Materials Letters 182 (2016) 253–256

Contents lists available at ScienceDirect

Materials Letters

journal homepage: www.elsevier.com/locate/matlet

Formation of low-angle boundaries accompanying the deformation process by twinning in titanium

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ARTICLE INFO

Article history:
Received 17 May 2016
Received in revised form
29 June 2016
Accepted 30 June 2016
Available online 1 July 2016

Keywords:
Twinning
Titanium
Defects
Dislocation walls
Grain boundaries
Stress
Mathematical modeling

ABSTRACT

The structure of the transition zone of the wedge twin formed inside the grains of polycrystalline titanium was experimentally investigated. The accumulation of low-angle grain boundaries formed during the deformation by twin growing was discovered. Mathematical modeling of the stress state close to the twin zone was described in context of the macroscopic dislocation model. The model allows describing physical processes responsible for the formation of low-angle grain boundaries in a form of dislocation walls close to the transition zone of the wedge twin.

1. Introduction

Mechanical twinning in real polycrystalline materials is a complex multistage process of movement and interaction of dislocations. On the one hand, the stress concentration at the boundaries of structural fragments and areas of intersections of twinning layers can lead to brittle fracture, and on the other hand, the presence of twinning layers significantly increases the durability of metals [1]. The direct result of the mechanical twinning process is a formation of high-angle grain boundaries in a metal structure. It affects the mechanical and performance properties of the products manufactured by twinning materials [2]. In the present work we demonstrate generation of low-angle grain boundaries in commercially pure titanium samples.

2. Materials and methods

Titanium samples were deformed by rolling at $\varepsilon = 75\%$ and annealed at 700 °C. The plates of size $(10 \times 10 \times 1.5)$ mm were sanded, polished and electropolished. The technique of obtaining wedge shape twins by microindentation of grains, for which the crystallographic plane (0001) is aligned with the surface of the sample, was described in detail [3]. There were indented over 1000 grains in the experiment. The prepared twins were studied with optical and scanning probe microscopy. Then the titanium samples were subjected to electropolishing and chemical etching with a subsequent investigation of the surface relief changes.

3. Results of the experiment

Study of the etched samples relief (Fig. 1b) showed that the transition zone of the twin layer has an inhomogeneous structure. The picture obtained after etching characterizes the level of the cumulative elastic stresses in this area and the formation of zones of the minimum and maximum defect density.

It was found that the wedge shape region III (Fig. 1b) was generated along the twin layer boundary with minimal stresses. Thus, the width of this zone increases up to 1 μm at the twin top and disappears completely in the twin's mouth. The area I of maximal stresses (Fig. 1b) was formed in the vicinity of zone III. The width of this zone in the mouth is about 1 μm and decreases up to 0 at the top of the twin. Zone II has an uniform thickness and the low internal stresses. The dislocations uniformly distributed over the entire length of the boundary as well as along the zone IV boundary.

It should be noted that the micro optical observations of the investigated grains confirmed that the structure of the transition zone is typical for all of the twins obtained in the experiment. Due

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http://dx.doi.org/10.1016/j.matlet.2016.06.127
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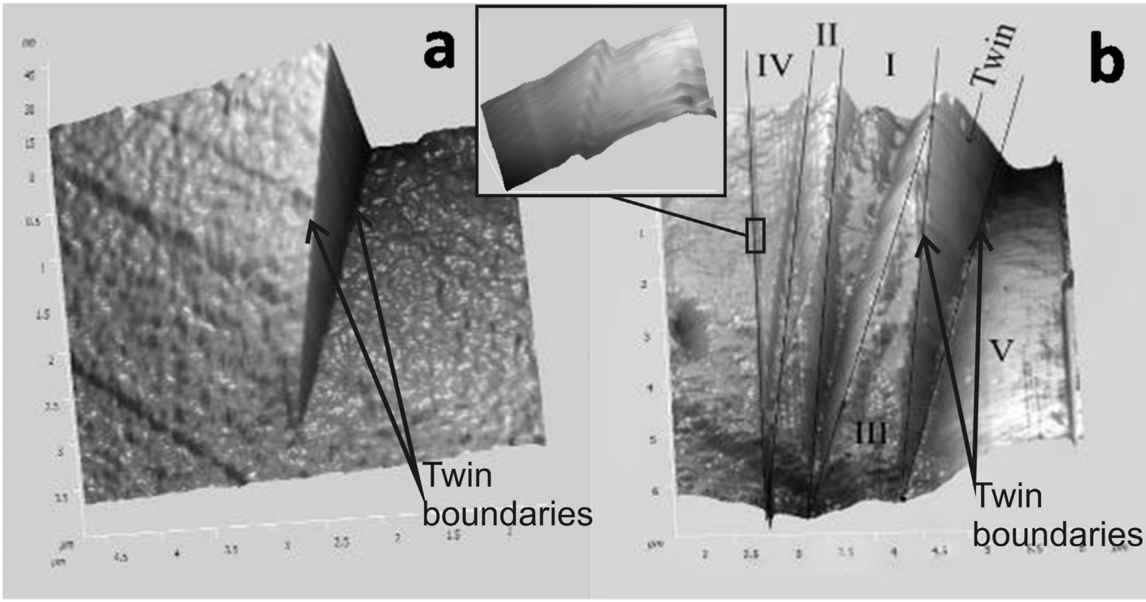

Fig. 1. The images obtained with scanning probe microscopy: the part of titanium surface with the wedge twin before (a) and after (b) etching.

to the appearance of brightly expressed peaks of stresses near the twin boundary, there is possible the formation of low-angle boundaries by the dislocation walls generation.

4. Discussion

Generation of low-angle boundaries in the transition zone and the inhomogeneous distribution of stresses can significantly affect the mechanical properties of metal [4]. The considered effect is well consistent with the fact of increasing the number of low-angle boundaries in the structure of twinning materials at high degree of deformation [5]. It can be explained by increasing the number of the fragments in the twin layers transition zone. To obtain a total picture of the processes taking place during the deformation it should be considered mechanisms of sliding and twinning not only as competing ones but also as the phenomena accompanied each other and responsible for the formation of a structure in the twin layer zone. So, in the work [6] it was experimentally shown that the stresses localized in the twin area had been relaxed by the dislocation gliding in the accommodation areas. It can be assumed that there is a regular structural rearrangement in these areas forming dislocation clusters and the crystal areas of the minimal and maximal defect density. Generation of the block structure in the transition areas was observed on single crystals of zinc earlier [4]. The authors studied a distinction of a crystallographic orientation in the transition zone and the parent crystal by the X-ray graphic method. It was detected the formation of variety of the structure fragments in the accommodation area.

It is known that in HCP crystals the formation of the block with a structure different from the rest part of a transition area occurs close to the twin layer boundary because of the dislocation reaction:

$$2\left[-100\right] + 1/14\left[-211\right] \rightarrow \left[011\right] \quad (1)$$

This reaction is not favorable energetically, and full dislocations repel from the twin boundary in the transition zone. Therefore, an area near the boundary is purified of all dislocations. This theory explains well the presence of a zone III detected in the experiment (Fig. 1b). Also, the high stresses in a zone I are well explained by a dislocation drain from the twin layer boundary and from a zone III during the relaxation process of the stresses resulting from the growth of the twin layer. Interaction of dislocations well explains the emergence of low-angle boundaries and therefore the maximum stresses in a zone I (Fig. 1b). But this theory cannot explain the presence of the stresses minimum in a zone II and the dislocation wall on the boundaries of zone IV. To understand the processes occurring in the transition zones, it is necessary to consider not only influence of the defect motion, but also the stress field arising as a result of formation of the twin layer. Significant influence of residual stresses confirms mismatch of a twin angle on the crystal surface to estimated parameters and reducing the misorientation angle between the twin layer and a pattern crystal with regard to values calculated by symmetry considerations.

For a detailed analysis of the field of the residual internal stresses, it was carried out the mathematical modeling of a stress state in a vicinity of the twin zone described in the framework of the macroscopic dislocation model [7]. The stress field near the twin of the wedge shape is defined as follows:

$$\sigma_{ij}(x, y) = \int_0^L \sqrt{1 + (f_1'(x_0))^2}\,\rho_1(x_0)\sigma_{ij}^{(1,0)}(x, y, x_0)dx_0 + \int_0^L \sqrt{1 + (f_2'(x_0))^2}\,\rho_2(x_0)\sigma_{ij}^{(2,0)}(x, y, x_0)dx_0, \quad (2)$$

where L is the length of the twin; $f_1(x_0)$, $f_2(x_0)$ – functions describing the shape of the twin boundaries; $\rho_1(x_0)$, $\rho_2(x_0)$ – densities of twinning dislocations on the twin boundaries; $\sigma_{ij}^{(1,0)}$, $\sigma_{ij}^{(2,0)}$ – stresses created by individual dislocations on the twin boundaries. Based on the experimental data the form of the incoherent boundaries of mechanical wedge twin in the investigated metal is approximated by straight-line functions:

$$f_1(x_0) = \frac{H}{2}\left(1 - \frac{x_0}{L}\right),\ f_2(x_0) = -\frac{H}{2}\left(1 - \frac{x_0}{L}\right). \quad (3)$$

Here H is a twin width at the mouth. Assuming the density of twinning dislocations at the boundaries is identical, the symmetry of shear stresses about the twin axis is observed (Fig. 2).

It should be noted that the point defining the conjunction of the functions describing the elastic wedge twin boundaries is singular. Therefore, the values of stresses calculated in its vicinity

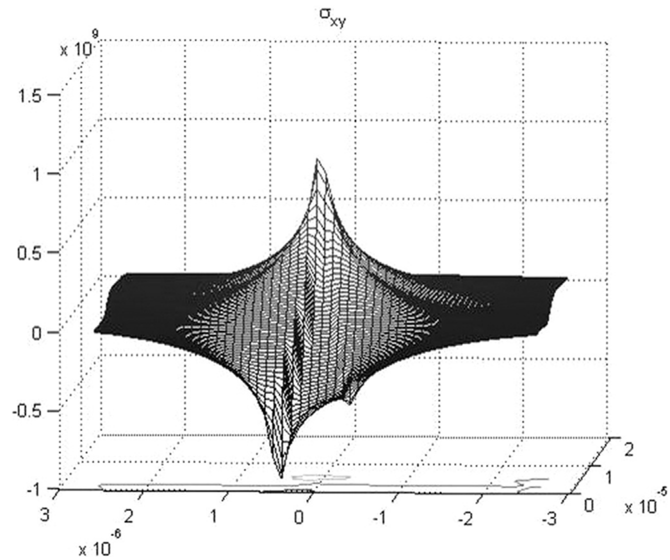

Fig. 2. Distribution of stresses in the twin lamella, determined according to the current model.

exceed the real ones significantly. The shear stresses take negative values near the mouth of the twin and are close to zero in the middle part of the twin. The stress level exponentially changes with increasing distance near the boundaries. The stress plot represented by this model does not explain the physics of formation of the low-angle boundaries found by the experiment in the transition zone. For a correct mathematical description of the processes occurring in a metal, it is necessary to take into account the presence of the above dislocation wall formed by the interaction of twinning dislocations with defects in the transition zone. As mentioned earlier, the full dislocations and partial twinning dislocations with collinear Burgers' vectors form the wall in the accommodation area by repelling from each other. Considering the above fact of the presence of low-angle boundaries generated by the interaction of dislocations, it was carried out the additional mathematical modeling. The obtained results (Fig. 3) show that there is the extra stress maximum and minimum in addition to the maximum stress formed by the twin boundary and the low-angle boundaries taken into account in the process of modeling. It can be a result of a superposition of fields from different sources.

The data obtained by the modeling are in agreement qualitatively with the experimental results (Fig. 1b). Thus, the present model enables to explain the physics of the processes responsible for the formation of a zone III (Fig. 1b). As shown in Fig. 3b, the area corresponding to the stress maximum deviates from the twin boundary with approaching to its top on account of the superposition of the fields created by the twin boundary and the dislocation wall. The mathematical modeling of residual stresses was made in condition of low-angle boundaries parallel to a twinning plane. It has to be noted that the modeling results do not indicate the formation of minima and maxima that were seen in the experiment. Location of the low-angle boundaries parallel to the twinning plane indicates its continuous formation in the process of generation of the twin layer and the high stresses at the top of the twin. The proposed model shows that the formation of the low-angle boundaries, due to the interaction of the existing defects in the material and the twinning dislocations, leads to changes of the stress distribution in the transition zone. This, in turn, generates some of the low-angle boundaries in the form of dislocation walls.

5. Conclusions

It was discovered and studied the ordered dislocation structure in the area of transition zone of wedgelike mechanical twin in the titanium. In the work we suggest dislocation mechanism of formation of the structure through the generation of several low-angle boundaries. This generation arises as the result of high internal stresses in the transition zone of twinning layers and moving defects due to relaxation of these stresses.

Carrying out the mathematical modeling confirmed the correctness of the proposed mechanism.

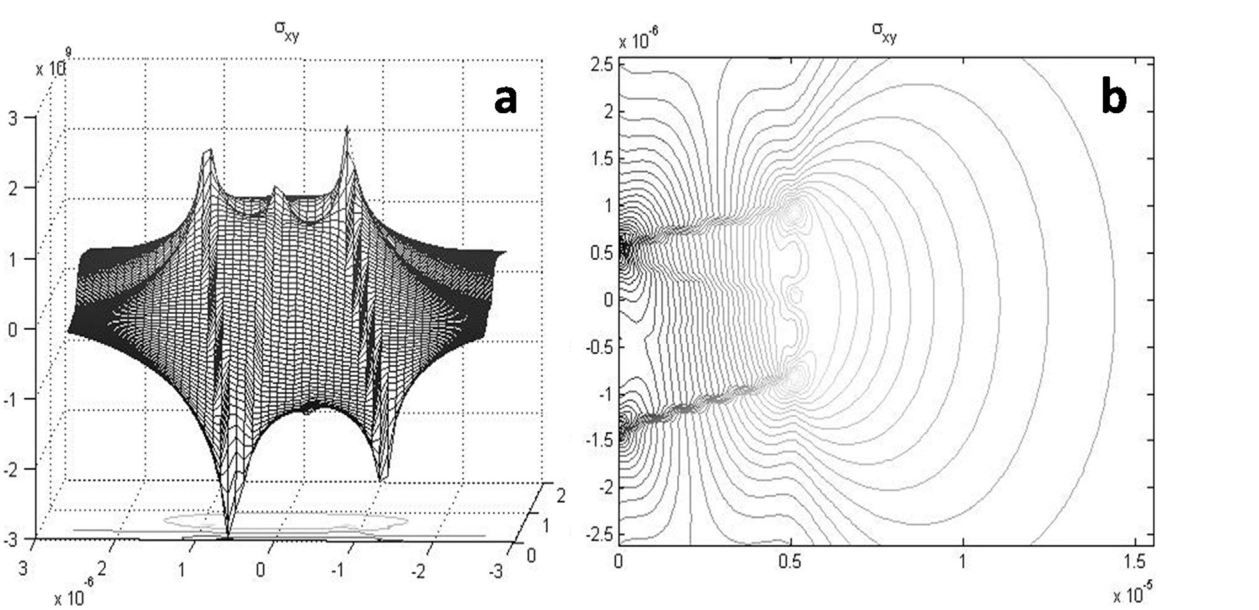

Fig. 3. Distribution of stresses in the twin lamella, based on the availability of dislocation walls parallel to the twinning plane: a) a visual representation of the results, and b) a presentation of results using isolines.

Acknowledgment

Work is performed with assistance of the Ministry of Science and Education of Russia, the Project no. 14.578.21.0063 (RFMEFI57814 × 0063), and the authors would like to thank Prof. Vadim Glebovsky (The Institute of Solid State Physics RAS) for the critical assistance in preparing this article.

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