
A PHYSICAL MODEL OF THE FORMATION OF A SURFACE LAYER BROKEN BY MECHANICAL TREATMENT IN MATERIALS FOR OPTICAL-ELECTRONIC AND SENSOR DEVICES

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We investigate changes of the ellipticity parameter of polarized light in the case of its reflection from a polished surface of optical glass caused by the presence of defects and microdeformations formed in it during final operations of a mechanical treatment. The most widespread industrial grades of optical glass were used as samples for investigations. A physical model of the formation of a surface layer broken by a mechanical treatment was proposed. According to the model, due to the thermofluctuation breakage of interatomic bonds, the distribution of defects has a form similar to the temperature distribution in the process of transfer of the thermal energy from the treated surface to internal layers of the material. That's why one of the physical characteristics that can be used for the description of the distribution of defects in the broken surface layer is the thermal diffusivity of the treated material.

1. Introduction

The main task of the traditional shaping technology of high-precision parts of optical devices lies in the obtaining of ultimate geometric parameters and a quality of the surface providing their functionality. For this purpose, they are successively ground and polished using lapping workbenches with oscillating instrument. Optical glasses belong to brittle materials, that's why the mechanical removal of technological allowances takes place due to the interaction of abrasive grains with a treated surface, which is accompanied by the origination of brittle cracks, their development, and the slivering of microparticles of a treated material. In order to reduce the roughness of the treated surface, one successively decreases the dimensions of abrasive grains after each operation of the abrasive treatment. Thus, on each stage of the abrasive treatment, the surface layer broken during the previous operation is removed, and a broken layer characteristic of the given stage of the abrasive treatment with smaller dimensions of abrasive grains is formed. In [1–3], it was established that the depth of the layer broken by treatment is proportional to the size of abrasive grains and depends on physical properties of the treated material. For

crystalline materials, various methods of investigation of the structure of the surface layer are developed and described in the literature demonstrating that, in the case of deformation, the density of dislocations in surface layers of such crystals as nickel, silicon, copper, aluminum, and ionic crystals is higher than that inside a crystal. The presence of the dislocation density gradient was established in the case of layer-by-layer etching from the surface inside a crystal [4–6]. However, the analysis of literature data on the structure of surface crystal layers demonstrated their inconsistency and ambiguity. To a large extent, these results are influenced by structural and phase inhomogeneities of crystals caused by the technology of their growing [7]. There also exists a technique of exoemissive control of the surface of details after a treatment [8] that establishes the correlation between the exoemissive parameters and the imperfection of the material surface. The broken layer structure for glasses and glass ceramics is insufficiently studied, which is explained to a large extent by the scantiness of the known techniques of its investigation. For example, the method of optical and electron microscopy allows one to investigate only a relief and cracked layers. In [9], the broken surface layer was investigated in the course of a mechanical treatment of glass photomasks by means of the method of vertical breakings with the use of scanning electron microscopy. However, these methods are more often used for the solution of scientific problems or control problems in the laboratory environment, because they require an additional physical preparation of a sample, as well as the solution of problems related to the deciphering of the results of measurements.

In the given work, the parameters of the broken layer on the surface of details made of optical glass are described with the use of ellipsometric parameters of the material, in particular, the minimal ellipticity.

2. Experimental Technique

As is known, ellipsometric parameters are the ratio of the amplitude of p - and s -components of the electric vector of a light wave reflected from a sample – the azimuth of the reconstructed linear polarization (ellipticity $\text{tg}\rho$) and the phase difference between them (Δ). The magnitudes of these parameters are determined by the processes of interaction of light with substance. For isotropic dielectrics, the intensity of the p -component of a reflected light at the Brewster angle (ϕ_B) and the ellipticity $\text{tg}\rho$ are equal to 0, whereas the phase difference Δ experiences a jump from π ($\phi < \phi_B$) to 0 ($\phi > \phi_B$). Such an approach is substantiated by the point that, in the course of development of a brittle crack, there takes place a deformation and the breakage of interatomic bonds at its top. All surface breakings of the material density (relief layer, cracked layer, and sublayer with changed structure) represent an aggregate of these deformed and broken atomic bonds that finally decrease the refractive index of the substance and change the magnitude of the minimal ellipticity. Thus, in the case of layer-by-layer removal of the broken layer by means of polishing, one can investigate the distribution of defects in the broken layer by measuring the minimal ellipticity on each stage. The technique of ellipsometric investigations is described in [2,3,5,6]. As samples for investigation, the most widespread industrial grades of optical glass were used: flint glasses – TF10, TF7, TF1, BF28; crown glasses – BK10, STK3, TK23, K8, LK7. Physical characteristics of these grades of glass are given in GOST 13659-78 “Optical Colorless Glass. Physical-Chemical Characteristics. Basic Parameters”.

3. Results and Their Discussion

In the case of layer-by-layer removal of the broken layer by means of polishing, the typical experimental dependence of the ellipticity variation caused by the distribution of defects and microdeformations in the broken layer can be described by the equation

$$\text{tg}\rho = (\text{tg}\rho_0 - \text{tg}\rho_{\min})e^{-bx}, \quad (1)$$

where $\text{tg}\rho_0$ represents the ellipticity on the treated surface, $\text{tg}\rho_{\min}$ denotes the minimal ellipticity of the polished surface after the layer-by-layer removal of the broken layer by polishing, b is the constant characteristic of the treated material, and x is the distance from the treated surface.

The established dependence of the distribution of defects in the broken layer and the comparison of these

results with those in [10] on the regularities of abrasive wear of solid bodies allow one to represent the process of treatment of materials of optical-electronic devices as a continuous process of accumulation of defects in the surface layer resulting in the separation of wear fragments from the treated surface.

The thermofluctuation mechanism of development of microcracks (that forms a broken layer) provides for the fact that an essential part of the mechanical work of abrasive breakage will transform to the work of deformation of interatomic bonds. The interaction of abrasive grains with a glass surface and the mechanical treatment can be presented as a combination of the processes of indentation of abrasive grains, scratching, and formation of brittle microcracks. According to the estimate made in [11], in the course of development of a brittle microcrack in glass, there takes place a release of the thermal energy at a distance of several tens of angstroms from it, and the temperature in this local zone can amount to hundreds of Celsius degrees, which is close even to the sintering temperature of glass. Thus, the formation of a broken layer is accompanied by a change of the temperature during non-stationary thermal local processes, which coincides, by definition, with the thermal diffusivity of a treated material. It is of interest to establish the interrelation between the obtained experimental values of the parameter of the broken layer $\text{tg}\rho$ and the thermal diffusivity of treated materials. As a working hypothesis, a physical model of the formation of a surface layer broken by a mechanical treatment was proposed, according to which, due to the thermofluctuation breakage of interatomic bonds in the process of mechanical treatment, the distribution of defects has a form similar to that inherent in the process of transfer of the thermal energy from the surface inside the treated material.

In the case of a mechanical deformation of surface layers, atoms shift from the equilibrium positions. If we denote a shift by $u_i = x'_i - x_i$ in the direction i ($i = x, y, z$), where x'_i is the coordinate of an atom shifted in the direction i , and x_i is the coordinate of the equilibrium position, then the volume element ΔV after the deformation will be changed by $\Delta V' \approx \Delta V(1 + u_i)$, whereas $u_{ii} = \text{div}\bar{u} = \sum_i \frac{\partial u_i}{\partial x_i}$ [12]. In turn, deformation waves give rise to a change of the density of the substance $d = \frac{m}{V}$, where m is the unit volume mass. After the deformation, the density is equal to $d' = \frac{m}{V'} = \frac{m}{V(1 + \text{div}\bar{u})}$. In the small-deformation approximation, $d' \approx d(1 - \text{div}\bar{u})$. A change of the substance density manifests itself as a variation of the

refractive index n . The latter is determined by the ratio of the dielectric permittivities of the adjacent media $n = \sqrt{\frac{\varepsilon_2}{\varepsilon_1}}$; for air, $\varepsilon_1 \approx 1$. For a weakly polarized medium at a constant temperature, one can use the formula [13]

$$\varepsilon - 1 = 4\pi d\beta \frac{N_0}{M}, \tag{2}$$

where β denotes the substance polarizability, M is the molecular weight, and N_0 is the Avogadro number.

Thus, there exists a direct relation between the refractive index and the density:

$$n = \sqrt{\varepsilon} = \sqrt{1 + 4\pi d\beta \frac{N_0}{M}}. \tag{3}$$

For a deformed medium,

$$\begin{aligned} n' &= \sqrt{1 + 4\pi d'\beta \frac{N_0}{M}} \approx \\ &\approx \sqrt{1 + 4\pi d\beta \frac{N_0}{M}} (1 - \text{div } \bar{u}) \approx n - \frac{\text{div } \bar{u}}{2n}. \end{aligned} \tag{4}$$

A deformation can be also created in other ways, for example by means of a variation of the temperature. For example, if a body in the non-deformed state has temperature T_0 , then, even in the absence of external forces, the change of the temperature to the value T will result in its deformation due to thermal expansion.

As is known from elasticity theory [12], the change of the temperature and the deformation are linked by the linear dependence

$$\text{div } \bar{u} = \frac{1 + \mu}{3(1 - \mu)} \alpha (T - T_0), \tag{5}$$

where α stands for the coefficient of thermal expansion, μ is the Poisson's ratio. The problem on a mechanically created deformation can be reduced to the heat conduction problem. In our case, the problem is one-dimensional, as we investigate the depth of the broken surface layer. In this case, the heat conduction equation has a form

$$\frac{\partial T}{\partial \tau} = a \frac{\partial^2 T}{\partial x^2}, \tag{6}$$

where $a = \lambda/C_p d$ is the thermal diffusivity coefficient, λ is the thermal conductivity coefficient, C_p is the specific heat capacity, and $\frac{\partial}{\partial \tau}$ and $\frac{\partial^2}{\partial x^2}$ are, respectively, the derivatives with respect to the time and the coordinate. As the mechanical surface treatment represents a

periodic process, the problem has no initial conditions. The boundary conditions are presented in the form $T(0, \tau) = T_{\max} \cos(\omega \cdot \tau)$, where ω is the frequency, whereas T_{\max} is the amplitude of thermal oscillations of ions near the equilibrium positions.

The solution of this problem has the form [14]

$$T(x, \tau) = T_0 + T_{\max} e^{-\sqrt{\omega/(2a)} x} \cos\left(\sqrt{\frac{\omega}{2a}} x - \omega\tau\right). \tag{7}$$

With regard for the real conditions ($\tau \gg \frac{1}{\omega}$), the value of $\cos\left(\sqrt{\frac{\omega}{2a}} x - \omega\tau\right)$ can be assumed equal to $1/2$. Combining formulas (5) and (7), we obtain

$$\text{div } \bar{u} = \frac{1 + \mu}{3(1 - \mu)} \alpha \frac{1}{2} T e^{-\sqrt{\omega/(2a)} x}. \tag{8}$$

The value of T can be determined from the energy balance. The mechanical work spent for the surface treatment partially transforms to the thermal energy and partially to the destruction of a material. The mechanical work W depends on the force F applied to the surface of the sample that exceeds the friction force, the rate of motion of the instrument during the mechanical treatment v_{instr} , and the duration of treatment, i.e. $W = F v_{\text{instr}} \tau$. On the other hand, the thermal energy

$$Q = cdSLT, \tag{9}$$

where c stands for the specific heat capacity, d is the density, S is the surface area of the treated sample, L denotes the thickness of the broken layer, and T is the heating temperature of the sample surface. The part of the internal energy spent for the breakage of a material can be determined only experimentally, by analyzing the amount of the dispersed substance and the rate of dispersion.

Assuming that $Q = kW$, we obtain

$$T = k \frac{F v_{\text{instr}} \tau}{cdSL}. \tag{10}$$

The specific mechanical stress acting on the surface of a sample is equal to

$$\sigma = \frac{F}{S}, \tag{11}$$

then

$$T = k \frac{\sigma v_{\text{instr}} \tau}{cdL}. \tag{12}$$

The refractive index changes in the direction from the surface inside a sample as

$$n' = n - \frac{\operatorname{div} \bar{u}}{2n} = n - \frac{A}{n} e^{-\sqrt{\omega/(2a)} x}, \quad (13)$$

where

$$A = k \frac{\alpha}{4} \frac{1 + \mu}{3(1 - \mu)} \frac{\sigma v_{\text{instr}} \tau}{cdL}.$$

The measured ellipticity of the polarized light reflected from the sample surface is proportional to the difference of the refractive indices on the surface and in the bulk of a sample:

$$\operatorname{tg} \rho = n - n' = \frac{A}{n} e^{-\sqrt{\omega/(2a)} x}. \quad (14)$$

The formula coincides with formula (1), i.e. the constant $b = \sqrt{\frac{\omega}{2a}}$.

In order to estimate the possibilities of the use of the developed model, we give a numerical example. For optical TF1 glass, $a = 0.38 \times 10^{-6} \text{ m}^2/\text{s} = 0.38 \times 10^6 \mu\text{m}^2/\text{s}$; $\omega = 10^4 \text{ 1/s}$, $n = 1.6619$, so $b = \sqrt{\frac{\omega}{2a}} = \sqrt{\frac{10^4}{2 \cdot 0.38 \times 10^6}} \left[\frac{\mu\text{m}\sqrt{\text{s}}}{\sqrt{\text{s} \cdot \mu\text{m}}} \right] = 0.115$. Formula (14) can be presented as $\operatorname{tg} \rho = \frac{A}{1.6619} e^{-0.115x}$. The grinding with an abrasive having a grain size of $10 \mu\text{m}$ results in the formation of a broken layer of $30 \mu\text{m}$ in thickness (which was experimentally determined by the authors). Then the quantity $e^{-0.115x}$ for the surface polished to the depth $x = 30 \mu\text{m}$ is equal to 0.032. Since the experimental value of $\operatorname{tg} \rho_{\text{min}}$ for this polished glass amounts to 1×10^{-2} , $A = 0.5193$. Thus, $\operatorname{tg} \rho$ for TF1 glass will vary according to the formula $\operatorname{tg} \rho = 0.31 e^{-0.115x}$. In the case of the variation of x from 0 to $30 \mu\text{m}$, the calculated and experimentally determined values of $\operatorname{tg} \rho$ coincide to within an error which is at most 20%.

With regard for the performed investigation, it is possible to supplement the results of work [15], in which it was established that the ellipticity factor for polished surfaces of brittle nonmetallic materials depends on the physical quantities that characterize the strength of interatomic bonds. One can also relate the thermal diffusivity of this material to such quantities.

4. Conclusions

1. We have proposed a physical model of the formation of a surface layer of brittle glass-type materials broken by a mechanical treatment. According to the model, due to the thermofluctuation breakage of interatomic bonds in

the course of the treatment, the distribution of defects has a form similar to that inherent in the process of transfer of the thermal energy from the treated surface inside a material.

2. One of the physical characteristics that can be used for the description of the distribution of defects in the surface layer broken by a mechanical treatment is the thermal diffusivity of this material.

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ФІЗИЧНА МОДЕЛЬ ФОРМУВАННЯ ПОРУШЕНОГО МЕХАНІЧНОЮ ОБРОБКОЮ ПОВЕРХНЕВОГО ШАРУ МАТЕРІАЛІВ ОПТИКО-ЕЛЕКТРОННИХ І СЕНСОРНИХ ПРИЛАДІВ

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Резюме

Вивчено зміну параметра еліптичності поляризованого світла в процесі його відбивання від полірованої поверхні оптичного скла, що зумовлено наявністю дефектів і мікродеформацій, які формуються у ньому на фінішних операціях механічної обробки. У ролі зразків для досліджень було використано найбільш поширені промислові марки оптичного скла.

Запропоновано фізичну модель формування порушеного механічною обробкою поверхневого шару, згідно з якою в результаті термофлуктуаційного руйнування міжатомних зв'язків, розподіл дефектів має вигляд, аналогічний до розподілу температури в процесі передачі теплової енергії з поверхні об-

робки у внутрішні шари оброблюваного матеріалу. Тому однією з фізичних характеристик, що може бути використана для опису розподілу дефектів у порушеному поверхневому шарі, є температуропровідність оброблюваного матеріалу.