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Anisotropy of elastic modules of the planes of a hexagonal crystal and damage of titanium sheets

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A Fourier analysis of the anisotropy of the elastic properties of the crystallographic planes of hexagonal crystals, given by their angle of inclination to the isotropic plane of the basis (0001), is carried out. It was found that the anisotropy of Young's modulus of titanium for all planes is monotonic with a minimum in [10$\bar{1}$0] and a maximum in [1010] + $\pi/2$. For the zirconium and magnesium crystallographic planes forming an angle $\alpha \neq 0$ with the (0001) plane, the values of E take the minimum in the direction [10$\bar{1}$0] + $\pi/4$, and the maximum — in [10$\bar{1}$0] + $\pi/2$. We used the dynamic method to study the anisotropy of E for annealed and tensile-deformed titanium samples cut from sheets at different angles to the rolling direction (RD) and estimated the level of integral damage (D) of deformed samples (strips) relative to undeformed ones. The anisotropy of D is similar to the anisotropy of E; it is approximated by a Fourier series with harmonic amplitudes A_0 = 1.38, A_2 = −0.99, A_4 = −0.2 %. Prevailing influence of A_2 in the anisotropy of D indicates damage as a property of the second tensor dimension. This is expressed in the characteristic shape of pores in the form of ellipsoids, which are observed on microstructures.

Keywords: hexagonal crystal, Young and shear moduli, Fourier analysis, titanium, zirconium, magnesium, damage, pores.

Анізотропія пружних модулів площин гексагонального кристала та пошкодження титанових листів. *Н.А.Волчок, Я.Д.Клубіс, А.П.Начев, А.Ф.Тарасов, Г.Герштейн*

Проведено Фур'є-аналіз анізотропії пружних властивостей кристалографічних площин гексагональних кристалів, заданих кутом нахилу їх до ізотропної площині базису (0001). Отримано, що анізотропія модуля Юнга (E) титану для всіх площин носить монотонний характер з мінімумом в [10$\bar{1}$0] і максимумом в [10$\bar{1}$0] + $\pi/2$. Мінімальні значення E для площин кристалів цирконію і магнію, що утворюють кут з площиною (0001), приймає в напрямку [10$\bar{1}$0] + $\pi/4$, а максимальні — в [10$\bar{1}$0] + $\pi/2$. Вивчено анізотропію E відпалених і деформованих розтягуванням зразків титану, вирізаних з листів під різними кутами до напрямку прокатки (НП), динамічним методом і оцінено рівень інтегрального пошкодження (D) деформованих зразків щодо недеформованих. Анізотропія D подібна анізотропії E, апроксимується рядом Фур'є з амплітудами гармонік A_0 = 1.38, A_2 = −0.99, A_4 = −0.2 %. Переважаючий вплив A_2 на анізотропію D говорить про пошкодження як про властивість другої тензорної розмірності. Це виражається у характерній формі пір у вигляді еліпсоїдів, які спостерігаються на мікроструктурах.

Проведен Фурье-анализ анизотропии упругих свойств кристаллографических плоскостей гексагональных кристаллов, заданных углом наклона их к изотропной плоскости базиса (0001). Получено,что анизотропия модуля Юнга (E) титана для всех плоскостей носит монотонный характер с минимумом в $[10\bar{1}0]$ и максимумом в $[10\bar{1}0] + \pi/2$. Минимальные значения E для плоскостей кристаллов циркония и магния, образующих угол $\alpha \neq 0$ с плоскостью (0001), принимает в направлении $[10\bar{1}0] + \pi/4$, а максимальные — в $[10\bar{1}0] + \pi/2$. Изучали анизотропию E отожженных и деформированных растяжением образцов титана, вырезанных из листов под различными углами к направлению прокатки (НП), динамическим методом и оценили уровень интегральной поврежденности (D) деформированных образцов относительно недеформированных. Анизотропия D подобна анизотропии E, аппроксимируется рядом Фурье с амплитудами гармоник $A_0 = 1.38$, $A_2 = -0.99$, $A_4 = -0.2$ %. Превалирующее влияние A_2 на анизотропию D говорит о поврежденности как о свойстве второй тензорной размерности. Это выражается в характерной форме пор в виде эллипсоидов, которые наблюдаются на микроструктурах.

1.Introduction

Polycrystals have anisotropy of properties, which is determined by the orientational distribution of its individual elements (texture) and the anisotropy of the elements themselves, which are single crystals with a high degree of approximation. The general approach to specifying textures is to represent them in the form of three-dimensional orientation distribution functions (ODF) of polycrystal elements [1]. Methods for reconstructing ODF from experimental data are complex, require a large amount of primary information, and ODFs themselves contain redundant information in terms of the anisotropy of the properties of polycrystals.

The texture of cubic polycrystals with external symmetry elements (rolling direction, dragging axis, etc.) can be conveniently described in two-dimensional representation using ideal orientations (IO). In this case, the characteristics of the texture are: the crystallographic plane of individual crystals $\{hkl\}$, which coincides with the rolling plane; the crystallographic direction <uvw>, which coincides with the rolling direction (RD) or the transverse direction (TD) or the direction normal to the sheet plane (ND) [2]. The anisotropy of the properties of a polycrystal is determined by the relative content of the IO in the texture and the anisotropy of the properties of the ideal orientation itself.

In [3], the anisotropy of Young's modulus (E) in the crystallographic planes of the main ideal orientations of the textures of α-iron sheets was studied. The dependences of E on the direction of measurements, the anisotropy coefficients and average values of E in various IO of textures of annealing and rolling of α-iron were obtained.

Hexagonal crystals are substantially anisotropic not only in relation to the properties of the fourth tensor dimension (Young's and shear modules, Poisson's ratio), but also in relation to the properties described by second-rank tensors (thermal conductivity, electrical conductivity, thermal expansion, etc.) [4]. Due to the uniaxiality of the hexagonal crystal, the crystallographic planes of IO are convenient to set not by Miller indices, but by the angle α — their inclination to any of the principal planes, for example, the basis plane (0001). The direction is given by the angle φ relative to the direction $[10\bar{1}0]$.

The anisotropy of the properties of each of the IO in a real polycrystal is determined not only by the tensor dimension of the property itself, but also by the influence of the real structure with all its features and can serve as a basis for separating the contribution to the real anisotropy of the crystallographic and defect components of the texture, when assessing the level of structural defectiveness at the meso and microlevels [5]. For viscoelastic materials, such properties are the elastic properties of the fourth tensor dimension, which are preferred in methods for assessing the level of integral damage under various types of external influences on them.

The purpose of this work is to study anisotropy of elastic properties of the basic ideal orientations of textures in hexagonal metals with the ratio of the axes $c/a \leq 1.63$ and to determine the possibility of taking into account the contribution of texture in assessing the damage level of annealed and deformed titanium.

2. Anisotropy of the properties of crystallographic planes in a hexagonal crystal

The position of the crystal plane (*hkil*) is determined by the angle α of its inclination to the basal plane (0001). Let's introduce two coordinate systems x_i and x_i' with a common origin at point 0 (Fig. 1). The basal plane lies in the coordinate plane $0x_1x_2x_3$, and the [0001] axis coincides with the $0x_3$ axis. The plane (*hkil*) lies in the $0x_1'x_2'$ plane. In the plane (*hkil*), choose an arbitrary direction 0N and denote by φ the angle between it and the axis $0x_1'$. Let's find the dependences of the properties of the fourth tensor dimension of Young's (*E*) and shear (*G*) moduli on φ for different angles α, which determine the position of the (*hkil*) plane in the crystal.

From the spherical triangle ZBN we get:

$$\cos\theta = \cos(90^\circ - \alpha)\cos(90^\circ - \varphi) \qquad (1)$$

or for an arbitrary direction lying in the plane (*hkil*):

$$\cos\theta = \sin\alpha\sin\varphi.$$

We use the well-known expressions for the dependence of the elastic moduli on the direction in a hexagonal single crystal [4]:

$$\frac{1}{E} = s_{11} - (2s_{11} - s_{44} - 2s_{13})\alpha_{31}^2 + (s_{11} + s_{33} - s_{44} - 2s_{13})\alpha_{31}^4, \qquad (2)$$

$$\frac{1}{G} = s_{44} + \left(s_{11} - s_{12} - \frac{1}{2}s_{44}\right) + [2(s_{11} + s_{33} + s_{44} - 2s_{13}) - \left(s_{11} - s - \frac{1}{2}s_{44}\right)]\alpha_{31}^2 - 2(s_{11} + s_{33} - s_{44} - 2s_{13})\alpha_{31}^4. \qquad (3)$$

We represent the last expressions in the form:

$$\frac{1}{E} = s_{11} - a\sin^2\alpha\sin^2\varphi + b\sin^4\alpha\sin^4\varphi, \qquad (4)$$

$$\frac{1}{G} = s_{44} + c + (2b - c)\sin^2\alpha\sin^2\varphi - 2b\sin^4\alpha\sin^4\varphi, \qquad (5)$$

where

$$a = 2s_{11} - s_{44} - 2s_{13}, \qquad (6)$$

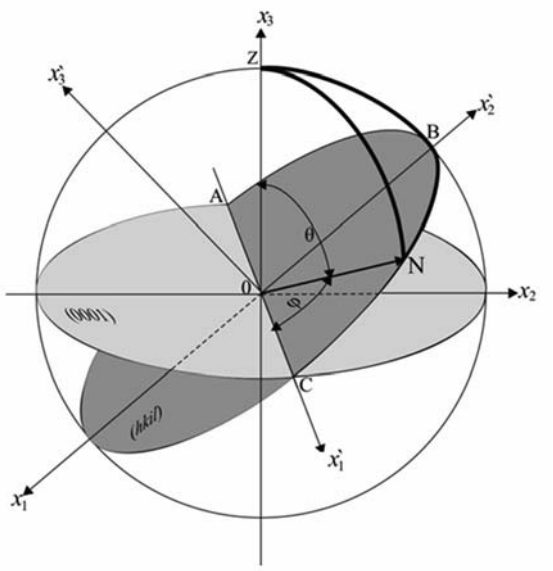

Fig. 1. To the derivation of the anisotropy of the elastic modules in the planes of a hexagonal crystal.

$$b = s_{11} + s_{33} - s_{44} - 2_{13}, \qquad (7)$$

$$c = s_{11} + s_{12} - \frac{1}{2}s_{44}, \qquad (8)$$

where s_{ij} are components of the compliance tensor, *E*, *G* are Young's and shear moduli, angle φ is measured from the direction [1010].

Further

$$2\sin^2\varphi = 1 - \cos2\varphi,$$

and

$$\sin^4\varphi = \frac{3}{8} - \frac{1}{2}\cos2\varphi + \frac{1}{8}\cos4\varphi.$$

After substituting the obtained expressions into (4) and (5), we get:

$$\frac{1}{E} = s_{11} - \frac{a}{2}\sin^2\alpha + \frac{3}{8}b\sin^4\alpha + \left(\frac{a}{2}\sin^2\alpha + \frac{3}{8}b\sin^4\alpha\right)\cos2\varphi + \frac{b}{8}\sin^4\alpha\cos4\varphi,$$

$$\frac{1}{G} = s_{44} + c + (2b - c)\sin^2\alpha(1 - \cos2\varphi) + 2b\sin^4\alpha\left(\frac{3}{8} - \frac{1}{2}\cos2\varphi + \frac{1}{2}\cos4\varphi\right).$$

After simplifications, we get:

$$E^{-1} = A_0 + A_2\cos2\varphi + A_4\cos4\varphi, \qquad (9)$$

$$G^{-1} = B_0 + B_2\cos2\varphi + B_4\cos4\varphi, \qquad (10)$$

Table 1. Compliance constants of hexagonal metals

Crystal	c/a	Compliance constants of single crystals and their combinations, $\times 10^{-11} m^2/N$							
		s_{11}	s_{12}	s_{44}	s_{33}	s_{13}	a	b	c
Titanium	1.591664	0.9581	−0.4623	2.1413	0.6979	−0.189	0.1534	−0.106	−0.57485
Zirconia	1.586121	1.0122	−0.4041	3.125	0.7977	−0.24	−0.618	−0.833	−0.9544
Magnesium	1.619938	2.2138	−0.7711	6.0241	1.9748	−0.491	−0.612	−0.851	−1.56935

where

$$A_0 = s_{11} - \frac{1}{2}a\sin^2\alpha + \frac{3}{8}b\sin^4\alpha, \quad (11)$$

$$A_2 = \frac{1}{2}a\sin^2\alpha - \frac{1}{2}b\sin^4\alpha, \quad (12)$$

$$A_4 = \frac{1}{8}b\sin^4\alpha, \quad (13)$$

$$B_0 = s_{44} + c + (2b - c)\sin^2\alpha - b\sin^4\alpha, \quad (14)$$

$$B_2 = -(2b - c)\sin^2\alpha - b\sin^4\alpha, \quad (15)$$

$$B_4 = \frac{1}{4}b\sin^4\alpha. \quad (16)$$

The expressions obtained are harmonic series describing the anisotropy of the elastic properties of a hexagonal crystal containing only even harmonics, the amplitudes of which depend on the single crystal characteristics and the angle of inclination of the plane $(hkil)$ to the plane (0001).

The anisotropy of Poisson's ratio in an arbitrary plane of a hexagonal crystal is calculated in the approximation [4] by the formula:

$$\nu(\varphi) = -s_{12}E(\varphi).$$

The anisotropy of elastic moduli for the crystallographic planes depending on their angle of inclination to the base plane (0001) was calculated for titanium, zirconium and magnesium. The stiffness constants c_{ijkl} from [6] were recalculated into the compliance constants s_{ijkl} [4] using the formulas:

$$s_{11} = \frac{1}{2(c_{11} - c_{12})} + \frac{S}{2}c_{33},$$

$$s_{12} = \frac{S}{2}c_{33} - \frac{1}{2(c_{11} - c_{12})},$$

$$s_{33} = S \cdot (c_{11} + c_{12}), \quad s_{13} = -S \cdot c_{13},$$

$$s_{44} = \frac{1}{c_{44}}, \quad S = \frac{1}{(c_{11} + c_{12})c_{33} - 2c_{13}^2}.$$

Using the values of the compliance constants and their combinations (Table 1), from (11)–(16),we calculated the amplitudes of the harmonics of the Fourier series of anisotropy $1/E(\varphi)$ for the hexagonal crystal planes depending on the angle of their inclination to the basal plane in the range from 0 to 90° with an interval of 15°; then the anisotropy of Young's modulus according to (4), as well as the average values of properties and anisotropy coefficients were calculated for each of the planes of the crystals of titanium, zirconium and magnesium. The calculation results are shown in Fig. 2 and Fig. 3.

The curves $E = f(\varphi)$ for titanium differ from those for zirconium and magnesium. In titanium, Young's modulus in each of the crystallographic planes increases monotonically from the prismatic direction to the direction of the projection of the c axis onto the normal to this plane. For zirconium and magnesium, for angles $\alpha \le 45°$, E decreases, and for $\alpha \ge 45°$, it increases after a minimum at $\alpha \approx 45°$.

Average elastic moduli for various crystallographic planes of titanium monotonically increase with increasing angle α between these planes and the basal plane. For zirconium and magnesium, this characteristic changes non-monotonically with increasing α; at first it drops to a minimum at $\alpha \approx 45°$, and then increases to its maximum value. The anisotropy coefficients $\eta = E_{max} - E_{min}/E_{max} \cdot 100$ % also behave dif-

3. Anisotropy of elastic properties of ideal orientations in hexagonal metals with $c/a \le 1.63$

Metals with a center to center ratio c/a less than ideal, which include titanium, zirconium, magnesium and their alloys, are of interest as structural materials for which the strength and elasticity characteristics are of paramount importance.

The anisotropy of elastic moduli for the crystallographic planes depending on their angle of inclination to the base plane (0001) was calculated for titanium, zirconium and magnesium. The stiffness constants c_{ijkl} from [6] were recalculated into the compliance constants s_{ijkl} [4] using the formulas:

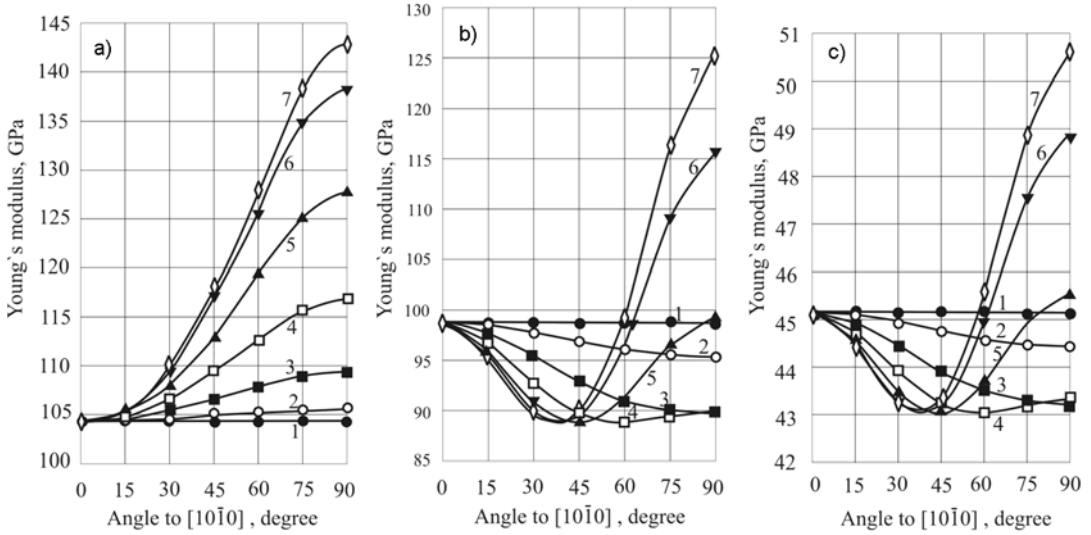

Fig. 2. Anisotropy of Young's modulus of crystallographic planes of hexagonal a) — α-titanium, b) — zirconium, c) — magnesium, depending on the angle of their inclination to the basal plane (0001): *1* — 0°, *2* — 15°, *3* — 30°, *4* — 45°, *5* — 60°, *6* — 75°, *7* — 90°.

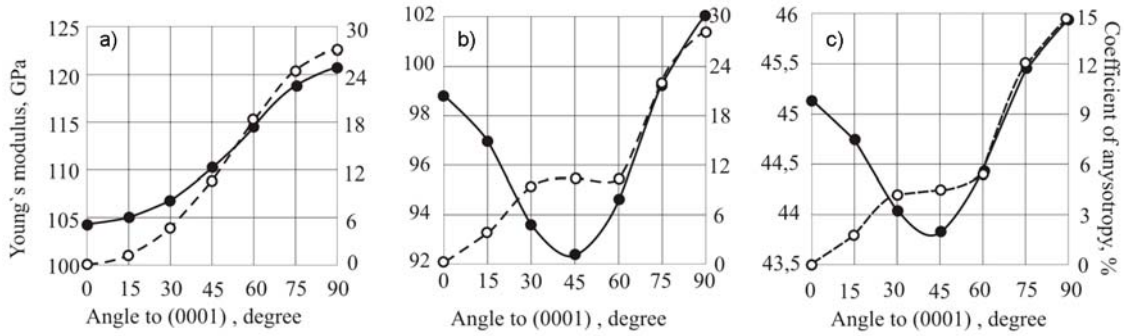

Fig. 3. Average Young's modulus (•) and anisotropy coefficient (°) of crystallographic planes: a) — titanium, b) — zirconium, c) — magnesium,depending on the angle of their inclination to the basal plane (0001).

ferently for these metals. For titanium, the anisotropy coefficient increases monotonically. For zirconium and magnesium, η increases monotonically with increasing α, but with some delay in the area of $\alpha \approx 45°$.

The textures of sheets of titanium and its α-alloys have been studied in sufficient detail. The textures of rolling and recrystallization of titanium differ mainly in the sharpness of the (0001) texture component: $\pm\alpha(ND - TD)$ [7–10]. There are also basic and prismatic components in titanium textures. Therefore, it should be expected that in the approximation of continuum mechanics, annealed and weakly deformed titanium samples should have the same anisotropy of elastic properties. The change in the elastic characteristics depends on the change in the defect structure, namely the resulting damage.

4.Research results

From titanium sheet VT1-0 with a thickness of 1.5 mm (as delivered — the initial state), two batches of samples were cut at different angles to the rolling direction (RD) with an interval of 15° in the form of a "dog bone" with a working part length of 120 mm and a width of 10 mm. The samples were subjected to prolonged annealing at a temperature of 325°C in an atmosphere of inert gas (argon) for 12 h. No visible damage was observed in the structure of the annealed samples in the cross section perpendicular to the RD (Fig. 4a).

Then the samples of one batch were subjected to stretching on a tensile testing ma-

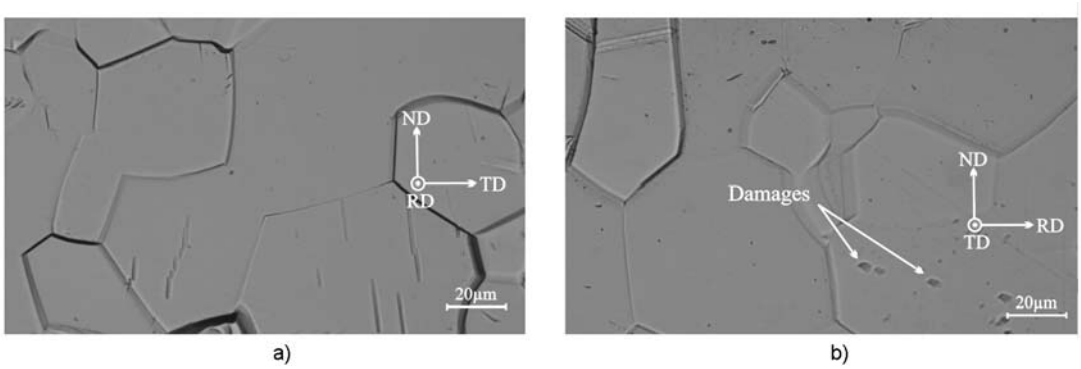

Fig. 4. Microstructure images: a) — titanium samples annealed at 375°C in a section perpendicular to the RD; b) — a sample deformed by tension in the TD, in a section perpendicular to the TD.

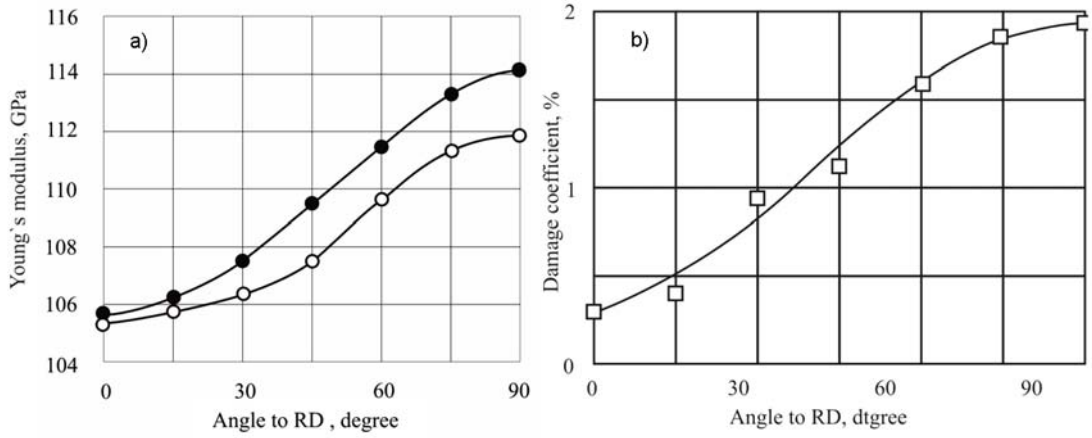

Fig. 5. Anisotropy: a) — Young's modulus in the rolling plane of titanium sheets • — after annealing at a temperature of 325°C and ° — subsequent deformations by tension up to 5 % of the samples, cut in different directions to the RD; b) □ — coefficient of damage of deformed samples relative to annealed ones.

chine "Zwick Z100 (100 kN)" up to 5 % permanent deformation. Rectangular plates 80 mm long were cut from the middle part of the samples of both batches. The plates thus obtained were processed in a pack to ensure uniform lengths.

Young's modulus was determined by the dynamic method [11] from the frequency of natural transverse vibrations of the plates. The vibration frequency was measured using the program [12]. Fig. 5a shows the results of measurements of Young's modulus by the dynamic method.

The curves of Young's modulus versus the direction of measurement for annealed and deformed titanium samples are similar in nature. Significant divergence of the curves starts from the measurement angles ~ 30° relative to RD. The maximum decrease in E in the deformed samples as compared to the annealed ones occurs in the transverse direction (TD). The curves for the annealed sheets are quite satisfactorily approximated by an even Fourier series with harmonic amplitudes: $A_0 = 109.61$; $A_2 = -4.28$; $A_4 = 0.19$ GPa, and for deformed samples: $A_0 = 108.08$; $A_2 = -3.14$; $A_4 = 0.4$ GPa. The anisotropy coefficient of the sheets has changed little. For annealed sheets and deformed samples, it was 7.4 and 5.8 %, respectively.

Fig. 3a shows that when describing the texture using a certain effective (statistical) angle α of inclination of the basal plane to the rolling plane, in both cases, the angle $\alpha = \pm 30 - 40°$ (ND – TD).

Thus,the effect of texture on the decrease in Young's modules of deformed samples with relation to annealed ones is not decisive.

Damage ratios $D = 1 - \tilde{E} / E_0$ (E_0 is Young's modulus for the annealed and $\tilde{E}$ for deformed samples) [5] were calculated for different directions in the range of RD – TD. The results are shown in Fig. 5b. The curve

$D = f(\varphi)$ is similar in shape to the curve of Young's modulus versus the measurement direction in titanium sheets. Coefficient D monotonically increases from the minimum value of the $D_{RD} = 0.28$ % to the maximum $D_{TD} = 2.63$ %.

If we consider the damage as a decrease in the effective interaction area in the cross sections of the samples due to the formation of pores and other discontinuities of the polycrystal [5], then our measurements indicate that the damage in the cross sections perpendicular to the TD is slightly higher than in the TD. Fig. 4b presents the microstructure of a titanium sample deformed by tension in the transversal direction in a section perpendicular to the rolling direction.

Damage to the structure in the form of pores of various shapes and sizes, distributed in grains in the form of clusters, are distinguishable in the images of the microstructure. Fourier analysis showed that the dependence of the damage coefficient of deformed samples (cut at different angles to the RD) compared to the annealed standards is satisfactorily approximated by the series:

$$D = (1.38 - 0.99 \cdot \cos 2\varphi - 0.2 \cdot \cos 4\varphi)\%.$$

The anisotropy $D = D(\varphi)$ is mainly determined by the contribution of the second harmonic. That is D, as a tendency to damage, can be regarded as a property of the second tensor dimension. This is expressed in the presence of pores that are close to elliptical in shape. The influence of the fourth harmonic is five times less; however, this does not exclude the appearance of elliptical damage with constrictions or thickenings.

5. Conclusions

The crystallographic planes of a hexagonal crystal, depending on the inclination angle α to the basal plane (0001), have a characteristic anisotropy of elastic properties. The anisotropy of Young's modulus (E) of titanium for all planes is monotonic with a minimum in $[10\bar{1}0]$ direction and a maximum in $[10\bar{1}0] + \pi/2$. The minimum values of E for the planes of zirconium and magnesium crystals, forming an angle $\alpha \neq 0$ with the plane (0001), occur in the direction $[10\bar{1}0] + \pi/4$, and the maximum — in $[10\bar{1}0] + \pi/2$.

2. The anisotropy of E of annealed titanium sheets with an intact structure is approximated by a Fourier series with harmonic amplitudes $A_0 = 109.61$; $A_2 = -4.28$; $A_4 = 0.19$ GPa. In the microstructure of titanium samples cut at different angles to the rolling direction (RD), damages in the form of pores are observed, their Young's modules decreased unevenly relative to the annealed samples.

3. The anisotropy of the integral damage coefficient D is similar to the anisotropy of E, it is approximated by a Fourier series with harmonic amplitudes $A_0 = 1.38$, $A_2 = -0.99$, $A_4 = -0.2$ %. Prevailing influence of A_2 on the anisotropy of D indicates damage as a property of the second tensor dimension. This is expressed in the characteristic shape of pores in the form of ellipsoids.

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