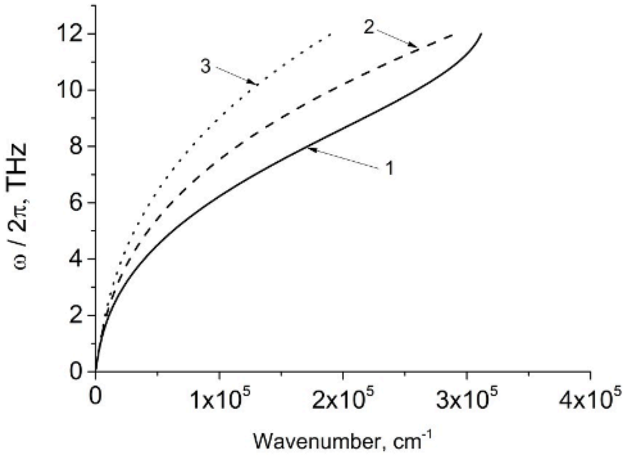

Figure 3 – The dependence of the wave vector of plasmon oscillations on the frequency of external EMR at various chemical potential values (1 – μ = 0 meV, 2 – μ = 15 meV, 3 – μ = 30 meV) and at a temperature of 300 K

The decrease of the wavelength of plasmon oscillations in graphene in the region of terahertz frequencies caused by the decrease of the propagation coefficient, is due to the strong localization of plasmons in graphene.

V. CONCLUSIONS

Thus, the plasmon effects were modeled in a single-layer graphene nanostructure, depending on the chemical potential and temperature. The obtained frequency dependences of the EMR propagation and absorption coefficients have shown that in the frequency range considered, the EMR can not only propagate due to plasmon oscillations, but also be amplified by them.

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ELECTRON TUNNELING TO THE SURFACE STATES AT PHOTOCATALYSIS

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I. INTRODUCTION

Composites with titanium dioxide nanoparticles (nanocomposite) have the widest prevalence in heterogeneous photocatalytic processes of organic compounds oxidation [1]. Titanium oxide possesses substantial photocatalytic activity in UV range, and characterized by high resistance to the photocorrosion processes and absence of toxicity, which helps to apply it as a component of self-purifying surfaces as well as in purification of domestic and industrial water and air [6]. The sunlight produces generation of electron-hole pairs in the near-surface area of TiO_2. In order to eliminate their recombination and ensuring of electron transition to the surface states, the necessity in the effective division of such pairs occurs. In many cases for this purpose heterojunctions contained titanium oxide with, e.g., silicon, are used. The electron-hole pairs, generated in titanium oxide, are divided: holes are moving to the silicon interface, where they are recombined, while electrons are moving to the surface and participate in the tunneling process on the surface states.

A spectrum of non-equilibrium electrons light-generated in the conduction band of titanium dioxide is resulted from the dependence of sunlight intensity on the photon wavelength [2]. A transfer of generated electrons to the surface states, which is determined by the tunneling transmission coefficient, depends on the surface potential reliefs created by the organic compounds on TiO2 surface. A real potential relief has a very complex form and includes alternated potential barriers and wells. As a result, the energy spectrum of tunneling electrons to the surface states of absorbed organic compounds depends on the sunlight intensity. Consequently, the photocatalytic activity and effectiveness of organic compounds oxidation on titanium dioxide surface is also determined by the sunlight intensity. Therefore, in order to evaluate and predict the photocatalytic activity of titanium dioxide surface it is necessary to estimate the spectrum of electrons tunneling to the surface states in dependence on the sunlight intensity. For this purpose it is necessary to determine transmission coefficient of the tunneling electrons. The aim of this paper is the modeling of the tunneling transmission of electrons excited by the sunlight through barriers generated by the surface states potential relief produced due to absorption of impurities and organic compounds.

II. MODEL

To determine transmission coefficients of the tunneling electrons, we developed the model based on the phase functions method. The model takes into account bulk and interface barrier parameters and the image force potential and allows including the potential relief of the wide-gap semiconductor. The principal feature of the phase functions method is the ability to find out the transmission coefficients. According to this method, only wave function variation, as a result of potential actions, is calculated rather than the proper wave function. This process is time-consuming for complex potentials. Besides, it is difficult to estimate the faults of results derived.

The tunneling transmission coefficient through a barrier of the width d which is described by the potential U(x) is equal to: [4]

$$D(E) = \exp\left(\frac{1}{k}\int_0^d U(x)[b(x)\cos(2kx) - a(x)\sin(2kx)]dx\right) \tag{1}$$

where $k(E) = (8\pi^2 m^* E / h^2)^{1/2}$ is the tunneling electron wave vector, m* and E are the effective mass and energy of the tunneling electron, h is the Planck constant, d is the tunneling barrier width. Functions a(x) and b(x) are defined from

$$\frac{da(x)}{dx} = \frac{U(x)}{2k}[-\sin(2kx) - 2b + (a^2 - b^2)\sin(2kx) - 2abcos(2kx)] \tag{2}$$

$$\frac{da(x)}{dx} = \frac{U(x)}{2k}[\cos(2kx) + 2a + (a^2 - b^2)\cos(2kx) - 2absin(2kx)] \tag{3}$$

To describe the potential barrier U(x) the following equation is used:

$$U(x) = \frac{8\pi m^*}{h^2}\left(U_0 - \frac{q}{\varepsilon\varepsilon_0 x} + A_s \exp\left(\frac{(x-p_0)^2}{\sigma}\right) + \frac{\alpha}{\sqrt{\pi}}\exp\,[\alpha^2(\mathrm{x}-\Delta)^2]\right) \tag{4}$$

where U_0 is the maximal height of the TiO_2 surface potential barrier, φ(x) is the image force potential, q – electron charge, ε, ε_0 – relative dielectric TiO_2 permeability and absolute dielectric vacuum permeability, As, p_0, σ – parameters, characterized imperfection of the potential relief surface. The above model was implemented for tunneling electron transmission through the absorbed layer on titanium dioxide surface in TiO_2 nanostructure illuminated by the light in neutral gas environment with organic compounds. For the generated electron-hole pairs division TiO_2 nanocomposite is positioned on Si substrate $N = 2m\frac{x_0^2 kT}{(h/2\pi)^2}$ – coefficient, which has influence on the height and form of the potential barrier in particular on the height and form of the additional barrier. Expression $q/\varepsilon\varepsilon_0 x$ displays counting forces of the mirror images, which smoothed barrier. Expression $\frac{\alpha}{\sqrt{\pi}}\exp\,[\alpha^2(\mathrm{x}-\Delta)^2]$ describes infinitely high peak placed approximately in the middle of the potential well, where α is the parameter, which influences on the width of this peak.

III.RESULTS AND DISCUSSIONS

Electron tunneling through the absorbed layers on the titanium oxide surface as a part of Si /TiO2 heterostructure, illuminated by the light in the neutral gas environment, contain organic pollution, was considered. Two potential barriers divided by the potential well represent potential relief. Additional infinitely high barrier is situated between two barriers in the middle of the potential well. This barrier indicates position of the organic molecule on the potential relief.

Transmission coefficient is changed non-monotonically in the case when additional infinitely high barrier is placed in the middle of the potential well. Transmission coefficient increases monotonically beginning from E=0.5 eV. At E = 1-2 eV graph decreases drastically from 0.8 up to 0.4 after which graph continues increasing. But at the certain height of the additional barrier resonance fluctuations appear. These fluctuations becomes evident at higher α values. Duration and frequency of changes rise proportionally to the correction coefficient of the barrier growth.

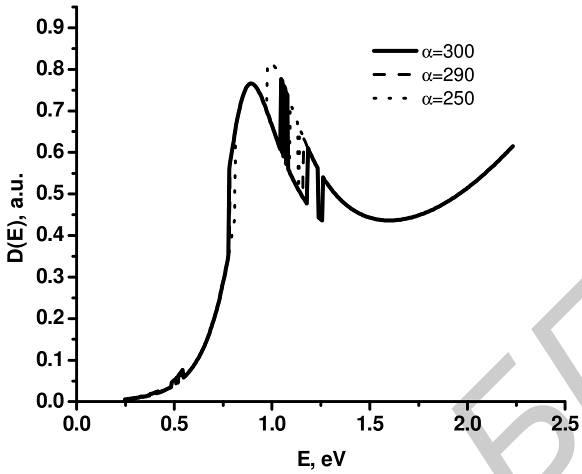

Figure 1 – Change of the transmission coefficient depending on additional barrier high

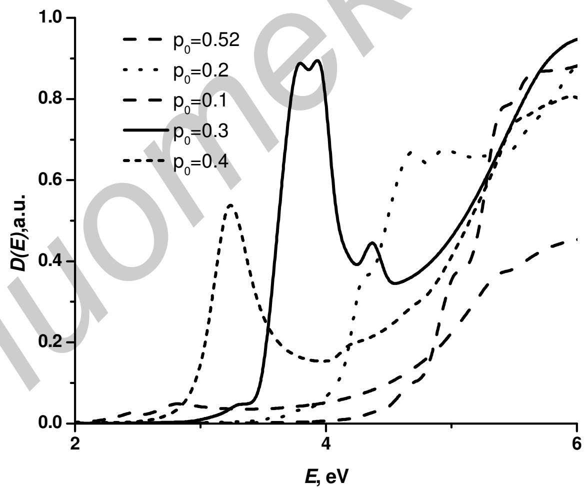

Figure 2 – Change of the transmission coefficient depending on value of the dispersion potential

The highest fluctuation in the form of two sequential additional peaks on D(E) characteristic is observed at p_0=0,3-0,4 (Fig. 3).

When parameter of the potential dispersion p_0 = 0, transmission coefficient has monotonic characteristic without peaks and fluctuations. Maximal value of the transmission coefficient is reached at p_0=0.3, but at further increasing up to p_0=0.4-0.52 peaks' high decreases and change of the transmission coefficient depending on the value of the dispersion potential parameter becomes monotonically again. (p_0=0.52) (Fig.4)

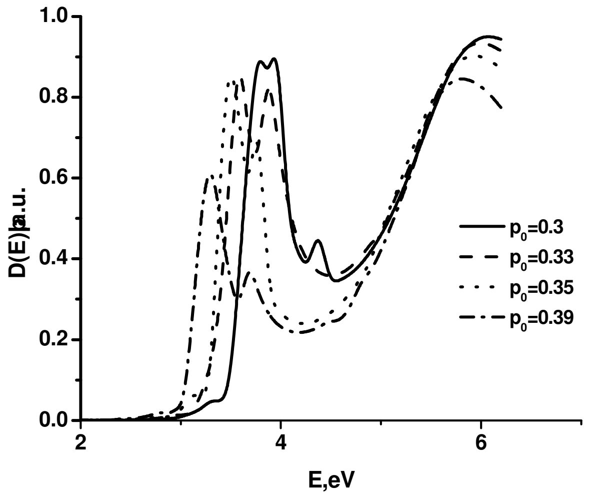

Figure 3 – Change of the transmission coefficient depending on the value of the dispersion potential parameter p_0= 0,3 – 0,4)

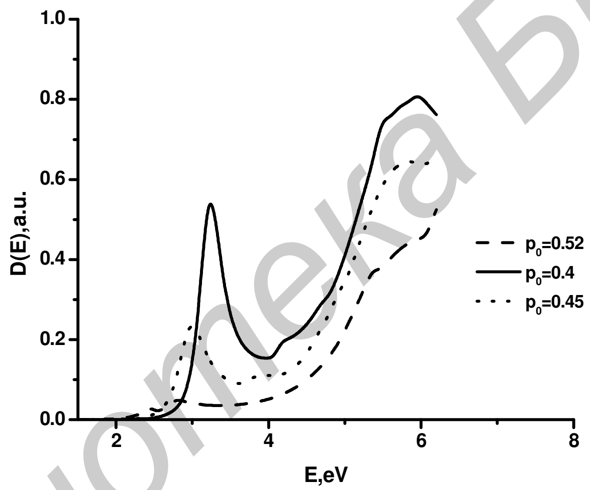

Fig. 4. Change of the transmission coefficient depending on the value of the dispersion potential parameter (p_0=0,4 – 0,5)

IV. CONCLUSIONS

Calculations of electron tunneling to the surface states, which are created by the organic compounds on the titanium dioxide surface under the light illumination, are performed. It is proved that potential barrier form on the titanium oxide surface, which contains organic compounds, leads to the non-monotonic dependence of the transmission electron coefficient at the surface states on the energy (N-type). At the maximal values of the transmission coefficient additional peaks with the fluctuations are appeared. Such features of the transmission coefficient of tunneling electrons are explained by the interference of transmitted and reflected waves, over barrier wave and reflected wave under conditions of the complex potential relief.

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