev i Rybin, 1973) attention was paid to crack initiation at the passage of deformation across the boundary due to accumulation of grain boundary dislocations with differential Burgers vector. However, since the details of dislocation structure forming at the boundary depend on mutual orientation of Burgers vector, misorientation vector, and the vector normal to the boundary, an interpretation of experimental results on polycrystals can only be speculative. In this connection experiments with bicrystals tested when the mentioned vectors are known, and their mutual orientation can be changed are of great interest. Such experiments were started by (Smirnov i Snezhkova, 1977; Smirnov, Snezhkova i Khannanov, 1979).

EXPERIMENTAL

The isoaxial LiF bicrystals investigated (Fig. 1) contained a plane symmetrical tilt boundary parallel to the specimen axis [001] and forming the angle $\alpha/2$ with the (010) planes. Bicrystals were grown from special constitutive seed crystals by the Kiropulos method. Final specimens have a dimention of about 4x5x15 mm.

Before deformation bicrystals were prepared for single slip (Smirnov,1968), what for they were X-ray hardened with the exeption of a narrow zone 2 mm high and oriented along the direction of slip. In the present work two versions were examined. In the first case (Fig. 1,a), further called case A, the boundary was attacked by screw dislocations, and the Burgers vector formed the angle ~45° with the vector of tilt boundary and the angle $\varphi \approx \alpha/2\sqrt{2}$ with the boundary plane. Two such slip systems exist: (101) [10$\bar{1}$] (Fig. 1,a) and (101) [$\bar{1}$01], though they don't differ from each other due to the symmetry of the boundary. In the second case (Fig. 1,b), case B, the boundary was attacked by edge dislocations, and the Burgers vector formed the angles ~45° with the boundary plane and the vector of the boundary inclination. There also exist two slip systems: (011) [011], (Fig. 1,b) and (011)[011]. After preparation for single slip the specimens were tested in compression along the axis. Dislocation structure of deformed bicrystals was revealed by the selective etching method.



a b

Fig. 1. A schematic picture of the deformation of bicrystals by single slip in case A (a) and in case B (b). The zone of plastic shear is marked off by circles. CDEF - a boundary of bicrystal, PTRO - a slip plane in crystal 1, ABSO - a slip plane in crystal 2.

RESULTS

Deformation Parameters

It was found that yield resistance for bicrystals tested in the way described above (5,8 MPa for 293 and 17,5 MPa for 77 K) was equal to that of monocrystals within the limits of errow. However, their plastic deformability may considerably differ. While monocrystals could be deformed up to several tens persent without crack formation (Smirnov, 1968), in bicrystals visible macrocrack may appear at yield point. In case A the critical deformation before crack initiation ε_c varied with the misorientation angle. The dependence of ε_c on α in that case at 293 and 77 K are shown in Fig. 2,a. In Fig. 2,b the same data are represented on the $\varepsilon_c - 1/\alpha$ coordinates. They can be obviously regarded as linear and described by an equation:

$$\varepsilon_c = K/\alpha \qquad (1)$$

K being $13\cdot10^{-3}$ and $6{,}5\cdot10^{-3}$ for 293 and 77 K, correspondingly.

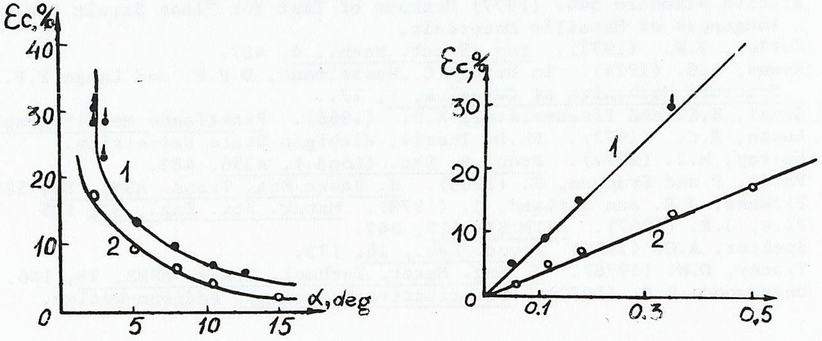


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Fig. 2. A dependence of the deformation before fracture ε_c on the misorientation angle α (1-293, 2-77 K). Arrows on full circles mean that the deformation degree before crack initiation in the boundary is higher, but compression was stopped at that point because of the fracture from the ends of specimens.

In case B crack initiation occurs at a low ε_c, ε_c not depending on α within the limits $\alpha = 5-12^{\circ}$ (Table 1).

TABLE 1 A Dependence of Shear Deformation ε_c before Fracture on Misorientation Angle α for case B

α (deg.)	ε_c (%)
5	5,0
8	5,5
10	4,2
12	4,3

Crack Parameters

Cracks were formed in the single slip zone of deformed crystals within the boundary plane. In case A one edge of a crack coincided practically with the definite edge of the deformation zone (MN line in Fig. 1,a), while the crack itself propagated along the boundary throughout the zone and could transgress it's limits. An angle of the crack opening ϑ near MN line can be determined by means of pattern observed with an interference microscope. The angle ϑ was found to be independent on misorientation angle α (Table 2).

TABLE 2 A Dependence of the Angle of the Crack Opening on Misorientation Angle for case A

α (deg.)	ϑ (min.)	
	T=293 K	T-77 K
5	29	15
8	31	19
10	30	17
12	27	16
14	28	19

In case B first cracks visible with a light microscope were shaped as sharp extensive horizontally directed wedges (Fig. 3) with angle α, their spike always lying on the convex part of bicrystals (MN line in Fig. 1,b). In other words, wedge-formed cracks in their pattern are similar to ROS triangle in Fig. 1, b, formed by lines of intersection of slip planes in crystals 1 and 2 with the boundary plane. At subsequent deformation cracks increase in size and join together occupying gradually the whole zone MNLK and even transgressing it's limits in the boundary plane.

Dislocation Structure

In case A the slip was single; slip lines approached the boundary from one crystal, passed through it and propagated into the other. The shear in slip bands, being measured by method (Smirnov and Efimov, 1966), was independent on the distance from the boundary. Basing on the constancy of shear in that case it is believered that mobile dislocations are not retarded by the boundary. The density of dislocations near the boundary is distance independent.

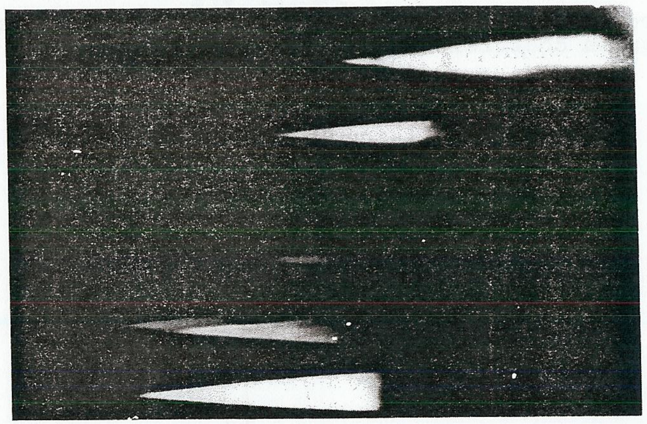

Fig. 3. Cracks in a boundary plane for case B ($\alpha = 10^{\circ}$)x300.

In case B dislocation structure of deformed crystals in the slip zone was represented by slip lines and bands with 4-5 % shear on AB line. Far from the boundary crystals were deformed along the single crystallographic plane system (011). The density of dislocations increase in the direction of the boundary. Orthogonal and inclined (101) and (10$\bar{1}$) slip systems were also observed near the boundary. It was shown by dislocation topography in the grain boundary region (Smirnov, Snezhkova i Khannanov, 1979) that slip lines occur on slip planes of corresponding crystals, and their lines of intersection with the boundary form within the boundary two systems of parallel lines, inclined at the angle of misorientation α. The schematic pattern of these lines within the boundary is shown in Fig. 5.

DISCUSSION

Case A

The main feature of case A is the formation of torn vertical wall of edge dislocations with differential Burgers vector $b_{\Delta}=b_1-b_2$, as a result of screw dislocations crossing the boundary during deformation (Fig. 4), (b_1 and b_2 are the Burgers vectors of dislocations in crystals 1 and 2). Here the value of $b_{\Delta}=(\alpha/\sqrt{2})b$, as geometry of slip shows, (b is the Burgers vector of mobile dislocations). The lower end of such a dislocation wall is under perpendicular tension stresses, that may cause a crack in this region. According to (Indenbom, 1961), if the wall is between M' and K' (M'K'=h), the L-sized crack will stretch from x_1 to x_2 ($x=0$ in M', $0<x_1<L<x_2$). In case $L>>h$ the following estimation holds, (Indenbom, 1961):

$$L=\frac{G}{32\pi(1-\nu)\gamma}\Theta^2h^2 \qquad (2)$$

where G is shear module, Θ - a wall misorientation angle, ν - Poiasson coefficient, γ - surface energy.

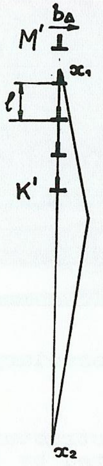

Fig. 4. A torn wall of edge dislocations (M'K') and crack formation (X_1X_2), (a schematic picture). Vector b_Δ is the differential Burgers vector of grain boundary dislocations.

The misorientation angle of the boundary dislocation wall is determinable from the value of deformation ε in the zone: $\Theta=b_\Delta/l$, where l is the distance between dislocations in the wall; $l=b/\varepsilon$, hence

$$\Theta=(\alpha/\sqrt{2})\varepsilon \qquad (3)$$

Comparing (3) with (1) for critical deformation ε_c one can deduce the value of the critical wall misorientation angle as:

$$\Theta_c=K/\sqrt{2} \qquad (4)$$

K=const. Therefore it occurs that crack development in bicrystals with different α values takes place at Θ_c=const, the Θ_c value being 0,5° for 293 and 0,25° for 77 K.

Obtained experimental results obviously correspond to the model (Indenbom, 1961), represented in Fig. 4. Really, cracks always extend to tension stress region from a grain boundary dislocation wall. A crack doesn't cover the whole deformation zone, it starts at some distance from MN line. The angle of the crack opening ϑ in x_1 for 293 K is about 0,5° (Table 2), and coincide practically with the critical wall misorientation angle at different α values. Quantitative accordance is also quite good. According to (2) visible cracks several millimetres in size must form at $\Theta\leqslant 0,5°$, while L=1 mm, (Θ =0,3° while L=4 mm), as it is experimentally ascertained. The increase of Θ_c at 293 K in comparison with that at 77 K may be caused by partial stress relaxation in dislocation wall due to a secondary slip.

Hence in case A fracture experimental results on bicrystals is in qualitative and quantitative accordance with the model of crack initiation within the boundary due to accumulation of grain boundary dislocations.

Case B

The main feature of case B is that lines of intersection of slip planes with the boundary in the neighbouring crystals don't coincide (Fig. 1,b), but form the angle α . Therefore a slip propagation from one crystal to another may perform either by edge dislocation crossing the boundary along OS line with formation of steps with linear density $n=tg\alpha/b$ on dislocations or by a retardment of primary dislocation on OS line with subsequent nucleation of dislocation loop and formation of opposite-signed dislocation on OR line or parallel to it. The observation of slip lines motion near the boundary ascertained that dislocations are retarded by the boundary, and slip develops along the slip system of the neighbouring crystal. Since the dislocations at the different sides

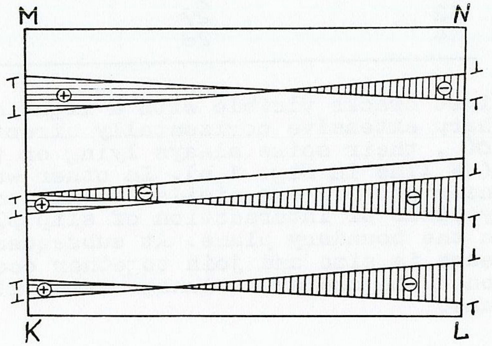

Fig. 5. An intersection of slip planes in neighbouring crystals with the boundary plane MNLK (a schematic picture). ⊖ - tension zones, ⊕ - compression zones.

of the boundary are opposite-signed, corresponding zones between slip bands within the boundary will also be under different stresses, according to Fig. 5, (tension or compression perpendicular to the boundary).Since shape and position of experimentally observed initial cracks (Fig. 3) correlate with shape and position of the tension zones (Fig. 5), it is suggested that just that tension leads to crack initiation and growth.

On the basis of the data obtained the conclusion is drawn that in case B crack initiation within the boundary occurs due to opposite pile-ups arising at the different sides of the boundary. An estimate of stresses needed for crack initiation can be done from the model of a single pile-up (Strow, 1957), and also from the calculation of opposite parallel pile-ups (Vladimirov i Khannanov, 1973). The calculation of the single pile-up approximately conform to the experiment ($\tau_{theor} \sim 6{,}0$ MPa, $\tau_{exp} \sim 5{,}8$ MPa); as for the opposite pile-ups crack initiation stresses are less by 1-2 orders of magnitude.

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