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Folding in Single Crystals Concavity Areas during Compression

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Abstract. The authors analyze folding in concavity areas. Special aspects of folding are determined both for natural concavities stipulated by specifics of crystallographic orientation and for deliberately created concavities inside a U-shaped cut. It is shown that at the macrolevel folding is caused by concavity areas, in other words the stress condition pattern has primary influence on initiation of folds. Development of folding structures is followed by misorientation of local areas inside the crystal. The misorientation leads to an increase in the Schmidt factor and initiating additional slide patterns inside the crystal at the mesolevel. Development and accumulation of misorientations at the microlevel correlate with those in the dislocation structure. A U-shaped incision helps to activate a larger number of slip systems and the emergence of additional deformation domains.

Previously, the authors showed that deformation in single crystals is caused by several factors [1], the stress condition pattern being one of them. Experiments demonstrated that when a sample undergoes compression the nature of the external stress field is changed due to end face friction. This is also caused by sample geometry (there are geometrical stress concentrators—ribs and corners).

S.I. Gubkin [2] has shown that during compression the end faces of the sample undergo all-around non-uniform compression and the central part of the crystal suffers from uniaxial compression. Compression leads to changes in the stress condition pattern. In the central part of the crystal, uniaxial compression is converted into all-round non-uniform compression in the central part of the sample, and along the side ribs “compression-extension” patterns occur.

Calculations made by a finite elements method in [3] show that the deformation tensor in local crystal areas is different. External stress is at its maximum at the tops and end ribs of the sample. The non-uniform distribution of stress in the crystal during compression affects deformational relief and non-uniform deformation in single crystals.

In the end face area of the sample a slip takes place when all the three main stress components are different from zero. Here the slip stress is calculated in general. Due to this the traces of the slip along the planes with a zero Schmidt factor can occur near the end faces of the sample. The Schmidt factor equals zero when a uniaxial stress pattern is suggested and calculated [4]. These factors lead to additional domain slides in the end face area of single crystals.

Special deformation conditions in the end face area cause surface bending and folding inside the crystal. This process is the most relevant in [111]-crystals. The complex stress pattern and special deformation conditions in the bending area lead to a more complicated deformation pattern known as folding. In [5] folding is defined as a separate independent surface deformation pattern.

The aim of this study is to find regularities in folding in the areas with a complex stress condition pattern based on an analysis of deformation relief and crystallographic orientation of local areas at different scale levels.

Compression tests were carried out using Instron ElektroPuls E10000 machine operated at strain rate 1.4×10^{-3} s^{-1} at an ambient temperature. Prior to testing the samples were polished and lubricated by graphite. Shear traces on the

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single crystal faces were obtained and then examined using optical microscope LeicaDM 2500P, SEM instrument Tescan Vega II LMU with EBSD-attachment for determining the disorientation value in local areas.

Figure 1 shows the folding morphology, changes in local areas orientation in the concavity area and orientation of areas in the standard stereographic triangle relative to the compression axis *X*. The folds in the concavity area are small, being about 15 µm wide and 35 µm long.

An EBSD device showed that from the plane perpendicular to the folds one can note interchanging stripes with an orientation close to initial (111) and reoriented to (110) direction. The stripes with an orientation close to initial are 10…20 µm wide, the reoriented areas are 20…40 µm wide. Reorientation leads to increasing the Schmidt factor up to 0.36…0.45 compared with initial 0.27, more reoriented areas having a higher value.

When the deformation reaches 16% the misorientation angles are within 2°–3°. Maximum values of 5° can be found at the boundaries of the areas with an orientation close to initial (111) outlining them. The misorientation angle changes in size along a transverse line perpendicular to the stripes in a quasi-periodic way.

The maximum registered misorientation angle values are within 5 µm, which corresponds to the misorientation value accumulated in the cellular dislocation substructure [6].

Thus, the inhomogeneity of a stress condition and specifics of single crystal geometry lead to non-uniform deformation and macrobending of the sample, which in turn conduces to folding as an additional way of deformation.

Hereafter we will consider an experiment to analyze how deliberately induced bending effects generation of the folding structure. Samples of a hexahedron shape with a U-shaped cut were used for the experiment. The cut was 0.1 mm in diameter at the top and 0.3 mm deep.

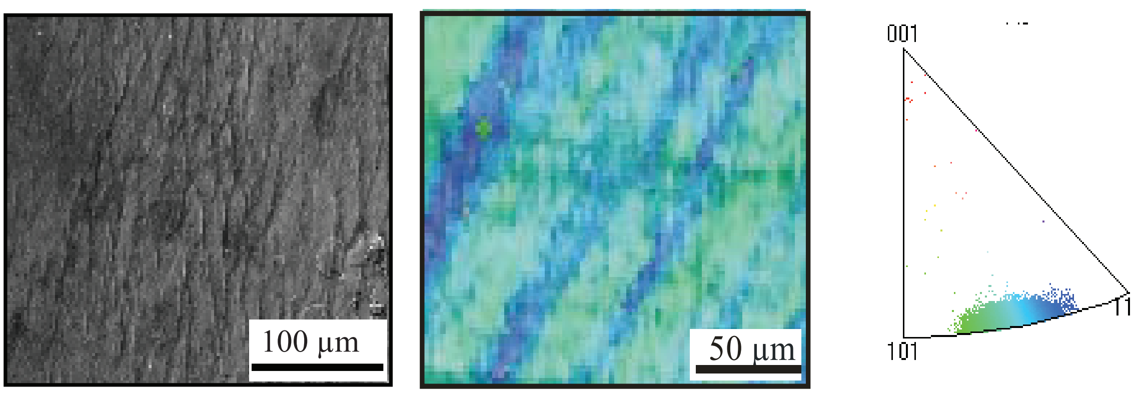
Samples with a compression axis [001] and side planes {100} were analyzed in the work. Previous works of different authors showed that single crystals with such an orientation are not subjected to folding and plastic deformation here is mainly of a sliding character and is rather uniform [7, 8].

The cut in the sample causes higher stresses at its top and promotes additional active slip systems. Due to this, those local sliding systems create additional deformation domains inside the sample. Herein above we have described this phenomenon with end face areas of [111]-single crystals.

Besides the cut there forms an additional free surface and changes in deformation conditions at the top and at the edges of the cut. It creates one more surface which is characterized as slight shear. The density of traces increases during deformation. Each cut edge has one active trace system (Fig. 2a).

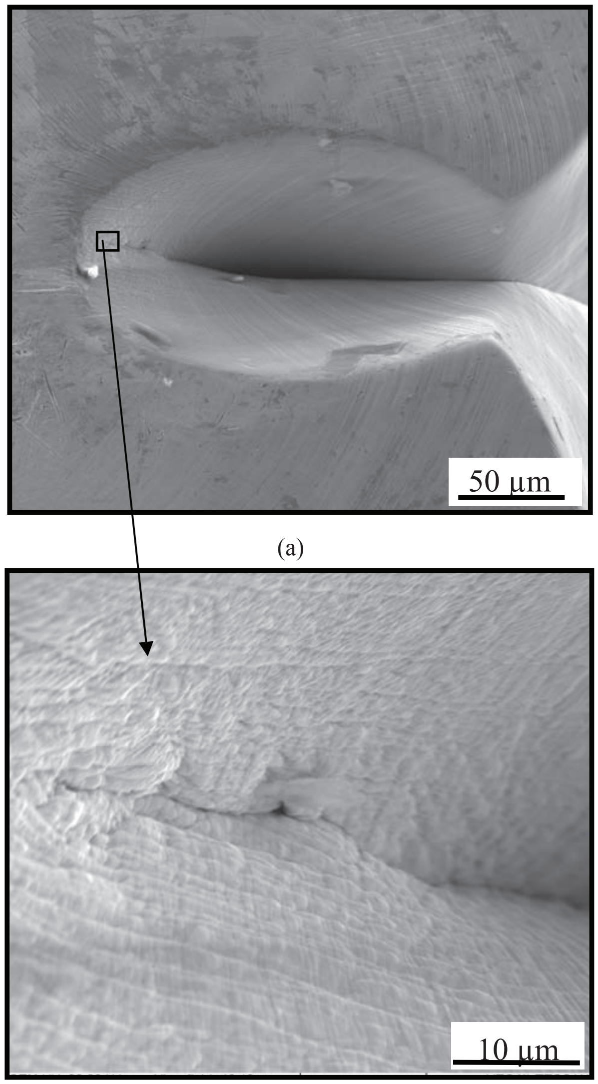
More complicated stress conditions and high stress values inside the concentrator predetermine the gradual activating of probable slide systems and their active interaction with each other. These processes lead to developing folds with a complex morphological structure inside the cut (Fig. 2b). Beside the folds, the relief consists of a system of steps left by mating slide planes with a high trace density at the top of the cut, which indicates intense plastic deformation in the stress concentrator area.

EBSD-analysis on the surface perpendicular to the cut (the side plane (010) showed that the orientation deviates from the initial direction [001] of the compression axis). In this case alternation of areas with a different orientation is not as strongly marked as that described above (Fig. 3).



(a) (b) (c)

FIGURE 1. Folding morphology (a), local areas reorientation (b), orientation of areas in the standard stereographic triangle relative to compression axis *X* (c), $e = 16\%$



(a)

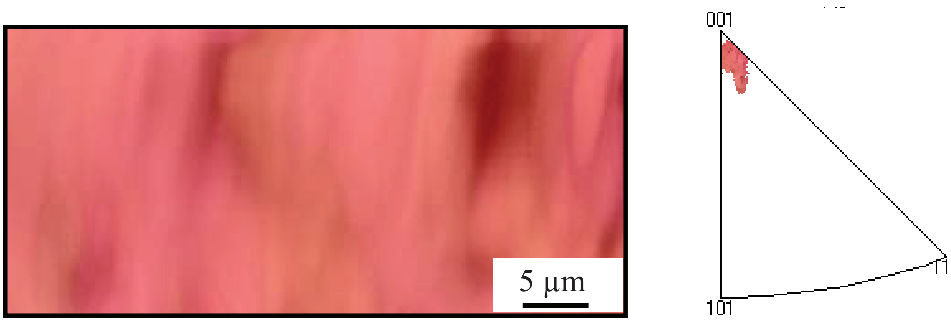
(b)

FIGURE 2. Deformation relief near stress concentrator (a), folds inside the stress concentrator (b), e = 41%

The reorientation process on the surface lying in the cut plane and on the mutually perpendicular surface reflects the specifics of a spatial distribution of stress fields near the cut. That is why it is viable to analyze misorientation on the side plane (100) which carries the cut. Near the cut there are systems of shear bands described above (Fig. 2). EBSD-analysis showed that the reorientation occurs smoothly. This is different from the previous case because the side plane (010) has some alternation of areas with a different orientation while the side plane (100) undergoes a gradient transition from one orientation to the other.

However there are some common features. For example, in both cases the misorientation angles of all boundaries are no more than 5°. In reoriented areas, the Schmidt factor increases up to 0.43…0.45 and on the side plane (100), it increases to the maximum possible value of 0.5. Therefore, a material under stress tends to reorient in the way which enables the most effective slide process.

Thus, the results of the research showed:



(a) (b)

FIGURE 3. Reorientation of local areas (a), orientation in the standard stereographic triangle for compression axis direction X (b), $e = 41\%$

(i) Macroscopic changes in the sample shape and as a consequence of the stress condition pattern are prerequisites to a developing folding structure. Concavity areas are preferable zones of folding. In such a case folding takes place even in [001]-single crystals with cubic plane sides which do not tend to develop folding. The folding process is connected with the development of misoriented structures inside single crystals.

(ii) The analysis of slip and reorientation process proved the interconnection of plastic deformation processes at different scale levels. Macroscopic changes in crystal shape correlate with the character of misorientation transformation near the cut. In this case macroscopic reorientation is followed by developing misoriented meso-zones. Due to such reorientation it is possible to activate slide systems favorable to the slip in the local deformation domains.

This is proved by the EBSD-analysis, which reveals an increase in the Schmidt factor. The ways of accumulating and changing of misorientation proved by the EBSD-analysis correlate with developing and accumulating misorientation in the dislocation structure which has been described before by different researchers [6, 9, 10].

(iii) Development of concavity areas in [111]-single crystals and in the stress concentrator top in [001]-single crystals as well as the maximal value of stress tensor components contribute to intensive folding and activating maximum slide systems. In such a case constant changes in the surface orientation inside concavity areas provide conditions for activating new slide areas. Such conditions will enable intensive development of misoriented micro- and nanostructures.

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