Supplementing a plastic deformation model in DAMASK software with twinning mechanisms in α-phase for two-phase titanium alloy VT16

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An approach to modeling texture formation in titanium alloys containing the hcp phase during plastic deformation is proposed using DAMASK software and taking twinning into account. The description of crystallographic slip implemented in the existing phenomenological model is supplemented by a developed algorithm for the nucleation and growth of deformation twins. Twin nucleation is implemented in accordance with the Schmid criterion and takes into account the local stress distribution, while growth is described using an energy criterion that accounts for the contribution of twin boundaries. The proposed model is verified using the experimental rolling texture of a zirconium single crystal, characterized by the same structure and lattice constant ratio c/a, and provides an excellent description of the observed fundamental patterns of crystal lattice reorientation. The model enables high-quality reproduction of the shape of twin lamella within the grain volume. The rolling texture of the VT16 polycrystalline alloy calculated using the developed model provides a good description of the observed experimental results of texture formation. At the initial stage of rolling, in grains whose basal axes are deviated from the normal direction in the sheet by an angle of more than 70 degrees, the main deformation mechanisms turned out to be twin planes $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$, which continue to act along with crystallographic slip until reaching 50%.

Key words: titanium alloys, VT16, twinning, slip, simulation, crystallographic texture, finite element model, plastic deformation, DAMASK.

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Introduction

Titanium alloys are widely used in aviation and astronautics, medicine, shipbuilding etc. due to their high specific strength, corrosion and thermal resistance [1]. Their properties are largely determined by alloying and phase composition. Thus, pure titanium belongs to the class of single-phase α-alloys and exhibits high ductility, while two-phase $\alpha + \beta$ alloys doped with V or Mo have low ductility and higher strength. An important factor that significantly affects the properties of titanium alloys is the volume fraction of the β-phase. The anisotropy of the properties of both single-phase and two-phase titanium alloys is largely determined by the α-phase texture, which depends not only on the deformation scheme but also on the presence of a second phase. According to [2], the content of the β-phase affects the crystallographic texture formed during thermomechanical processing. In [3], the influence of β-phase morphology on the plastic deformation of the α-phase in Ti-6242 alloy is associated with the interaction of phases at the interface and the involvement of β-phase particles in the deformation process. In metals with a hexagonal close-packed (hcp) structure, typical for α-titanium, not only crystallographic slip but also twinning, which provides the reorientation of the crystal lattice under conditions of obstructed slip, plays an important role in texture formation.

Optimization of the manufacturing routes using *X*-ray texture analysis is required to create the necessary anisotropy of properties in titanium products. Numerical modeling of plastic deformation is used to reduce the laboriousness of optimization processes. Despite the widespread implementation of the finite element modeling (FEM) of stress-strain states in parts and workpieces, it generally does not allow for predicting the evolution of crystallographic texture. For example, papers devoted to hot forging and upsetting of aircraft titanium alloys [4, 5] are aimed for studying the inhomogeneities of the stress-strain state in various sections of the product or billet. However, the texture is considered as the anisotropy of the yield strength along various directions, but its evolution during deformation is not taken into account in such calculations.

FEM models incorporating the regularities of crystalline plasticity (CPFEM), which directly determining the crystallites lattice rotations, are best suited for identifying the texture formation patterns. A freely available, open-source software DAMASK is the one of such tool [6]. DAMASK is a popular instrument for modeling the evolution of the microstructure and texture of single-phase and multiphase metallic materials, which has been most successfully used to study alloys consisting of phases with a cubic lattice structure [7–9].

However, there is no universal verified approach for predicting the texture of hcp-materials. Although DAMASK software states for the accounting for twinning, its realization fails in either an accurate description of their nucleation and growth, nor in the modeling the shape of twin platelets and the deformation texture of hcp metals. For example, [8] examines the evolution of the texture and structure of the Ti – 6Al – 4V alloy during tensile testing. In this study, twins in the microstructure are represented not as plates or needles, but as single points localized in areas with increased stress, and the typical reorientation of basal axes along the direction of compression, observed experimentally, is not reproduced in complete direct pole figures (DPFs).

Paper [9] shows the results of determining the anisotropy of the mechanical properties of rolled sheet made of technical-purity titanium with a stable rolling texture (the basal axes are deflected from the normal direction (ND) towards the transverse (TD) direction by 30°) using DAMASK modeling without taking any twinning processes into account. According to [10, 11], with such a basal axes distribution the main deformation mechanism is prismatic slip, which corresponds to the data obtained in the paper. However, despite the good agreement between the calculated stress-strain curves and the experimental ones, the model does not explain the observed difference in hardening at the initial stages, where deformation occurs predominantly by twinning.

A promising approach that allows for the correct incorporation of grain reorientation by twinning is described in [12]. It proposes to calculate the stress-strain state considering only crystallographic slip, and then to estimate the criterion for achieving the critical resolved shear stress (CRSS) for twinning activation for each point of representative volume. However, if some grain has an unfavorable for slip orientation, such approach leads to its whole reorientation by twinning rather than the formation of lamellae within, what makes impossible the microstructure prediction.

Thus, the aim of this work is to develop and verify a twinning model for metals with an hcp structure, integrated into the calculations of the DAMASK software and allowing to predict not only the crystallographic texture evolution, but also the twins morphology.

Modeling methodology

The rolling simulation was carried out using DAMASK software, in which the phenomenological law of plastic deformation describes a crystallographic slip as [8]:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left(\frac{\tau^{\alpha}}{\xi^{\alpha}}\right)^{n}\operatorname{sgn}\left(\tau^{\alpha}\right) \quad (1)$$

where $\dot{\gamma}^{\alpha}$ – slip rate in system α; τ^{α} – resolved shear stress; ξ^{α} – slip resistance; n – slip rate sensitivity. The hardening law is described by the slip resistance evolution ξ^{α} taking into account the interaction of the slip systems between each other.

Since the phenomenological model implemented in DAMASK does not provide a correct reconstruction of the deformation texture of titanium alloys containing the α-phase, the twinning mechanisms were elaborated using a developed by authors algorithm, which takes into account the nucleation and growth of twin lamellae, as well as stress relaxation [13, 14].

A necessary condition for the twinning activation is reaching by the resolved stress the CRSS value, but this is not sufficient [15–17]. Due to the lack of a universal criterion for twin nucleation within the FEM, we used a deterministic approach aimed at identifying the regions most favorable for its initiation. Therefore, it is assumed for twin nucleation the necessity of the CRSS achieving within regions with a high hydrostatic pressure gradient, characterizing local stress inhomogeneities [18–20]. The hydrostatic pressure p and its gradient are calculated using the following formulas:

$$p = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} \rightarrow \left|\nabla p\right| = \sqrt{\left(\frac{\partial p}{\partial x}\right)^2 + \left(\frac{\partial p}{\partial y}\right)^2 + \left(\frac{\partial p}{\partial z}\right)^2} \quad (2)$$

where σ_{xx}, σ_{yy}, σ_{zz} – principal stresses of Cauchy tensor. The calculation of the resolved stress at each point within the calculation cell is carried out for each of the possible twinning planes in α-titanium: $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$, reorienting the basal axes by an angle of 85°, 35°, 65° and 57°, appropriately [21, 22]. An energy criterion, accounting for the reaching by CRSS along the growth direction and the energy of the twin boundary, further controls the twin growing [23]. The change of the system energy $\Delta W(t)$ during the twin growth at the i-th point is described by the following equation:

$$\Delta W(i) = s \times \left[\Delta\tau(i)\right]_{+} \times \Delta V_i \quad (3)$$

where $\Delta\tau(t)$ is calculated by:

$$\Delta\tau(i) = \tau(i) - \tau_0 - \frac{2\gamma_{CTB}\kappa(i)}{s} \quad (4)$$

here $\tau(i)$ – resolved shear stress in the twinning system at the i-th point of space, τ_0 – CRSS of the twining system, γ_{CTB} – specific energy of a twin boundary; $\kappa(i)$ – the twin boundary curvature; s – amount of shear.

We consider the twin growth in this model as an anisotropic process: the priority elongation directions is the twinning direction and perpendicular to it within the twinning plane, the twin broadening along the direction normal to the twinning plane is also possible. The twin growth stops if there are no candidates for which $\Delta W(t)$ remains positive or if the twin reaches a grain boundary. It should be noted that in the present model a twin propagation through a grain boundary is possible only if the misorientation angle between adjacent grains is less than 15° [24].

Experimental data show that in two-phase $\alpha + \beta$ titanium alloys, twins of hcp α-phase never cross the boundary with the β-phase (bcc) [25, 26]. The boundary blocks the propagation of twin dislocations, so the strain transfer occurs only indirectly in this model — through elastic stresses or the emergence of new twins in adjacent α-phase grains. This effect is limited by stress fields, what is already taken into account by the DAMASK software. After completion of all growth processes, local elastic stress relief occurs within the twin.

The algorithm for modeling texture formation with twinning incorporation has been integrated into the calculation scheme using DAMASK software and includes the following steps:

1. Configuring the initial microstructure (grain structure and texture) and material parameters (slip systems, twinning and critical stresses of their activation) and the calculation termination frequency for twinning modeling;
2. Calculation of the stress-strain state in DAMASK software taking slip into account at a small increment of the deformation degree $\Delta\varepsilon$ and the calculation stopping;
3. Inspection of the criterion for achieving the CRSS and determination of twin nucleation centers;
4. Modeling of an anisotropic twin growth and crystal lattice reorientation;
5. Recalculation of the stress-strain state taking into account local stress relaxation and continuation of the calculation in DAMASK software.

Steps 3—5 are repeated until the target deformation is achieved.

The basic model parameters used in DAMASK and CRSS for the twinning model are given in the **Table** [8].

Table
Material parameters used in the model [8]

α-Ti			
Lattice periods ratio	c/a	1.587	
Stiffness coefficient of hcp-phase	C_{11} C_{33} C_{44} C_{12} C_{13}	160 181.1 46.7 90.1 66	GPa
Initial (ξ_0) and ultimate (ξ_∞) slip resistance for basal, prismatic and pyramidal along <c + a> direction systems	$\xi_0^{basal}/\xi_\infty^{basal}$	205/411	MPa
	$\xi_0^{prism}/\xi_\infty^{prism}$	126/291	
	$\xi_0^{pyr<c+a>}/\xi_\infty^{pyr<c+a>}$	654/700	
Hardening coefficient for sliding	h_0^{sl-sl}	2000	
Critical stress for twinning	$\tau_0^{\{10\bar{1}2\}}$	502	
	$\tau_0^{\{11\bar{2}1\}}$	550*	
	$\tau_0^{\{11\bar{2}2\}}$	620	
	$\tau_0^{\{10\bar{1}1\}}$	650*	
β-Ti			
Stiffness coefficient of bcc-phase	C_{11} C_{12} C_{44}	133 95 43	GPa
Initial (ξ_0) and ultimate (ξ_∞) slip resistance for $\{110\}\langle 1\bar{1}1\rangle$ system	$\xi_0^{\{110\}}/\xi_\infty^{\{110\}}$	430/500	MPa
Hardening coefficient for sliding	h_0	1500	
For both α- and β-Ti			
Relative strain rate	$\dot{\gamma}_0$	0.001	
Slip rate sensitivity	n	20	

*CRSS values for all four twinning systems are not presented in literature simultaneously therefore $\tau_0^{\{11\bar{2}1\}}$ value was chosen between $\tau_0^{\{10\bar{1}2\}}$ and $\tau_0^{\{11\bar{2}2\}}$ and $\tau_0^{\{10\bar{1}1\}}$ corresponds to CRSS for pyramidal slip system.

Results

To verify the presented model we used the crystallographic texture of zirconium single crystals with three different orientations, obtained as a result of experimental rolling in [21, 22] and presented by incomplete DPFs (0001) in **Fig. 1**, *a*. The twinning influence in the two-phase titanium alloy VT16 on its texture formation was established by the sheets texture in the initial state (**Fig. 2**, ***Aa***) and after rolling up to 21% (**Fig. 2, *Ab***), 31% (**Fig. 2, *Ac***) and 50% (**Fig. 2, *Ad***) deformation degree.

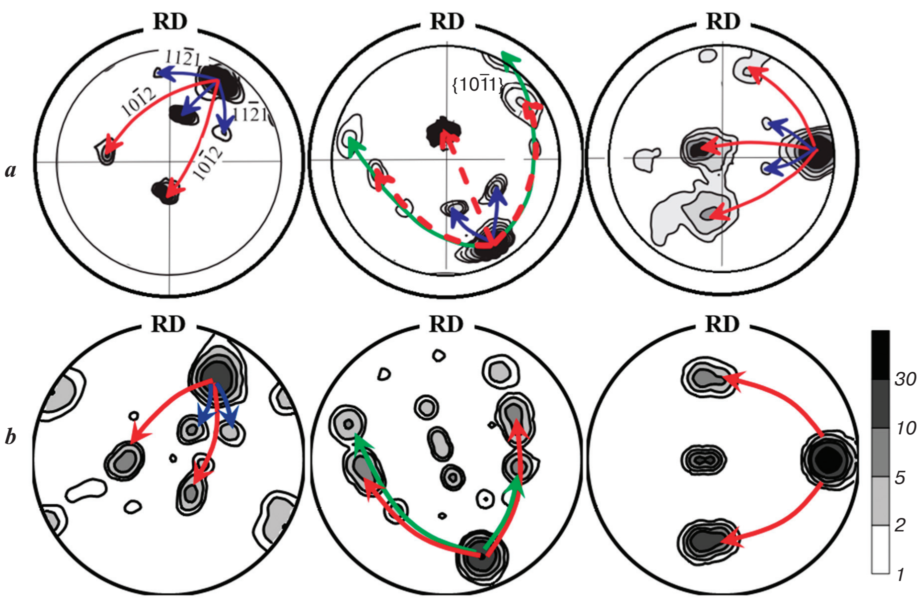

Fig. 1. DPFs (0001):
a — experimental sample;
b — simulated with taking twins into account [21, 22]

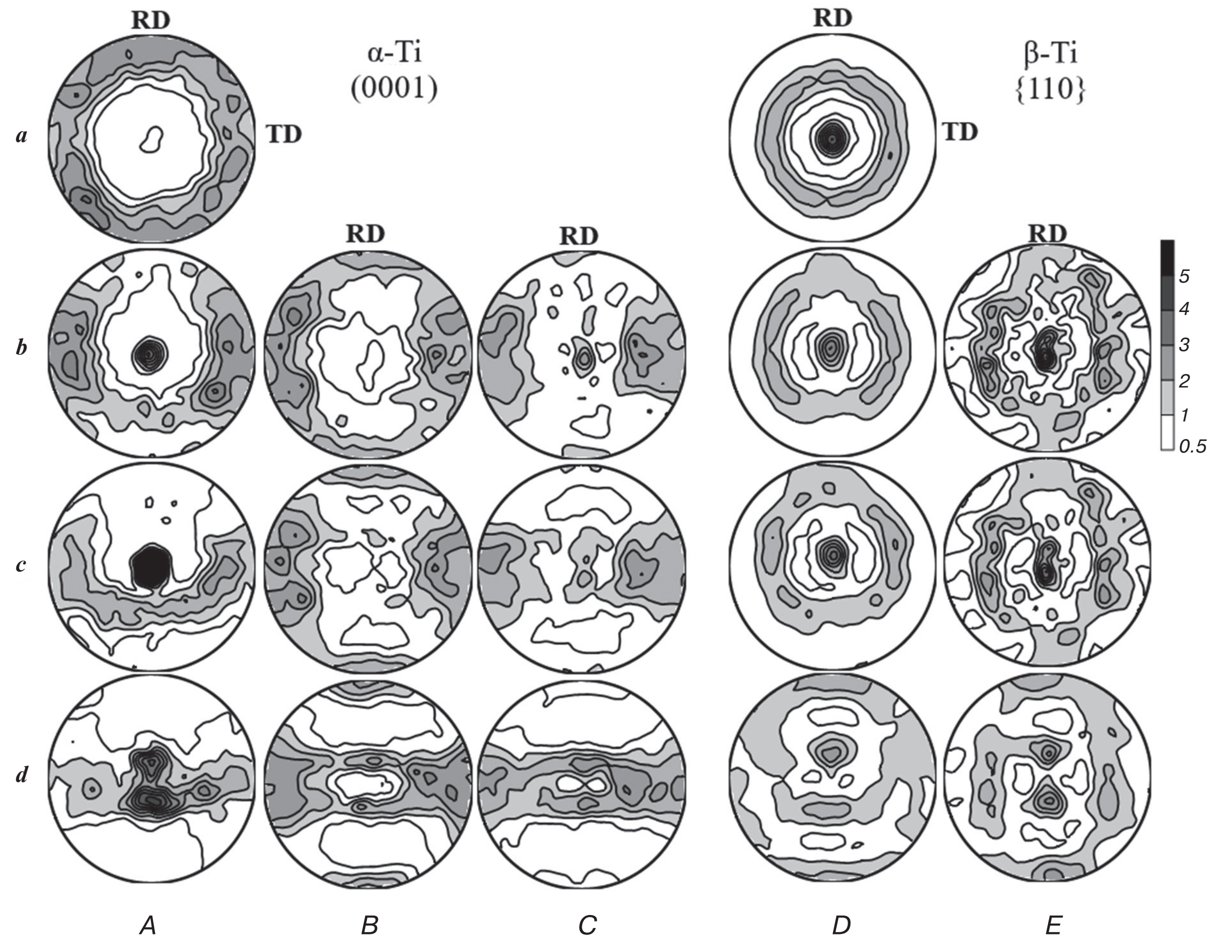

Fig. 2. Texture evolution of α-Ti on complete DPFs (0001): *A* – experimental; *B* – simulated with taking only slip systems into account, *C* – simulated with taking slip and twinning into account; texture evolution of β-Ti on DPFs {110}: *D* – experimental, *E* – simulated with taking slip and twinning into account in α-Ti at deformation degree:
a – 0%, b – 21%, *c* – 31%, *d* – 50%

Model verification

We verified the reorientation algorithm by the rolling texture of a zirconium single crystal with three different orientations subjected up to deformation degree of 5% and 7%. The initial orientations of the single crystal was chosen such that the predominant deformation mechanism should be twinning along the $\{11\bar{2}1\}$, $\{10\bar{1}1\}$ and $\{10\bar{1}2\}$ planes, which reorienting the basal axes by an angles of 35°, 57°, and 85°, respectively. When modeling the texture formation in a single crystal, we consider the action of four twinning systems along the $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ planes, however, under the specified loading conditions, which are closed to experimental rolling, the activity of only three systems was observed: $\{11\bar{2}1\}$, $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$, what corresponds to the experimental results.

Texture formation during rolling of polycrystalline of VT16-allo

The formation of texture in a polycrystalline material consisting of α- and β-phase grains was calculated during rolling up to deformation degree of 50%. If calculate the deformation without taking the twinning mechanism into account for the initial texture of axial type, there is no reorientation of the basal axes away from the RD, what is inconsistent with the experimental results. When we involve the twins nucleation and subsequent growth into the model, a qualitative texture change is observed on the complete DPF (0001): the activity of $\{10\bar{1}2\}$-twinning reorients the basal axes from the RD to the ND, accompanying by a formation of central maxima, which cannot be explained only by crystallographic slip (**Fig. 2, *Bd***). At the same time, in the β-phase one can see the formation of a texture typical for the slip action with a component $\langle 110 \rangle \parallel$ RD.

Discussion

The obtained modeling results for the texture formation in Zr single crystals we explain by the fact, that the orientation of basal axes along the RD results in the close-to-zero Schmid factor for the slip systems $(0001)\langle 10\bar{1}0 \rangle$ and $\{11\bar{2}0\}\langle 10\bar{1}0 \rangle$, while a higher shear stress is usually required to activate the pyramidal slip systems. Therefore, reorientation occurs via twinning along the systems with the highest resolved stress, generally $\{10\bar{1}2\}$ and $\{11\bar{2}1\}$. Many researchers consider when modeling only two types of twinning systems with $\{10\bar{1}2\}$ and $\{11\bar{2}2\}$ planes [8, 12], suggesting that they provide a large deformation fraction, however, the modeling carried out in this work confirms the experimental result obtained for Zr (**Fig. 1**): twinning along the $\{10\bar{1}2\}$, $\{11\bar{2}1\}$, as well as $\{10\bar{1}1\}$ planes is active in hcp metals. The presence of maxima on the complete DPF (0001), deviated from the initial position by the typical reorientation angles of the basal axes, illustrates this fact. However, the $\{11\bar{2}2\}$-twinning was not detected either in the experiment or in modeling.

In the texture formation model of the VT16 alloy, which takes into account the appearance and growth of twins, the dominant deformation mechanism is prismatic slip and twinning along the $\{10\bar{1}2\}$, $\{11\bar{2}1\}$ planes. This is evidenced by their high activity **(Fig. 3)**. In this case, high activity of basal and prismatic slip systems is observed, while pyramidal ones are practically not involved in plastic deformation at the early stages. The inclusion of 20% (volume fraction) of the β-phase in the model leads to an increase in the activity of all plastic deformation systems at its initial stages. This is explained by the fact that the main slip systems {110}<111> in β-Ti are characterized by higher critical shear stresses compared to the basal and prismatic systems in α-Ti. Therefore, plastic deformation of β-Ti grains begins later. Twinning is initially more active in the presence of a second phase, as the α/β phase boundary can act as an additional stress concentrator. As the degree of deformation increases to ε = 1–2%, the activity of prismatic and basal slip decreases steadily in the presence of an additional phase, unlike in a single-phase α-alloy.

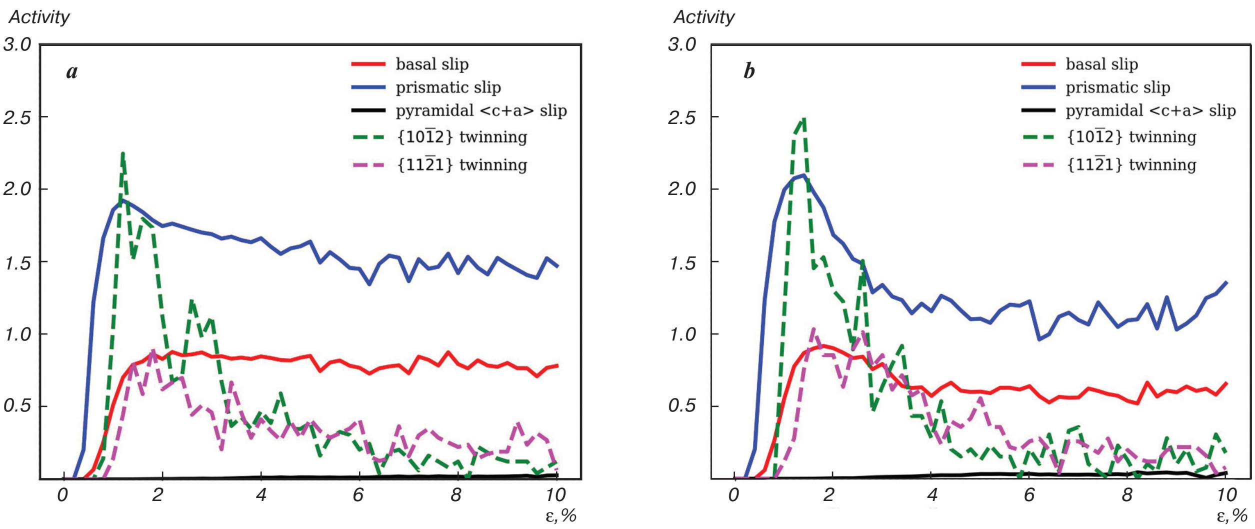

Fig. 3. α-Ti twinning and slip system activities at initial polycrystalline deformation stage:
a – without β-phase; *b* – with 20% of β-phase

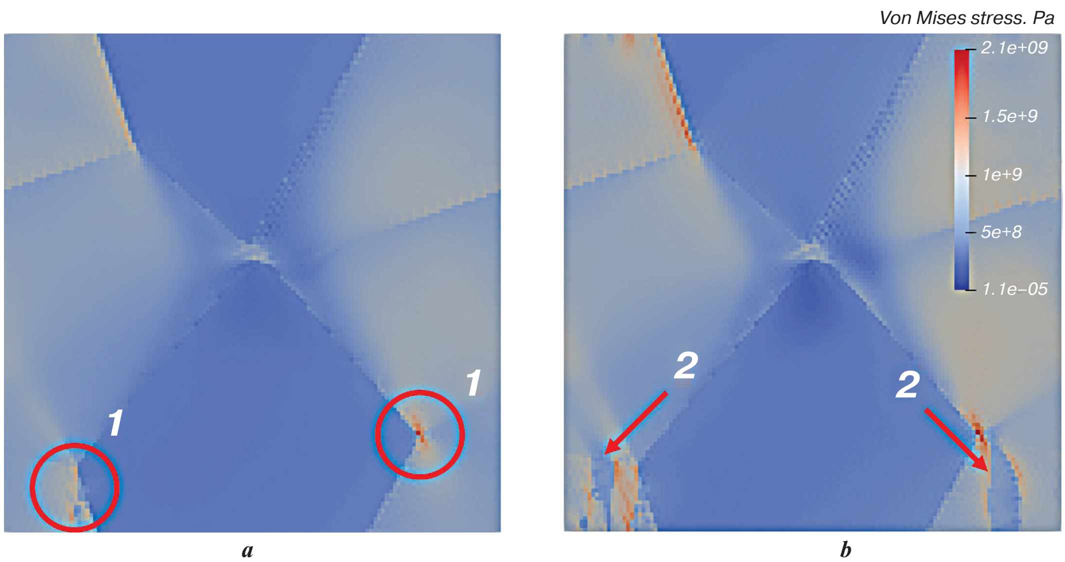

Fig. 4. Von Mises stress distribution map:
a – ε = 0,4%; *b* – ε = 0,6%. stress localization areas which are beneficial for twinning nucleation are marked as *1*; stress relaxation areas within twin lamellae are marked as *2*

Since the model uses an additional criterion for selecting potential nuclei with the maximum hydrostatic pressure gradient, such concentrators are regions of active nucleation and twin growth, which, unlike [12], allows for modeling the microstructure of twins within the grain. As **Fig. 4** shows, equivalent stress localization occurs at grain boundaries and triple junctions, which is explained by localized deformation heterogeneity in grains, where slip is possible and where it is hindered. Further growth of twin plates in the direction of twinning leads to reorientation of a portion of the grain, and the proportion of twins in grains is not predetermined, but is determined by the stress distribution within the grain itself. Thus, twins most often nucleate in regions of stress localization induced by the interaction of grains of different orientations or phases, while the formation of twins within the grain body is less likely.

Fig. 4 shows maps of the von Mises equivalent stress distribution at the moment of first twin nucleation. Near grain boundaries (region 1), localized elastic stresses are observed, caused by different grain orientations relative to the external stress. In these regions, stress accumulation leads to the attainment of the CRSS and the formation of twin nuclei. Twinning activation occurs not directly at the points of maximum stress, but in adjacent regions with a high hydrostatic pressure gradient. This distribution of nucleation sites ensures the preferential development of twins deeper into the grain rather than their localization in boundary zones. This behavior is due to the fact that near grain boundaries, in addition to high reduced stresses, there is an increased density of defects that impede twin growth, reducing the likelihood of their stable development from these regions.

Conclusions

1. A model and algorithm for the simulating of texture formation during cold rolling of two-phase titanium alloys are established, taking into account the twinning mechanism in the α-phase. The model includes the identification of the most favorable regions for twin nucleation, as well as the growth of twin platelets. The proposed algorithm expands the calculation of crystal lattice rotation involving slip mechanisms in the DAMASK software with the reorientation regularities during twinning.

2. The developed model of grain reorientation involving twinning was verified using the results of rolling a zirconium single crystal, which is characterized by the same set of twinning systems as titanium. The model reproduces the action of twinning systems with the $\{11\bar{2}1\}$, $\{10\bar{1}2\}$ and $\{10\bar{1}1\}$ planes observed experimentally, what confirms its validity.

3. The model of twin nucleation and growth describes adequately their shape and location within the material volume. Nucleation occurs in the areas of stress localization, and growth occurs predominantly in the twinning plane.

4. Using the developed model, we calculated the texture formation during rolling of VT16 titanium alloy up to a deformation degree of 50%. The resulting texture corresponds to the experimental results, explains the reorientation of basal axes towards the sheet normal direction, and allows for the prediction of texture formation in two-phase titanium alloys during cold rolling.

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