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ANALYSIS OF THE DEFORMATION BEHAVIOR OF CP Ti WITH DIFFERENT GRAIN SIZES BY MEANS OF KINETIC MODELING

ANALIZA PRZEBIEGU ODKSZTAŁCENIA Ti O ZRÓŻNICOWANEJ WIELKOŚCI ZIARNA W OPARCIU O MODEL KINETYCZNY

A kinetic composite dislocation-based model of the deformation behavior of pure metals has been developed. The model incorporates the known approaches by M. Zehetbauer and M. Barnett and allows considering both dislocation activity and dislocation twinning in the process of plastic deformation.

The model is employed to analyze the deformation behavior of CP Ti subjected to upsetting in three different microstructural states, namely, as-received coarse-grained state, intermediate and ultrafine-grained states. The last two states were obtained by means of equal-channel angular pressing with 1 and 8 passes. Available published data for microstructure and experimental "true stress-true strain" plots obtained at close conditions of upsetting ($\dot{\varepsilon}$ = 2×10^{-2}-10^{-3} c^{-1}, T = 473-573 K) were taken as source information for modeling.

It is shown that grain refining activates the processes of dislocation accumulation and annihilation in cell – grain interiors, activates dislocation accumulation and suppresses dislocation annihilation in cell walls – grain boundaries. On the other hand, grain refinement activates annihilation of dislocations in cell – grain interiors and suppresses it in cell walls – grain boundaries.

It has been found that at the investigated temperatures and strain rates the role of deformation twinning is significant in the coarse-grained state, in the intermediate state it is noticeable, and in the UFG state it is negligible.

The obtained modeling results correlate well with the available experimental results and complement them considerably.

Keywords: dislocation-based model, titanium, dislocation slip, twinning

Rozwinięto kinetyczny, dyslokacyjny model mechanizmu odkształcenia czystych metali. Model ten obejmuje znane podejście M. Zechetbauera i M. Barnetta pozwalające uwzględnić zarówno aktywność dyslokacji jak i dyslokacyjnego bliźniakowania w procesie odkształcenia plastycznego. Model ten zastosowano w analizie procesu odkształcenia Ti o czystości handlowej w trzech różnych stanach mikrostruktury, mianowicie; dostarczonego o grubym ziarnie, średnio- i ultra-drobnoziarnistego. Ostatnie dwa stany mikrostruktury były uzyskane w procesie 1- i 8-krotniego przeciskania przez kanał równo-kątowy. Osiągalne dane literaturowe odnośnie mikrostruktury i zależności doświadczalnych "true stress-true strain" uzyskane w zbliżonych warunkach obciążenia ($\dot{\varepsilon}$ = 2×10^{-2}-10^{-3} c^{-1}, T = 473-573 K) uwzględniono jako informacje źródłowe w procedurze modelowania. Wykazano, że rozdrobnienie ziarna uaktywnia proces akumulacji, spiętrzania i anihilacji dyslokacji we wnętrzach komórek (dyslokacyjnych) oraz ziaren jak i na granicach tych obszarów.

Stwierdzono, że przy określonej temperaturze badania i prędkości odkształcenia, rola bliźniakowania odkształceniowego jest znacząca w przypadku struktury gruboziarnistej, zauważalna w przypadku strukturydrobnoziarnistej i pomijalnie mała w przypadku struktury o ultra-drobnym ziarnie. Wyniki modelowania potwierdzają rezultaty uzyskane na drodze doświadczalnej, uzupełniając się znacznie.

1. Introduction

Study of the mechanisms of plastic deformation of commercially pure (CP) Ti is a subject of numerous investigations [1-12]. By now it has been stated that dislocation slip and crystallographic twinning are main deformation mechanisms [8-12]. As it is noted in [10, 11], the directions $\langle 11\bar{2}0\rangle$ in the planes $\{10\bar{1}0\}$ (**a** – slip) and the directions $\langle 11\bar{2}3\rangle$ in the planes $\{10\bar{1}1\}$ and $\{11\bar{2}\bar{2}\}$ (**a+c** – slip) are typical of the dislocation slip in CP Ti. In [13] the directions $\langle 11\bar{2}0\rangle$ in the planes $\{10\bar{1}0\}, \{10\bar{1}1\}$ and $\{0001\}$ are referred to this type in the decreasing order of feasibility of the dislocation slip over these planes.

The necessity for twinning activation during plastic deformation of CP Ti is conditioned by a limited number of potential slip systems (SS). At room temperature

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twinning, as a rule, occurs over the planes $\{10\bar{1}2\}$, $\{11\bar{2}1\}$ and $\{11\bar{2}2\}$, their actualization depends on the deformation conditions [12].

Dislocation slip and twinning compete with each other in the process of plastic deformation of CP Ti. The contribution of each of the mentioned mechanisms into the realization depends on a temperature, rate, scheme and degree of deformation.

It is well known that an increase in the plastic strain degree results in radical changes in the microstructure. At the same time grain refinement takes place. The dislocation density increases. Misorientations between neighboring cells and cell blocks grow. As a result some important structure-sensitive properties of metallic materials, for example strength, enhance [14]. Therefore, a grain size is one of the main parameters which define the character of the deformation behavior and acting mechanisms of plastic deformation [15].

The recent development of the severe plastic deformation (SPD) method made it possible to achieve extremely high strain degrees ($\varepsilon > 1-100$) with no change of geometrical dimensions and no failure of deformed bulk metallic ingots [16]. As a result it was managed to form ultrafine-grained (UFG) and nanocrystalline states in different metallic materials including CP Ti [3].

Equal-channel angular pressing (ECAP) is one of the ways of SPD realization [16]. During ECAP a bulk billet is multiply pressed through the two intersecting channels with identical cross sections. Increase in the number of passes during ECAP results in a gradual transformation of the coarse-grained microstructure into a cell microstructure with low-angle cell walls, then into an intermediate submicrocrystalline structure with low-angle grain boundaries and, finally, into a UFG or nanocrystalline structure with dominantly high-angle grain boundaries. 8-12 passes of a billet through the die with a definite geometry are required for the microstructure to be refined till UFG and nanocrystalline states. A route, temperature and ECAP velocity play an important role here [16].

Recent experimental investigations of the deformation mechanisms do not give an unambiguous answer to the question about the role of different mechanisms during the plastic deformation of CP Ti in different states [1-13]. On the other hand, a kinetic modeling is one of the important tools employed to analyze the plastic deformation mechanisms [17].

The kinetic modeling is conducted within the frames of developed models which consider the features of the simulated microstructure and potential deformation mechanisms. The dislocation-based model by M. Zehetbauer and his colleagues is one of the most successful models of this kind [18, 19]. The model takes into account the dislocation activity both in cell interiors and walls. The cell interiors contain screw dislocations, which interact only with each other via their shear fields. Edge dislocations in cell walls interact only with each other via their dilatation fields.

L. Remy based on the conducted experimental investigations developed the kinetic equation of f.c.c. deformation twinning in which the volume fraction of twins is expressed as an implicit function of strain [20]. M. R. Barnett and coworkers [21] modernized this approach and applied it to predict twinning dominated flow in Mg.

The aim of the investigations, the results of which are presented in this paper, was to develop the dislocation-based model which considers the possibility to activate dislocation slip as well as deformation twinning and the possibility to employ it to analyze the deformation mechanisms in CP Ti in coarse-grained, intermediate and UFG states.

2. Mathematical model of the deformation behavior

Let us describe main provisions of the model which was used to investigate the deformation behavior of CP Ti samples.

The flow stress τ was considered summed up by the stress $\tau_s = \sigma_s/M^*$, associated with the dislocation slip (where M^* – the Taylor factor averaged over the deformation interval during tension), and the stress $\tau_t = \sigma_t/M^*$ connected with twinning [20, 21]

$$\sigma(\varepsilon) = (1 - f_t)\sigma_s(\varepsilon_s) + f_t\sigma_t, \qquad (1)$$

here f_t is the volume fraction of twins.

To consider additional strengthening due to deformation twinning, there was applied an approach discussed in [22]. It was assumed that the stress σ_s in the crystal areas free of twinning is described by Zehetbauer's model [19]. The model takes into account all the potential dislocation slip systems implemented at this degree of stress. The stress in the areas subjected to deformation twinning is ξ times higher than the stress in the similarly textured material without deformation twins. The growth of the stress is conditioned by the formation of twin boundaries and interaction between dislocations and twins

$$\sigma_t = \xi\sigma_s. \qquad (2)$$

The strain ε is assumed to consist of the dislocation slip (ε_s) and shear connected with twinning (ε_t). Using the expression $\varepsilon_t = (1/M*)\gamma_t = c/a\sqrt{3} - a\sqrt{3}/c$ [2, 21], ε_t results to be 0.056. The total strain increment can be described as [20]:

$$d\varepsilon = (1 - f_t)d\varepsilon_s + \varepsilon_t df_t. \quad (3)$$

Here f_t means the volume fraction of twins.

In this paper the resolved stress τ_s associated with the dislocation slip (as included in (1)) was calculated on the basis of Zehetbauer's composite model [19], which considers separate kinetics of edge and screw dislocations. Edge dislocations are supposed to be arranged within the cell walls, while the screw dislocations are ruling the deformation within the cell interiors with no interaction between them.

As Zehetbauer's model is a composite one, it describes microscopic hardening ($\theta = d\tau_s/d\gamma_s$) in terms of contributions by the cell interiors θ_1 and by the cell walls θ_2. γ_s is the resolved shear strain caused by the dislocation slip. The stresses in the cell interior τ_1 and cell walls τ_2 vary according to:

$$\frac{d\tau_1}{d\gamma_1} = C_1 - C_3\tau_1, \quad (4)$$

$$\frac{d\tau_2}{d\gamma_2} = C_2 - C_4[\tau_2 - \tau_2(0)]\tau_2^5. \quad (5)$$

The parameters C_1 and C_2 are associated with the dislocation accumulation rate in cell interiors and walls, respectively. The parameter C_3 reflects the annihilation rate of screw dislocations due to activation of cross slip in cell interiors. The parameter C_4 characterizes annihilation of edges in cell walls being governed by non-conservative motion. The initial values of the resolved flow stresses in the cell interiors $\tau_1(0)$ and cell walls $\tau_2(0)$, corresponding to the strain $\gamma_s = 0$, are set with the help of equations:

$$\tau_1(0) = \tau_0/(2 - f_1), \quad (6)$$

$$\tau_2(0) = 2\tau_1(0), \quad (7)$$

where τ_0 is the resolved yield stress of material, and f_1 is the volume fraction of cell interiors.

The resolved shear stress for a crystal with account of the compatibility condition of deformation of cell walls and interiors $\gamma_s = \gamma_1 = \gamma_2$ is described as:

$$\tau_s = f_1\tau_1 + f_2\tau_2, \quad (8)$$

where

$$\tau_1 = \alpha_1 Gb\sqrt{\rho_1}, \quad (9)$$

$$\tau_2 = \alpha_2 Gb\sqrt{\rho_2}, \quad (10)$$

$$\gamma_s = \varepsilon_s M^*. \quad (11)$$

Here α_1, α_2 are the parameters characterizing the interaction of dislocations in the cell walls and interiors, respectively, $f_2 = 1 - f_1$ is the volume fraction of cell walls, G is the shear modulus, b is the Burgers vector, ρ_1 and ρ_2 are the dislocation densities in cell interiors and walls, respectively.

The dislocation densities in the cell interiors ρ_1 and cell walls ρ_2 make up the total (average) dislocation density ρ:

$$\rho = f_1\rho_1 + f_2\rho_2. \quad (12)$$

The volume fraction of cell walls f_2 is considered as constant and equal to the value measured in [19].

However, no experimental data on the strain dependence of the volume fraction of twins for Ti with different grain sizes have been available. Because of relatively small tensile strains $\varepsilon \approx 0.4$ applied here, we assume that the volume fraction of twins follows the law used in [16] for coarse-grained Ti (for definition of s, q and e see [23]):

$$f_t = \frac{s}{1 + \exp(-q(\varepsilon - e))}. \quad (13)$$

3. Modeling results and their discussion

The experimental data on the microstructure and the "true stress-true strain" plot were taken as initial parameters of modeling. The least-square method was applied to fit the experimental and modeling "true stress-true strain" curves. The parameters C_i and ξ served as adjustable parameters.

In all the considered cases the relative volume fraction of cell walls- grain boundaries was $f_1 = 0.97$ and $f_2 = 0.03$ [19].

The initial stress values in the cell bodies $\tau_1(0)$ and cell walls $\tau_2(0)$ corresponding to the value $\gamma = 0$ were defined in the following way $\tau_1(0) = \tau_0/(2 - f_1)$, $\tau_2(0) = 2\tau_1(0)$, where τ_0 is the material yield stress.

By adjusting the parameters C_i and ξ, the modeling curve (1) obtained as a result of solution of equations (3) – (5), (8), (11) and considering expression (2) was approximated to the experimental "true stress-true strain" curve. The evolution of the crystallographic texture was not taken into account during deformation. Only the average value of the Taylor factor $M*$ was considered. The modeling parameters α_1, α_2 were defined as a result of approximation of the modeling "dislocation density-true strain" curve obtained after solving equations (9), (10), (12) to the experimental values of the dislocation density.

3.1. Coarse-grained state

CP Ti in the coarse-grained state was characterized by an average grain size ~ 40 μm [2]. The experimental results obtained during upsetting with a strain rate 10^{-3} s^{-1} at a temperature of 473 K were taken as initial parameters for modeling [2].

Fig. 1 shows the experimental points and the modeling "true stress-true strain" plot. The modeling plots describing the contribution of dislocation slip and twinning into the stress flow depending on the strain degree are also presented here.

As it proceeds from Fig. 1, the modeling "true stress-true strain" plot adequately describes the corresponding experimental data. One can single out three stages of strain hardening, namely, slow, fast and slow. Such a character of strain hardening can be explained by analyzing the contribution of dislocations and deformation twins into it depending on the strain degree. As is seen, at the initial stage the flow stress caused by dislocation slip grows quickly and then slows down. This corresponds to the fact that the Frank-Read dislocation sources start operating in the interiors and boundaries of coarse grains. A cellular microstructure with low-angle cell walls forms. The cell walls become sources of dislocation piling-up and sink. However, the total dislocation density is small (~ 5.8×10^{13} m^{-2} at $\varepsilon = 0.1$). The processes of dislocation accumulation and annihilation in the cell interiors and dislocation accumulation in the cell walls run slowly. The dislocation annihilation in the cell walls runs actively (C_1 = 180 MPa, C_2 = 3.3 GPa, C_3 = 1.60, $C_4 = 4.58 \times 10^{-10}$ MPa^{-5}).

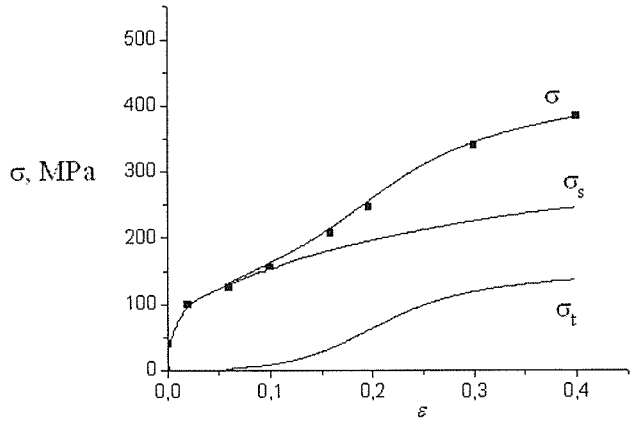

Fig. 1. The modeling "true stress-true strain" plots for total stress σ, stress σ_s related to dislocation slip, stress σ_t related to twinning and experimental data (■) [2]. Coarse-grained CP Ti. Compression. $\dot{\varepsilon} = 10^{-3}$ s^{-1}. T = 473 K.

A small number of possible dislocation types in CP Ti makes it necessary for twinning systems to activate. As it is seen from Fig. 1, the contribution of twinning into the flow stress of coarse-grained CP Ti becomes conspicuous at $\varepsilon > 0.06 - 0.10$ and reaches just more than half of the corresponding contribution of dislocations at $\varepsilon > 0.30$. This implies that the contribution of twinning into hardening of CP Ti in the coarse-grained state may be rather convincing. This is also evidenced by a high value of the parameter $\xi = 1.35$, which reflects the contribution of twinning into strain hardening of the metal.

It may be concluded from the above-said, that a complex view of the "true stress-true strain" plot (Fig. 1), which corresponds to upsetting of CP Ti in the coarse-grained state, can be explained by competition between dislocation slip and deformation twinning.

3.2. Intermediate state

The intermediate state was formed in CP Ti as a result of the 1st ECAP pass [7]. According to [4] this state is characterized by the flow lines oriented at an angle ~ 30° to the longitudinal axis of a billet and connected with formation of small shear bands in the process of ECAP. The question is the longitudinal vertical section of a billet which is in agreement with the plane possessing the channels of the ECAP die-set. TEM investigations point to the presence of very thin parallel elongated bands about 70 nm wide. These bands are identified as twins which formed in the initial coarse-grained structure as a result of plastic shear up to high strain degrees $\varepsilon > 1$.

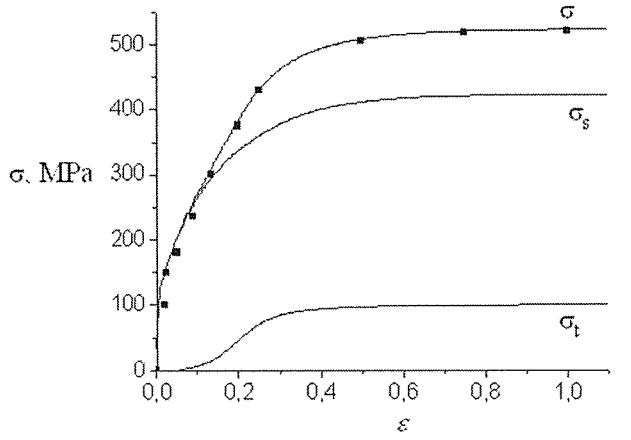

Fig. 2. The modeling "true stress-true strain" plots for total stress σ, stress σ_s related to dislocation slip, stress σ_t related to twinning and experimental data (■) [7,8]. CP Ti after 1 ECAP pass. Compression. $\dot{\varepsilon} = 2 \times 10^{-2}$ s^{-1}. T = 548 K.

The experimental data on the microstructure and the "true stress-true strain" plot, obtained during upsetting with a strain rate 2×10^{-2} c^{-1} at a temperature of 548 K, were taken as initial modeling parameters [7, 8]. The initial stress flow τ_0 was 30 MPa.

The modeling "true stress-true strain" plot describes the experimental dependence very well [7, 8] (Fig. 2). The plot has a monotonous character with a gradual attenuation of strain hardening. After $\varepsilon \approx 0.4$ saturation of the flow stress is observed. The modeling plot which describes the contribution of the dislocation slip into the flow stress against the strain degree saturates at $\varepsilon \approx 0.5$. The modeling plot which describes the contribution of twinning depending on the strain degree saturates at $\varepsilon \approx 0.3$. The contribution of twinning into the flow stress reaches $\sim 1/4$ of the contribution of dislocations. Thus, it may be concluded that the role of twinning during upsetting of the intermediate state is substantially smaller than in the case of the coarse-grained state.

The compared states differ from each other significantly by their microstructures before being upset. In the first place, the grain size decreased 10 times after 1 ECAP pass. In the second place, the dislocation density grew. In the third place, a high density of twins can be observed in the microstructure after 1 ECAP pass. At the same time the upsetting conditions (temperature and rate) differ little (473 K and 548 K, 10^{-3} s^{-1} and 2×10^{-2} s^{-1}). It may be concluded that the very initial (before upsetting) structure of the deformed samples affected the choice of active deformation mechanisms in the investigated states of CP Ti.

As it proceeds from the conducted analysis, at the above-mentioned upsetting conditions the intermediate microstructure that formed after 1 ECAP pass is more predisposed to activation of the dislocation slip than the coarse-grained structure. This is evidenced by the fact that during upsetting to the intermediate strain degree $\varepsilon = 0.1$ the total dislocation density in the intermediate structure is much higher ($\sim 2.3\times10^{14}$ m^{-2}), than in the coarse-grained structure ($\sim 5.8\times10^{13}$ m^{-2}) at $\varepsilon = 0.1$. Besides, the processes of dislocation accumulation in cell interiors and walls and their annihilation in cell interiors activate essentially, but annihilation is suppressed in cell boundaries (C_1 = 425 MPa, C_2 = 7.2 GPa, C_3 = 2.72, $C_4 = 5.68\times10^{-11}$ MPa^{-5}). At that the role of twinning in metal hardening reduces considerably. This is evidenced by the coefficient ξ, the value of which decreased by more than 2 times.

3.3. Ultra-fine grained state

The UFG state was formed in CP Ti as a result of 8 ECAP passes (route B_C) at a temperature lowering in the range 723-673 K [3, 24]. This state is characterized by a rather homogeneous microstructure with an average grain size ~260 nm and mainly high-angle grain boundaries [3].

The data on the microstructure and experimental results obtained during upsetting with a strain rate 10^{-3} s^{-1} at a temperature 523 K [24] were taken as initial parameters for modeling (Fig. 3). The initial flow stress τ_0 was 50 MPa.

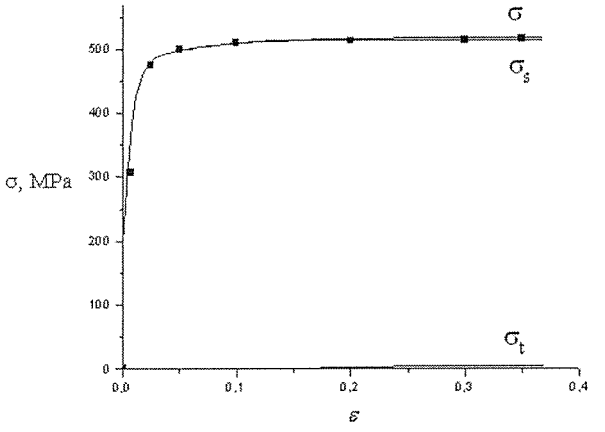

Fig. 3. The modeling "true stress-true strain" plots for total stress σ, stress σ_s related to dislocation slip, stress σ_t related to twinning and experimental data (■) [7]. CP Ti after 8 ECAP passes. Compression. $\dot{\varepsilon} = 10^{-3}$ s^{-1}. T = 573 K.

The modeling "true stress-true strain" plot describes the experimental dependence well (Fig. 3). The plot has a monotonous character with a gradual attenuation of strain hardening. After $e \approx 0.2$ saturation of the flow stress is observed.

The modeling plot which describes the contribution of the dislocation slip into the flow stress depending on the strain degree almost aligns with the modeling "true stress-true strain" plot. The dislocation density reaches 3.9×10^{14} m^{-2} at a strain degree $\varepsilon = 0.1$. The processes of dislocation accumulation and annihilation in grain interiors and boundaries as well as the annihilation of dislocations in grain interiors activate considerably. Annihilations of dislocations in grain boundaries are considerably suppressed (C_1 = 5600 MPa, C_2 = 13.5 GPa, C_3 = 27.30, $C_4 = 8.65 \times 10^{-12}$ MPa^{-5}).

The modeling plot which describes the contribution of the twinning into the flow stress depending on the strain degree practically aligns with the X-axis and manifests itself weakly at $\varepsilon > 0.15$. At that the coefficient ξ = 0.02 is very low. This points to a minor role of twinning during upsetting of UFG CP Ti.

4. Summary

The kinetic model allowing for implementation of the plastic deformation by activating both dislocations and deformation twinning was developed. The model was employed to investigate CP Ti in different structural states. They were the annealed coarse-grained state, the intermediate state after 1 ECAP pass with a large number

of twins and the UFG state after 8 ECAP passes with an average grain size 260 nm.

It was demonstrated that at almost identical temperature-rate conditions of upsetting the coarse-grained state witnesses the activation of twinning and dislocation processes. In the intermediate state the role of twinning diminishes. In the UFG state the role of twinning is negligible.

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