Short Communication

Structure and Stresses in a System of Two Mechanical Twins in Titanium

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(Received 25 July 2018; revised manuscript received 07 December 2018; published online 18 December 2018)

In the work we have presented the results of experimental studies and mathematical modeling for the
processes of the structure formation in a transition zone of wedge-type twins system in commercially pure
titanium. The process of interaction of structure defects with twinning dislocations during the formation of
a wedge-type twin was taken into consideration. It is shown that the interaction alters the stress maxi-
mum in vicinity of boundaries in the system two wedge-type twins.

Keywords: Twinning, Dislocation walls, Grain boundaries, Stress, Mathematical modeling.

DOI: 10.21272/jnep.10(6).0604 PACS number: 68.49.Jk

1. INTRODUCTION

The intensification of twinning at certain stages of the deformation processing reduces the average grain
size, which positively affects on improving the strength properties of metals and alloys. However, at a certain
stage, the twinning process ceases to contribute to the refinement of structure. Mechanical twinning in real
polycrystalline materials is a complex multi-step process of motion and interaction of dislocations. On the
one hand, the concentration of the stress on the borders of the fragments of the structure and in the areas of
intersection of the twin inter layers can lead to a brittle fracture and on the other – the existence of twin inter
layers greatly increases the strength of metals [1]. It is believed that a direct consequence of the mechanical
 twinning is the formation of the large-angle boundaries in the deformable metal.

However, in experiments on commercially pure tita-
nium it is found that due to both the high internal stresses in the transition areas of the twinning inter
layers and movement of defects at the relaxation of the stresses, there is a natural formation of the low-angle
boundaries. This, in turn, can influence the mechanical and operational properties of products manufactured
from the twin-able materials. Since at the real deformation of polycrystalline materials there is a formation of
the ensembles of the twin wedges, it is of great interest to reveal both the superposition of the stress fields
of the different twins and its impact on the structure in the transition zone.

2. MATERIALS, METHODS AND MODEL

As an experimental material was titanium
(grade VT1-0), which was subjected to the rolling de-
formation ε = 75 % and annealed at 700 °C. The pro-
cessing techniques and twin studies by the wedge mi-
cro-indentation of the grains for which the crystallo-
graphic plane (0001) is aligned with the sample surface
were described earlier [2]. In the experiments more
than 1,000 grains were indented. The study of the
etched samples relief showed that the area of the trans-
ition of the twin interlayer has a non-uniform struc-
ture. Since the pattern obtained after etching charac-
terized the level of the total elastic stress in this area,
it can be assumed that the zones are formed with the
minimum and maximum density of defects.

For a more detailed analysis of the field of the resi-
dual internal stresses, the mathematical modeling of a
continuous distribution of the twinning dislocations at the borders of the twinning zones described within
the framework of the macroscopic dislocation model [3].

A system of wedge-type twins arising on the sur-
fase of titanium sample is considered. In the general
case, in the XOY plane, the shape of the boundaries of
a wedge-type twin is described by the functions f₁(x₀),
f₂(x₀), f₃(x₀) and f₄(x₀) (Figure 1). The densities of twin-
nig dislocations at the boundaries of a wedge-type twin are different and are given by functions of linear
dimensions of the twin. Then the stresses created by
the system under consideration of wedge-shaped twins
can be determined from the formula [3]:

\[ \sigma_{ij}(x, y) = \sigma_{ij}^0(x, y) + \sigma_{ij}^1(x, y) + \sigma_{ij}^2(x, y) \]

where

\[ \sigma_{ij}^0 = \int_{L_{AB}} \rho_1 \sigma_{ij}^{(1,0)} ds; \]
\[ \sigma_{ij}^1 = \int_{L_{CB}} \rho_2 \sigma_{ij}^{(2,0)} ds; \]
\[ \sigma_{ij}^3 = \int_{L_{DE}} \rho_3 \sigma_{ij}^{(3,0)} ds; \]
\[ \sigma_{ij}^4 = \int_{L_{FE}} \rho_4 \sigma_{ij}^{(4,0)} ds. \]
Here \( \sigma^{(1)}_{ij}, \sigma^{(2)}_{ij}, \sigma^{(3)}_{ij} \) and \( \sigma^{(4)}_{ij} \) are stresses created by each boundary of the system of wedge-shaped twins. The stresses are determined using the curvilinear integral along the twin-boundary profiles LAB, LCB, LDE and LFE, respectively; \( \sigma^{(1,0)}_{ij}, \sigma^{(2,0)}_{ij}, \sigma^{(3,0)}_{ij} \) and \( \sigma^{(4,0)}_{ij} \) are stresses created at the twin boundaries of single dislocations respectively.

The curvilinear integrals (1) turn into definite integrals [3]:

\[
\sigma^{(1)}_{ij}(x, y) = \int_0^L \left[ 1 + \left( f'_1(x_0) \right)^2 \right] \rho_1(x_0) \sigma^{(1,0)}_{ij}(x, y, x_0) dx_0;
\]

\[
\sigma^{(2)}_{ij}(x, y) = \int_0^L \left[ 1 + \left( f'_2(x_0) \right)^2 \right] \rho_2(x_0) \sigma^{(2,0)}_{ij}(x, y, x_0) dx_0;
\]

\[
\sigma^{(3)}_{ij}(x, y) = \int_0^L \left[ 1 + \left( f'_3(x_0) \right)^2 \right] \rho_3(x_0) \sigma^{(3,0)}_{ij}(x, y, x_0) dx_0;
\]

\[
\sigma^{(4)}_{ij}(x, y) = \int_0^L \left[ 1 + \left( f'_4(x_0) \right)^2 \right] \rho_4(x_0) \sigma^{(4,0)}_{ij}(x, y, x_0) dx_0;
\]

here \( L \) is the length of the twin. The Burgers vector of the partial twinning dislocations has two components – the edge \( b_e \) and the screw \( b_s \) ones. The stresses field near the twin of the wedge shape (in figure 1) is defined as follows [3]:

\[
\sigma_{ij}(x, y) = \int_0^L \left[ 1 + \left( f'_1(x_0) \right)^2 \right] \rho_1(x_0) \sigma^{(1,0)}_{ij}(x, y, x_0) dx_0 + \int_0^L \left[ 1 + \left( f'_2(x_0) \right)^2 \right] \rho_2(x_0) \sigma^{(2,0)}_{ij}(x, y, x_0) dx_0 + \int_0^L \left[ 1 + \left( f'_3(x_0) \right)^2 \right] \rho_3(x_0) \sigma^{(3,0)}_{ij}(x, y, x_0) dx_0 + \int_0^L \left[ 1 + \left( f'_4(x_0) \right)^2 \right] \rho_4(x_0) \sigma^{(4,0)}_{ij}(x, y, x_0) dx_0,
\]

here \( L \) is the length of the twin; \( f_1(x_0), f_2(x_0), f_3(x_0) \) and \( f_4(x_0) \) are functions describing the shape of the borders of the wedge twin (in figure 2); \( \rho_1(x_0), \rho_2(x_0), \rho_3(x_0) \) and \( \rho_4(x_0) \) are densities of the twinning dislocations at the borders of the twin; \( \sigma^{(1,0)}_{ij}, \sigma^{(2,0)}_{ij}, \sigma^{(3,0)}_{ij} \) and \( \sigma^{(4,0)}_{ij} \) are stresses created at the twin borders of the single dislocations.

Based on the experimental data, the form of the incoherent borders of the mechanical wedge of the twin in the sample is given by the linear approximation. In the simulation it was assumed that the density of the twinning dislocations on the borders is the same, resulting in the shear stresses symmetry.

3. RESULTS AND DISCUSSION

The shear stresses have negative values near the mouth of the twin and close to zero in the middle of the twin. The stresses change near the borders exponentially.

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**Fig. 1** – Scheme The schematic illustration of twins in the simulation

The full and partial twinning dislocations with the collinear Burgers vectors, repelling, form the wall in the transition zone. The correct mathematical description of the stress field created by two twins should be based on the presence of the twin borders and the wall formed by the interaction of the twinning dislocations with defects in the transition zone. This is confirmed by experimental data [4].

**Fig. 2** – The image of titanium surface after etching in the area of the formed twin obtained with a scanning probe microscopy (a) and modeling of stress distribution in the area of twinning (b).
Obtained results (Figure 2a) demonstrate that in addition to the high stresses, formed by the twin border and accounted for in the simulation by the small-angle border, there are additional high and low stresses, resulting from the superposition of the fields from the different sources. The data, obtained using the simulation, agree qualitatively with the experimental data (Figure 2b). Thus, the present model provides an opportunity to explain the physics of the processes responsible for the formation of the additional zone situated between the twins. From Figure 2b, it follows that the zone corresponding to the maximum stresses deviates from the twin border and approaches its apex due to the superposition of fields generated by the twin border and dislocation wall.

Twining can in some ways be deemed to be analogous to slip, in that an activator of the both processes is the same when shear stresses reaches the critical value in slip plane. Some experimental results imply that twinning effect may also depend on stress components other than the shear stress. It can be assumed that formed stresses in transition zone of wedge deformed twin help generation and growth of new twin in the same plane.

The local stress concentration needs to be high enough for twin embryos to reach the critical size but as soon as they reach the critical size, the twin propagation can then proceed at a relatively low local stress. It is proved experimentally that in transition zone full and partial twinning dislocations with collinear Burgers’s vectors when repulsing form a wall in accommodation zone. It causes heterogeneity of a value of stresses and this provides further formation of twinning wedge in the area [4].

It should be mentioned that dividing one large twin into several twins does create additional interface between the twin and grain matrix, increasing the total interfacial energy, which would slightly alter the relative balance in favor of a large twin [5].

In Figure 2a are shown experimental results describing areas of stresses in two twins formed in the same plane of twinning. Unlike area of stress of one twin discussed in [4] in case of two twins should be considered redistribution of stresses in area of first as result of relaxing stresses caused by growing of second twin.

It is stated that maximum level of stresses in case of single twin is situated on tip. It could be explained by high density of dislocations and as well by superposition of stress fields from two borders of the twin.

According to experimental results Figure 2a in area of tips of wedge twins there is no concentrations of stresses. This indicates that there have place relaxing processes directly connected with pair forming of wedge twins.

Mathematic model took in account reorganization of dislocations in transition zones twin-matrix approves experimental result Figure 2b. In this case mathematic model and experiment results point that in transition zones it is observed the same dislocation structure as in case of single twin [4].

4. CONCLUSIONS

While forming of wedge twin in poly-crystal of titanium are forming conditions of formation of additional twin in its transition zone. Forming of the extra twin is some way of relaxation of high stresses in the tips.

The proposed model indicates that the formation of low-angle boundaries due to the interaction of existing material defects and twinning dislocations leads to a change in the stress diagram in the transition area, which, in turn, generates multiple low-angle borders in the form of the dislocation walls.

Shown physical mechanism and mathematic model gives rather clear picture of forming of structure and spreading stresses in zone of forming of two parallel twins.

ACKNOWLEDGMENTS

The work was financially supported by a program of the ministry of education and science of The Russian Federation for higher education establishments, project №14.578.21.0192 (RFMEFI57816X0192).

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