Influence of Lateral Incision on Inhomogeneous Deformation of a Nickel [001] – Single Cristal at Axial Compression

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Abstract. We used the scanning electron microscopy and the electron backscattered diffraction to investigate a deformation relief and a crystallographic disorientation of a nickel [001] single crystal with {100} faces with a lateral incision. We identified that the lateral incision can change the shear domains distribution pattern in the sample by creating additional deformation domains near the incision. The change in the patterns of the misorientation accumulation on the mutually perpendicular faces accompanies this deformation. We established that the orientation alteration occurs toward the increase of the Schmid factor for the slip systems in two of the four (previously equally loaded) slip planes. This method of shear deformation contributes to an optimal mutually consistent deformation in the adjacent areas of the single crystal.

1. Introduction

A fracture process ductile materials and possible failure play important role in material science and practice. The study of this process dealing with no only nucleation and propagation of dislocations, but also the initiation and extension of a crack. Fracture failure has been investigated by simulations and experiments at various length scales (see some examples in [1-5]). The literature gives us a set of different models proposed to describe dislocation nucleation from a crack tip [6-10].

From a practical point of view, an assessment of the product efficiency with stress concentrators is very important. The stress concentration areas intensify the processes of local deformation and destruction. They are a cause of reduction of generic plastic deformation before destruction. Numerous theoretical and experimental studies (e.g. [11, 12]) and handbooks (e.g. [13]) are devoted to investigations of the stress concentration. Mainly, the studies are dedicated to investigations of the incision shape, location and influence of an external load. The majority of studies on stress concentrators focus on the modeling, explore the processes of stress and deformation distribution in the incision areas, and do not examine the strain relief and the nature of the misorientation in this area. Meanwhile, the size, shape and orientation of the incision specify the deformation process characteristics.

The studies on single crystals represent the characteristics of the slip evolution under an inhomogeneous stress caused by the incision. The results, obtained by the authors earlier [14, 15], allowed to take into account the effects of the basic stress concentrators, and compression axis and lateral faces orientations on a plastic deformation in FCC single crystals. The most detailed studies were carried out on nickel single crystals [16, 17]. In these studies, we examine the inhomogeneity of the plastic deformation under the above-mentioned factors the lattice method. The electron-backscattered diffraction (EBSD) allows to explore the development of misorientations in relation to strain relief elements and formability of single crystals.

The aim of this paper is to investigate the deformation in nickel [001] single crystals with incisions on lateral faces, analyzing the deformation relief and crystallographic reorientation areas.

2. Materials and method

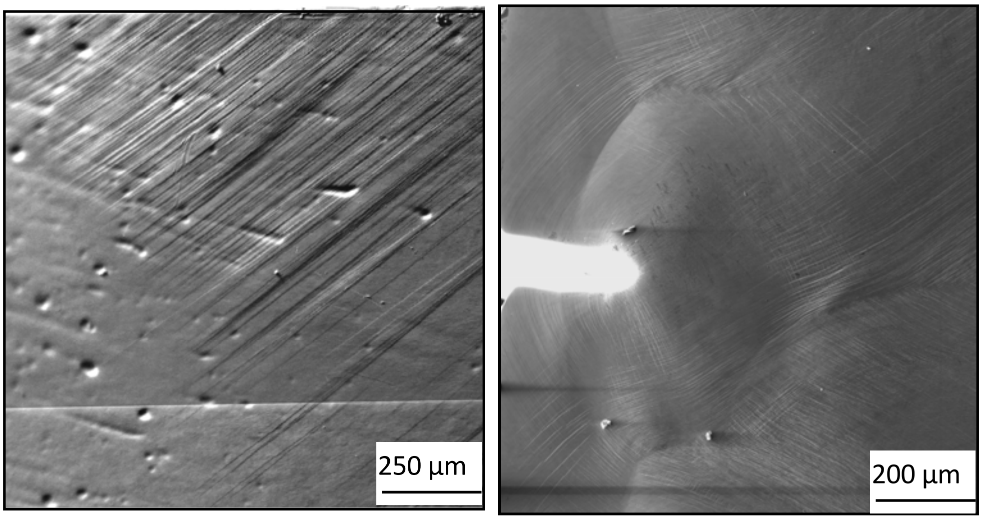
The object of the investigation is a nickel single crystal with compression axis orientation [001] and lateral faces {100}. The single crystals were prepared of a pure nickel containing less than 0.01% of impurities. The Bridgman method was used to grow the single crystals. The orientation was performed on the X-ray diffractometer. After the electroerosion cutting and polishing the deviation from the cubic orientation of the sample faces was ± 1 °. The study was carried out with samples of a size 3x3x3 mm and with a horizontal incision on a lateral face. The incision was made by the electroerosion cutting. It had a semicircular shape with radius at vertices R = 0,05 mm and depth t = 0,3 mm. The surface of samples was firstly mechanically polished and then electropolished in the saturated solution of the chromic anhydride and phosphoric acid at 20 V. The compressive deformation was done by the Instron ElectroPuls E10000 at rate 1,4 · 10-3 s-1 at room temperature. The graphite lubricant was used to reduce friction on lateral faces. The total sample strain was 0.41in relative units. The optical microscope Leica DM 2500P and scanning electron microscope Tescan Vega II LMU equipped with EBSD were used to investigate the deformation relief.

3. Experimental results

The presence of a horizontal incision on a lateral surface {100} of the [001] nickel single crystal changes the distribution of stresses and strains in a sample, when compared to the common deformation pattern where the sample is compressed in the form of a hexahedron and in the presence of an end friction. In the incision area, the stress conditions change. The incision area manifests as a stress concentration area. The magnitude of the stress concentration depends on: 1) the incision orientation with respect to the applied load and temperature; 2) the incision size compared to the size of the sample; 3) the shape of incision, determined by its geometric parameters. The geometric parameters of the stress concentrator are its linear dimensions (depth and radius) and an angle between the faces of the concentrator, in our case $\alpha = 0$.

When a strain increase, the incision edges come closer, and the radius of incision tip decreases. Under compression, the width of a sample a increases together with the depth of an incision t. The ratio of these parameters a / t = 10. We can assume that a >> t. In this case, the stress concentration coefficient $\alpha\sigma$ depends very little on a, and largely it depends on t. The greater the t, the higher the stress concentration factor is, i.e. $\approx \sqrt{t}$. Moreover, as the radius R decrease, the value of the stress concentration coefficient increases. When $\alpha = 0$, the value of the stress concentration coefficient depends on the geometrical parameters as following $\alpha\sigma \approx \sqrt{t}/R$. Therefore, during the deformation process, the maximum stress in the incision area is constantly greater than the average. It is directly proportional to the incision depth increase and inversely proportional to the radius of the incision tip. This creates conditions for a more active deformation in the incision area.

For a [001] nickel single crystal there are four equally loaded octahedral planes with two slip directions in each. The total number of slip systems is eight. The Schmid factor is equal to 0.41. Despite the fact that the slip systems of the given single crystal are equally loaded, the condition of an uniform volume alteration at compression of sample results in enabling of only some slip systems, not all of them. In single crystals without incisions first to activate are the slip systems near the primary stress concentrators, which are the near-end areas of the sample. The crystallographic diagram, the fragmentation pattern and the deformation relief are discussed elsewhere [14, 16]. Note, that the relief and the nature of the sample fragmentation, with concentrators and without concentrators, differ substantially (Figure 1). The analysis of the deformation relief shows that the introduction of the incision creates an extra surface and changes the deformation around the incision. The increase of density of shear bands accompanies the facilitated slip in the extra surface.



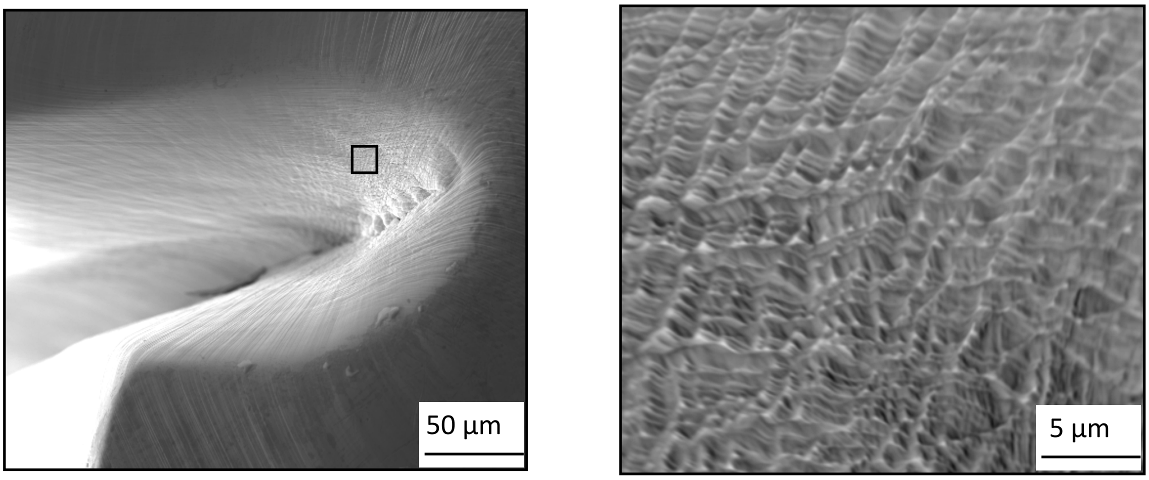
a) b)

Figure 1. The deformation relief of [001] single crystals without lateral incisions (a) and with the incision (b) on the lateral face (100).

We are able to observe the activation of two systems of shear bands according to two sides of the incision. The convergence of the incision edges leads to the curvature of the lateral edges, and as a result to the bending of the shear bands. The appearance of additional active slip systems is due to the higher degrees of stress at the incision tip. The activation of these local slip systems lead to the appearance of an additional strain domains inside the single crystal.

Note, that the atomistic simulation study for two FCC materials (Cu and Al) indicates the favorable factors dominating dislocation nucleation from a crack tip [18].

High and complex stress in the incision tip creates an environment for consecutive activation of possible slip systems, as well as active interactions between them. As a result, at the incision tip appear folds (Figure 2a). We can see a system of steps as the result of deformation along to conjugated slip planes (Figure 2b). The high density of the shear bands in the incision tip indicates the presence of intensive plastic deformation in this area.



a) b)

Figure 2. The deformation relief at the stress concentration area (a). Amplified view of the selected area (b).

The EBSD analysis was performed on the lateral face (010) perpendicular to the incision. It has been found that in this zone there is an alternation of areas with the orientation close to the initial [001] with respect to the compression axis (Y), and reoriented in the directions [105] and [117] (Figure 3) (Z-axis normal to the lateral face). The width of the areas with the orientation close to the initial is about 4 ... 7 microns, with the new orientations - 2 ... 4 microns. In this case, it is interesting to note that the value of the Schmid factor in reoriented areas increases to 0.43 ... 0.45. Consequently, the reorientation occurs in the direction of the most active slip.

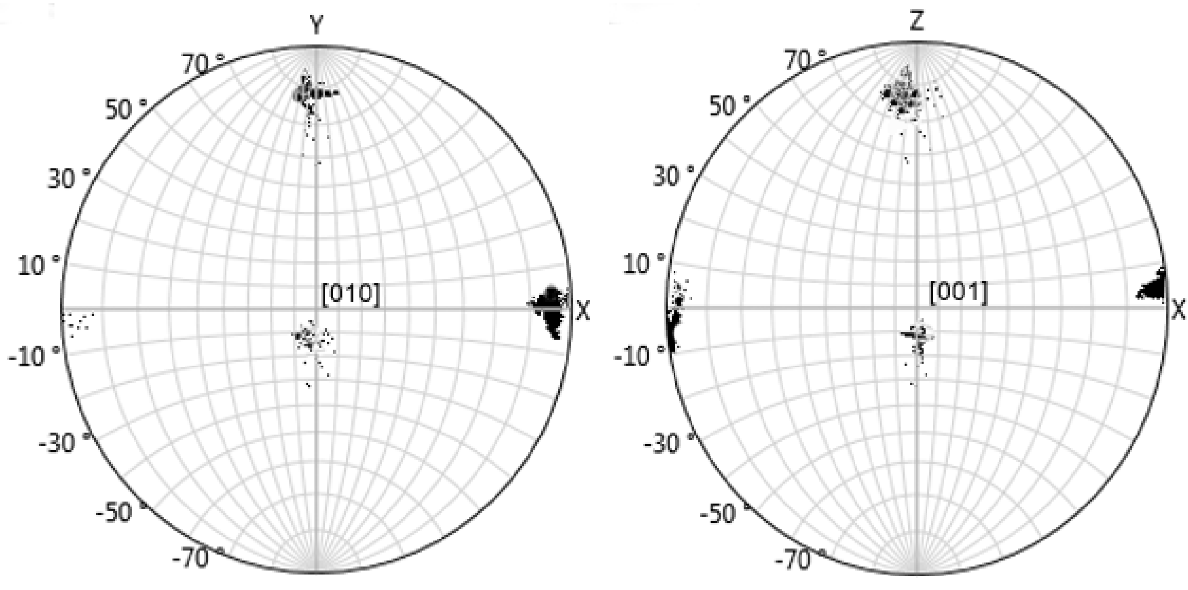


Figure 3. The direct pole figures obtained with the face (010) perpendicular to the incision.

Character of the folds formation at the incision tip is similar to the folds formation patterns occurring in a [111] nickel single crystals in areas of the macroscopic bending of face [17]. In fold structures the value of misorientation angles ranges from 2° to 5°. The maximum values of a misorientation angle are observed with a step of about 15 microns. The step in folds in a nickel [111] single crystal deformed by compression is about 5 microns. This fact agrees well with the misorientation value accumulating during a deformation in the cellular dislocation substructure.

The strain of the compression sample was equal to 0.16 (in relative units). The indicator for the sample with the concentrator was equal to 0.41. A cellular dislocation substructure occurs in nickel, when the strain is equal to 0.16. We are able to fix a microband substructure and a fragmented substructure, when the strain is equal to 0.41 [19]. In cellular substructure, it is possible to mark the accumulation of misorientations. This process goes through the excess density of dislocations in cell walls (about 10 cells are needed to accumulate this misorientation value). In the case of microband and fragmented structures, the misorientation emerges at the edges of microbands and fragments. Each edge may have a different misorientation value. Hatherly, Hutchinson, Karduck et. al. [20-22] and other researchers studied the accumulation of misorientation in microband and fragmented structure. They have shown that the accumulation of misorientation under condition of the transition from one microband to another contains three variants: 1) monotonous increase, 2) monotonous decrease, 3) periodically change of a misorientation. A comparison of our results with previously obtained shows that the greatest misorientation values are observed at the edges of microband deformation groups.

Misorientation gradient on the face lying in the incision plane is different from the one on the face perpendicular to the incision. It represents the spatial distribution of stresses near the incision. Therefore, the analysis of misorientation was also performed on the (100) face with the incision (Z-axis). Near the sample end, one can observe the slip systems discussed above (Figure 1). The EBSD analysis shows that the reorientation changes smoothly and in the same directions as in the mutually perpendicular face. However, if in the previous case, we observed an alternation of areas with different orientation, now we see the gradient change from one orientation (Figure 4, point 1) to another (Figure 4, point 2). The misorientation value of the adjacent areas is within 1°…2°, the maximum

value does not exceed 5°. The Schmid factor value approaches the maximum possible value of – 0.5.

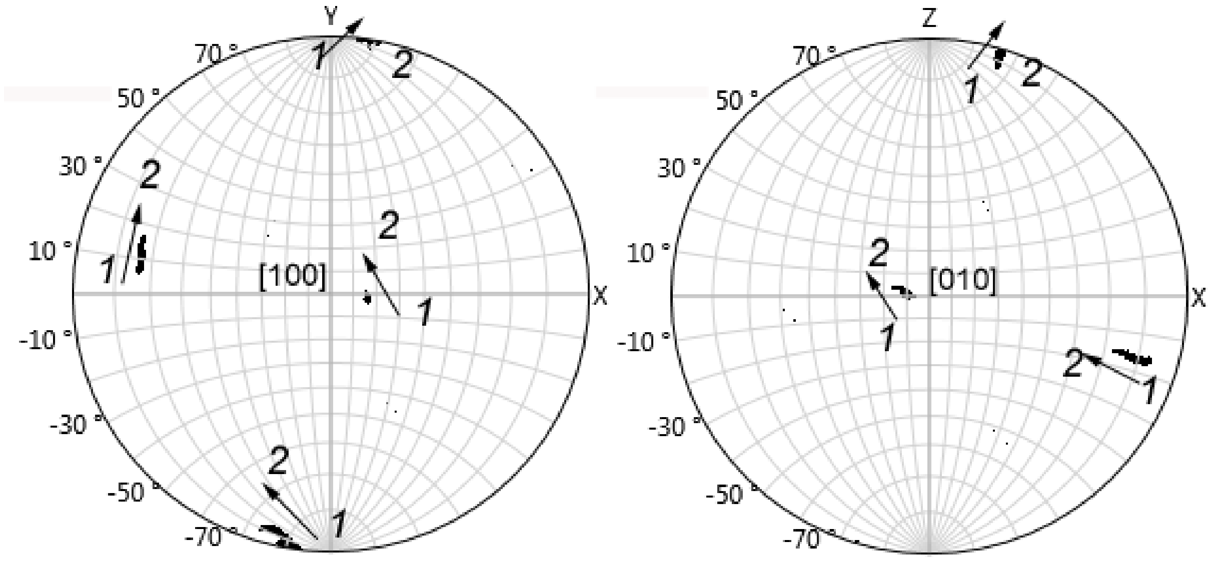


Figure 4. The direct pole figure obtained from the (100) on which the incision

We are able to observe the involvement of all equally loaded slip systems only in the situation when we consider a single crystal as a whole. The single crystal is broken on deformation domains (size 0.5 ... 2 mm). In each domain, only some of all possible slip systems are active. As a result, these macroscopic areas are the misorientation. This is due to accumulation of misorientation in meso-volumes of a material. The study presented in this article confirms this statement. On the meso-level there is a correlation between the change of orientation and active slip systems in them. When moving from the primary orientation [001] to the orientations [117] and [105], the Schmid factor changes for eight equally loaded slip systems. For four slip systems, it varies from 0.41 to 0.43, while for other four from 0.41 to 0.37. It is interesting to note that the increase of the Schmid factor is observed for systems of adjacent slip planes. According to authors, this slip feature contributes to the slip deformation of adjacent areas without disrupting the solidity of the material. This reorientation pattern and the Schmid factor alteration is typical for face with the incision and for the perpendicular to it face. The gradient increase of misorientation for the face with an incision can be explained by a smooth conversion of the curvature face due to the migration of the material to the incision area. On the face perpendicular to the incision, due to the nature of stresses, we observe a wavy surface alteration, which stimulates the formation of folded structures and periodic orientation change in slip systems at meso-level.

The deformation relief on the inner surface of the concentrator is a system of intersecting slip band that form a complex system of steps and folds. Substantial surface curvature in the tip of the concentrator, which occurs under the compressive deformation, contributes to folding. Involvement of a large number of slip systems becomes possible because of activation of the maximum value of all stress tensor components. As a result of the incision edges convergence and alteration of the surface orientation, inside the incision occurs the alteration of the crystallographic orientation in meso-areas toward favorable conditions for the slip.

4. Conclusions

Thus, the analysis of deformation relief and misorientation showed an interconnection between slipping and reorientation. The macroscopic forming in the incision area correlates with the nature of misorientation alterations. Its macroscopic alteration is accompanied by the formation of misoriented meso-areas where favorable to shear deformation in local domains slip system are activated.

Nature of change and accumulation of misorientations obtained by the EBSD method is in good agreement with the development and accumulation of misorientations in the dislocation structure observed in earlier works by authors and other researchers.

Significant surface curvature in the concentrator tip during the compressive deformation, as well as the maximum value of stress, leads to the formation of intense folding and to activation of the maximum number of slip systems. In addition, constant change of the surface orientation inside the incision creates favorable conditions for activation of new slip systems. Such deformation conditions should contribute to the intensive formation of the misoriented structure of micro- and nano-size.

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