COMPARISON OF PARAMETERS OF TWO-DIMENSIONAL (2D) AND THREE-DIMENSIONAL (3D) P-N-JUNCTION DIODES

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Abstract. The dependence of quasi-Fermi levels and current-voltage characteristics of electrons and holes of two-dimensional diodes with a p-n-junction on the wavelength of light was theoretically studied. The results obtained were compared with the experimental results. Theoretically, the differential conductivity and diffusion capacitance of a three-dimensional p-n-junction diode (3D) is shown to be relatively larger than that of a two-dimensional diode (2D).

Key words: p-n-junction, photocurrent, differential conductivity, diffusion capacitance, current-voltage characteristic, light.

1. INTRODUCTION

In recent years, two-dimensional (2D) semiconductor materials have attracted great interest in the field of electronics due to their high potential in the production of many-sided electronic devices. Semiconductor materials 2D showed the efficiency of light absorption. Therefore, these materials are the main source for optoelectronic devices, and especially for photodetectors [1–4]. In [5], an experimental and theoretical comparison of the properties and practical application of WSe_2 from two-dimensional 2D materials was carried out. In [6], for a two-dimensional 2D p-n-junction diode, the Poisson equation was combined with the equations, drift-diffusion and continuity equations, and the Shockley equation for an ideal current-voltage characteristic was also proposed. In addition, the processes of recombination and generation within the effective depletion layer (EDL) resulted in significant deviations from the ideal, and the capacitances and conductivities of a two-dimensional 2D p-n-junction diode were analyzed. Atomically thin MoS_2, due to its two-dimensional nature and low-power electronic potential, is important for newly created nanoelectronics, and especially important for space-related electronics. With this in mind, the results of experiments on the effect of vacuum ultraviolet radiation on two-dimensional field-effect transistors with MoS_2 are presented in [7]. In [8], the limited mobility of an acoustic phonon was studied using the Boltzmann equation and the principles of acoustic electron–phonon interaction for a temperature $T < 100$ K and a high charge carrier density in two-dimensional n-type MoS_2. Analytical expressions for the deformation potential and piezoelectric interactions are given together with a continuous elastic model.

Atomic thin films of layered materials such as MoS_2 are of great interest for studying two-dimensional phase transitions in an electrostatic field. To achieve such phase transitions, electrostatic field techniques are required to access high carrier densities. In [9], an electrostatic field method was developed that allows one to achieve a maximum density of $4 \cdot 10^{14}$ cm^{-2} n-type in multilayer MoS_2. It is also shown that with an increase in the charge carrier density, the transition of a dielectric into a metal and the transition of an incomplete metal into a superconductor in MoS_2 occur at a critical temperature of 10 K, and it is also shown that the superconducting transition temperature does not depend on the density of charge carriers for two-layer thin samples of MoS_2 after the onset of superconductivity.

When layered materials are reduced to a few atomic layers, their remarkable properties are demonstrated, in the production of innovative electronic devices, two-dimensional semiconductors (2D) play an important role. In recent studies in this area, molybdenum disulfide (MoS_2) is widely used as a prototype [10]. MoS_2 is an electronic range semiconductor. A semiconductor with a direct transition will be obtained at the boundary of one layer [11, 12], because the energy of an indirect transition is greater than the energy of a direct transition at points K, K` of the Bryullen zone.

At these points, the strong interaction of light with matter [13] and the enhancement of spin degeneration of the valence and conduction bands due to inversion symmetry breaking show that single-layer MoS_2 is an excellent material for transistors in electronics, optoelectronics, and developing nanoelectronics [14–17].

Modern semiconductor electronics has begun to study the transition metal family of dichalcogenides, graphite, black phosphorus, silicon, and germanium to create atomically sensitive p-n-junctions [18–24]. Using the capabilities and hyperfine nature of 2D materials that cannot be realized with 3D p-n-junctions, can be realized using p-n-junctions of a two-dimensional 2D diode. The use of a two-dimensional 2D diode in the creation of electronic and optoelectronic devices, transistors, solar batteries, photodetectors, etc. is shown in [24–35]. In [36], the effect of quantum capacitance and high linear field density on the statistics of carriers in two-dimensional semiconductor devices made of transition metal dichalcogenite was studied and compared with experimental data.

However, in the above studies, the effect of light on quasi-Fermi levels and on the current-voltage characteristics of electrons and holes of a two-dimensional 2D p-n-junction diode, as well as the parameters of two-dimensional 2D and three-dimensional 3D p-n-junction diodes, have not been sufficiently studied theoretically.

Based on the foregoing, our goal is to theoretically study the quasi-Fermi levels of electrons and holes of two-dimensional 2D p-n-junction diodes, the dependence of photocurrents of two-dimensional 2D diodes on the frequency of light, as well as the electrical conductivity and diffusion capacitance of 2D and 3D semiconductors.

2. RESULTS AND DISCUSSION

2.1. CHANGES IN THE QUASI-FERMI LEVELS OF ELECTRONS AND HOLES IN TWO-DIMENSIONAL 2D P-N-JUNCTION DIODES WITH INCREASING TEMPERATURE

For two-dimensional n-type semiconductors, the Fermi energy is determined by the following expression [36]:

$$E_{fn} - E_c = kT \ln\left(\exp\left(\frac{n}{g_{2D}kT}\right) - 1\right). \quad (1)$$

Here: E_f – Fermi energy, E_c – conduction band energy, k – Boltzmann's constant, T – grid temperature, n – electron concentration, g_{2D} – the energy density is $g_{2D} = \frac{m^*}{\pi\hbar^2}\sum_n \Theta(E - E_n)$. $\Theta(E - E_n)$ – Heaviside function, $\hbar$ – Planck's constant, $m^* = 0.57m_0$ – electron effective mass for a two-dimensional 2D single-layer diode SL MoS_2, the band gap is $E_g = 1.8$ эВ and for semiconductors type-p

$$E_v - E_{fp} = kT \ln\left(\exp\left(\frac{p}{g_{2D}kT}\right) - 1\right). \quad (2)$$

Here: p-hole concentration. Using expression (2), one can obtain a graph of the temperature dependence of the Fermi layer at different concentrations of single-layer SL MoS_2 (Fig. 1).

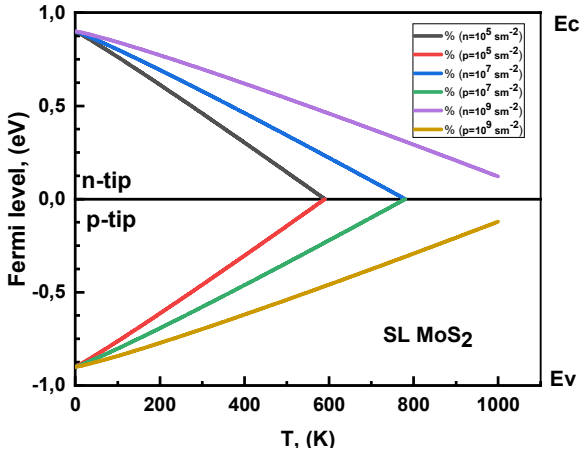

Fig. 1 – Temperature dependence of the Fermi layer of a two-dimensional 2D diode at various concentrations of single-layer SL MoS_2.

Influencing a strong electromagnetic field on the semiconductors of a two-dimensional 2D type-n diode, as a result, taking into account the heating of electrons and holes, expressions (1) and (2) can be written in the following form:

$$E_{fn1} - E_c = k\left(T_e - T\right)\ln\left(\exp\left(\frac{n}{g_{2D}kT}\right) - 1\right) \tag{3}$$

$$E_v - E_{fp1} = k\left(T_h - T\right)\ln\left(\exp\left(\frac{n}{g_{2D}kT}\right) - 1\right). \tag{4}$$

Here: E_{fn1} – energy of the quasi-Fermi level, T_e and T_h – respectively, the temperatures of electrons and holes. When in expressions (3) and (4) T_e, $T_h > T$ there is a separation of the Fermi level into quasi-Fermi levels (Fig. 2).

When the condition T_e, $T_h = T$ expressions (3) and (4) take the form: $E_{fn} = E_c$ $E_{fp} = -E_v$.

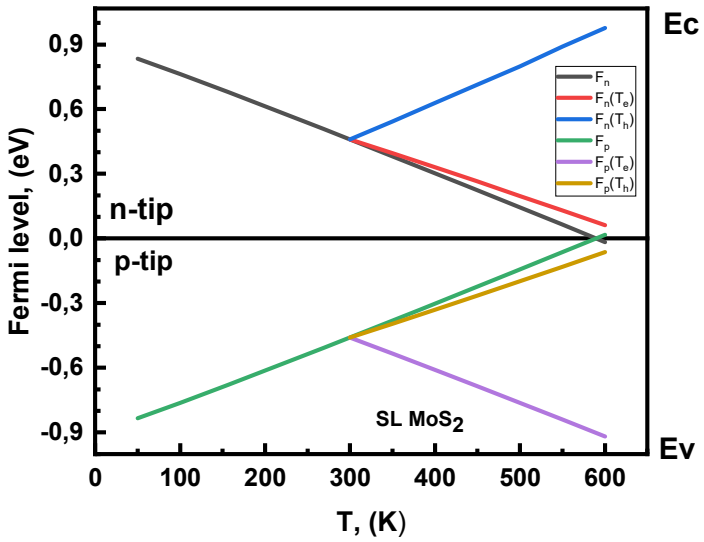

Fig. 2 – Temperature dependence of the Fermi layer of a two-dimensional 2D single-layer SL MoS_2 diode.

From here it will be possible to observe that the Fermi level of a two-dimensional 2D semiconductor diode under the action of a strong electromagnetic field is divided into quasi-Fermi levels. In addition, the quasi-Fermi levels of the minority current carriers in the regions and change more strongly than the quasi-Fermi levels of the main current carriers. Therefore, we can determine the EMF from the change in the Fermi quasi-levels of the majority and minor charge

carriers. That is, the EMF of a single-layer SL MoS_2 two-dimensional 2D diode can be found from the difference in the heights of the potential barrier:

$$\varphi_0 = F_n - F_p \qquad \varphi \equiv F_n\left(T_e\right) - F_p\left(T_h\right) \qquad \varepsilon = \varphi - \varphi_0 . \tag{5}$$

2.2. INFLUENCE OF LIGHT AND STRAIN ON QUASI-FERMI LEVELS OF SEMICONDUCTORS OF A TWO-DIMENSIONAL 2D DIODE IN A STRONG ELECTROMAGNETIC FIELD

In two-dimensional 2D semiconductors, the concentrations of electrons and holes can be determined from the following expressions [36]:

$$n = g_{2D} kT \ln\left(1 + \exp\left(\frac{E_f - E_c}{kT}\right)\right) \tag{6}$$

$$p = g_{2D} kT \ln\left(1 + \exp\left(-\frac{E_f - E_v}{kT}\right)\right) \tag{7}$$

The change in the quasi-Fermi level in two-dimensional 2D semiconductors due to an increase in the concentration of current carriers under the action of light is equal to

$$E_{fn} - E_c = k\left(T_e - T\right) \ln\left(\exp\left(\frac{n + I\beta\alpha\tau_e}{g_{2D} kT}\right) - 1\right) \tag{8}$$

$$E_v - E_{fp} = k\left(T_h - T\right) \ln\left(\exp\left(\frac{p + I\beta\alpha\tau_p}{g_{2D} kT}\right) - 1\right) \tag{9}$$

Here: α – light absorption coefficient [37]: $\alpha = A\left(h\nu - E_g - \Delta\varepsilon\right)^r$, $h\nu \approx E_g$ them, $\alpha = A\left(\Delta\varepsilon\right)^r$, β – quantum output, E_g – bandgap, ν – light frequency, h – Planck's constant, Δ – deformation potential, r – for a properly valid transition $r = \frac{1}{2}$ (correctly forbidden transition $r = \frac{3}{2}$), A – coefficient for a correctly admissible transition $A = 2 \cdot 10^4$ [37], I – light intensity, τ_e, τ_p – respectively, the lifetime of electrons and holes.

Considering the foregoing, we can write expressions (8) and (9), *i.e.*, the effect of light and deformation on the Fermi quasi levels.

$$E_{fn} - E_c = k\left(T_e - T\right)\ln\left(\exp\left(\frac{n + I\beta\tau_e A(\Delta\varepsilon)^r}{g_{2D}kT}\right) - 1\right) \tag{10}$$

$$E_v - E_{fn} = k\left(T_h - T\right)\ln\left(\exp\left(\frac{p + I\beta\tau_p A(\Delta\varepsilon)^r}{g_{2D}kT}\right) - 1\right). \tag{11}$$

Assuming that the degree r in expressions (10) and (11) is $r = \frac{1}{2}$ for a direct admissible transition, we see that the quasi-Fermi levels depend on the deformation at certain intensities.

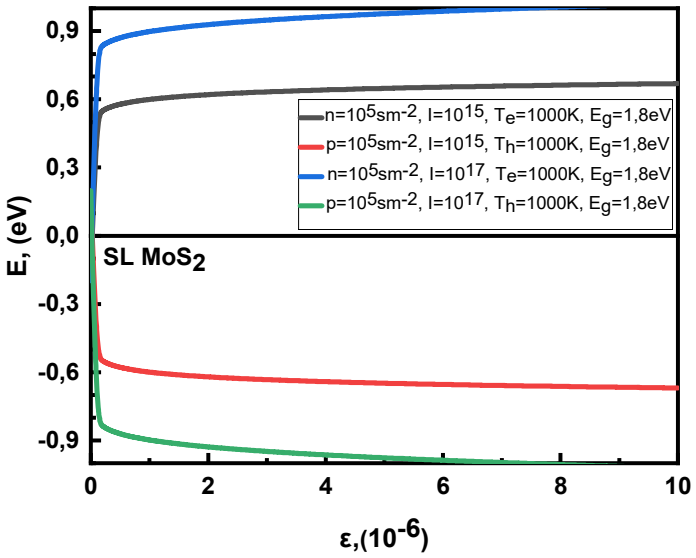

Fig. 3 – Dependence of light and strain on the quasi-Fermi level of a two-dimensional 2D single-layer SL MoS_2.

Figure 3 shows the change in the quasi-Fermi level under the action of deformation of different intensity of the two-dimensional 2D single-layer SL MoS_2. As can be seen from the figure, at high intensities one can observe a change in the quasi-Fermi level at high values. In addition, the quasi-Fermi levels of minority current carriers in the p and n regions change more strongly than the quasi-Fermi levels of the majority current carriers. Therefore, we can determine the photo-EMF under the deformation effect by the difference in the EMF formed by the change in

quasi-Fermi levels of the majority and minor charge carriers under the deformation effect for certain intensities.

2.3. DEPENDENCE OF PHOTOCURRENTS OF TWO-DIMENSIONAL 2D P-N-JUNCTION DIODES ON LIGHT FREQUENCY

Let us consider the current-voltage characteristic of a semiconductor due to the change in photocurrents depending on the frequency of light for photodetectors based on 2D semiconductor materials.

In this case, the Shockley equation can be used to calculate the total current of a two-dimensional 2D p-n-junction [25]:

$$I_{ds} = \frac{mU_T}{R_s} W\left(\frac{I_s R_s}{mU_T}\exp\left(\frac{U_{ds} + I_s R_s}{mU_T}\right)\right) - I_s . \tag{12}$$

Here: I_s – saturation current, m – coefficient of imperfection current-voltage characteristic of p-n-junction, $U_T = \frac{kT}{q}$ – thermal voltage, W – Lambert function, R_s – resistance in series with the diode. Using expression (12), one can obtain the current-voltage characteristic of a two-dimensional 2D p-n-junction (Fig. 4, line-1). Using expression (12), the total current of a two-dimensional 2D photodiode can be calculated as follows:

$$I_{ds} = \frac{mU_T}{R_s} W\left(\frac{I_s R_s}{mU_T}\exp\left(\frac{U_{ds} + I_s R_s}{mU_T}\right)\right) - I_s - I_c . \tag{13}$$

Here: $I_c = eI_0\left(1-\beta_0\right)$, $\beta_0 = \beta_s + \beta_v = \frac{\frac{d}{L_s} + \frac{1}{2}\left(\frac{d}{L_n}\right)^2}{1+\frac{d}{L_s}}$ – total losses for bulk and surface recombination, $\beta_c = \frac{\frac{d}{L_s}}{1+\frac{d}{L_s}}$ – relative losses for surface recombination, $\beta_v = \frac{1}{2}\frac{\left(\frac{d}{L_n}\right)^2}{1+\frac{d}{L_s}}$ – relative volumetric recombination losses, $L_s = \frac{D_n}{s}$, d – illuminated

area thickness, $I_0 = \alpha G(1-R)$ – light intensity, $G = \frac{W_i}{h\omega}$ – the number of photons incident on a unit surface, W_i – total light energy, $R = \left(\frac{n-1}{n+1}\right)^2$ – light reflectance, n – refractive index of the medium, $L = \left(\frac{2\varepsilon\varepsilon_0}{e}\frac{n_n + p_p}{n_n p_p}\right)(\varphi_0 + U)^{\frac{1}{2}}$ – space charge layer width, $L_s = \frac{D_e}{s}$, s – recombination rate [9].

In view of the foregoing, we have the following expression for the photocurrent

$$I_c = -\frac{eI_0}{1+\frac{L}{L_s}} = \frac{e\alpha G(1-R)}{1+\left(\frac{2\varepsilon\varepsilon_0}{e}\frac{n_n + p_p}{n_n p_p}(\varphi_0 + U)\right)^{\frac{1}{2}}\frac{s}{D_e}} = \frac{eG(1-R)A(h\nu - E_g - \Delta\varepsilon)^r}{1+\left(\frac{2\varepsilon\varepsilon_0}{e}\frac{n_n + p_p}{n_n p_p}(\varphi_0 + U)\right)^{\frac{1}{2}}\frac{s}{D_e}}. \quad (14)$$

Substituting (14) into (13) we have the expression

$$I_{ds} = \frac{mU_T}{R_s}W\left(\frac{I_s R_s}{mU_T}\exp\left(\frac{U_{ds} + I_s R_s}{mU_T}\right)\right) - I_s - \frac{eG(1-R)A(h\nu - E_g - \Delta\varepsilon)^r}{1+\frac{L}{L_s}}. \quad (15)$$

Using this expression, we obtain the following graph for the current-voltage characteristic of a semiconductor of a two-dimensional 2D diode (Fig. 4, line-2).

Theoretically, we outlined the change in the current-voltage characteristic of a two-dimensional 2D junction diode depending on the wavelength of light using expression (15) (Fig. 5(a)) and compared the result with the results of the experiment [1] (Fig. 5(b)). These comparisons show that the theoretical and experimental results agree qualitatively.

In Fig. 5(b), the experimental results show that the reverse current varies with the wavelength of the light. This corresponds to the photovoltaic mechanism and the generated photocurrent increases the reverse current. The electrical power

$\left(P_{el} = I_{ds}V_{ds}\right)$ generated by the device shown in the figure reaches approximately 13 pW at maximum light power.

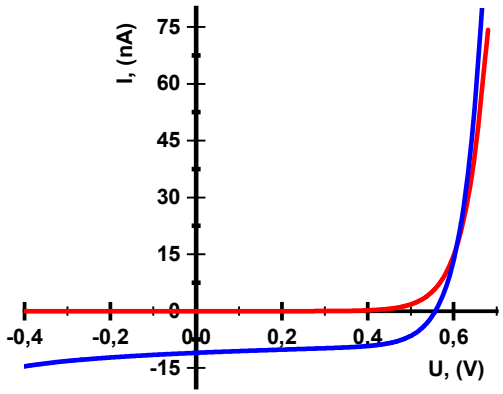

Fig. 4 – Current-voltage characteristic of a two-dimensional 2D junction diode.

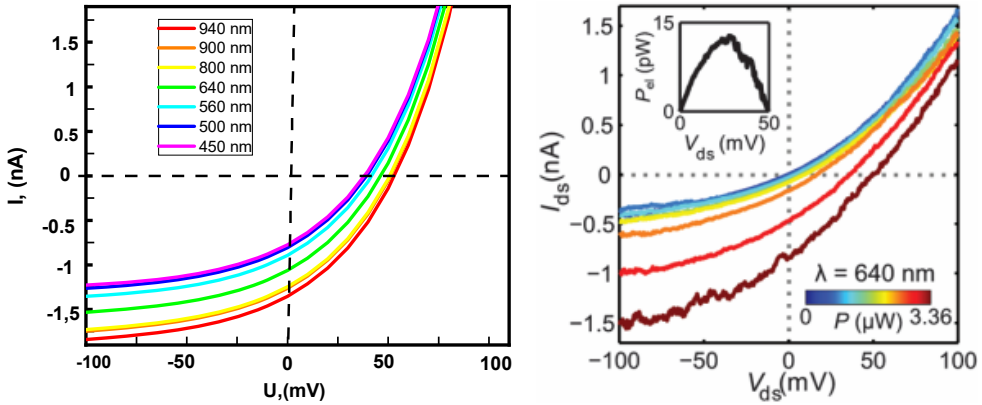

Fig. 5 – Current-voltage characteristic of a two-dimensional 2D junction diode:
a) theoretically; b) experimental [1].

2.4. COMPARISON OF DIFFERENTIAL CONDUCTIVITY OF THREE-DIMENSIONAL 3D AND TWO-DIMENSIONAL 2D P-N JUNCTIONS

The differential conductivity of a three-dimensional 3D p-n-junction is determined by the following relationship [38]:

$$G = \frac{\mathrm{d}I}{\mathrm{d}U} = \frac{eI_s}{kT}\exp\left(\frac{eU}{kT}\right) \tag{16}$$

Using expression (1), one can obtain a graph of the dependence of the differential conductivity of a three-dimensional 3D p-n-junction on a given voltage (Fig. 6).

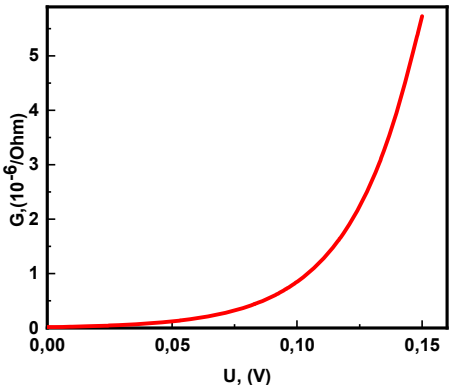

Fig. 6 – Dependence of the differential conductivity of the p-n junction on voltage.

Using the expressions given in [6], we obtain the following formula for the diffusion capacitance of a two-dimensional 2D diode p-n-junction:

$$G = \frac{q^2 n_i^2 \left(L_n + L_p\right)}{kTN_d} \exp\left(\frac{qU}{kT}\right) \tag{17}$$

In expression (17), $n_i = g_{2D} kT \exp\left(-\frac{E_g}{2kT}\right)$ $L_n = L_p = \sqrt{D_{n(p)}\tau_{n(p)}}$, $D_{n(p)} = \frac{kT\mu_{n(p)}}{q}$, $N_d = 4 \cdot 10^{12} \text{sm}^{-2}$ [6]. Using expression (17), one can obtain a graph of the dependence of the differential conductivity of a two-dimensional 2D junction diode on a given voltage (Fig. 7).

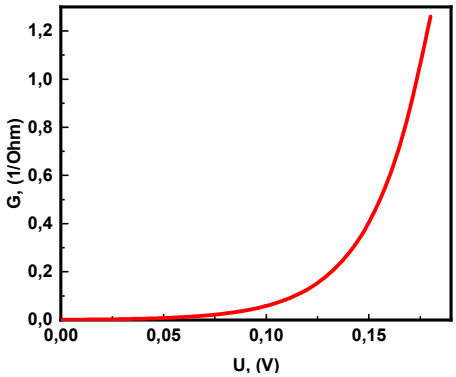

Fig. 7 – Dependence of the differential conductivity of the p-n-junction on voltage.

In Figs. 6 and 7, the dependence of the differential conductivity of three-dimensional 3D and two-dimensional 2D p-n-junctions on voltage is theoretically considered. The results show that the differential conductance of a two-dimensional 2D p-n-junction will be greater than that of a three-dimensional 3D p-n-junction. This shows that a two-dimensional 2D p-n-junction is more efficient than a three-dimensional 3D p-n-junction.

2.5. COMPARISON OF DIFFUSION CAPACITANCES OF THREE-DIMENSIONAL 3D AND TWO-DIMENSIONAL 2D TRANSITIONS

Comparison of diffusion capacitances of three-dimensional 3D and two-dimensional 2D transitions using the expression given in our previous work [38], for the diffusion capacitance of a three-dimensional 3D p-n-junction, we can obtain it's graph on a logarithmic scale

$$C = \frac{\tau e I_s}{2kT} e^{\frac{eU}{kT}} \tag{18}$$

using an expression, you can get its graph on a logarithmic scale (Fig. 8).

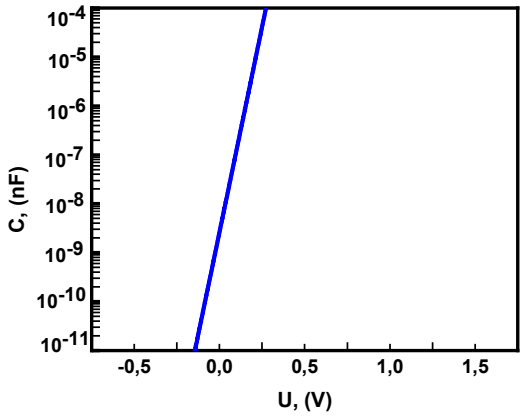

Fig. 8 – Dependence of the diffusion capacitance of a three-dimensional 3D junction on voltage.

The diffusion capacity of a two-dimensional 2D transition is determined by the following relationship [6]:

$$C_{dif} = \frac{q^2 n_i^2 \left(L_n + L_p\right)}{2kTN_d} \exp\left(\frac{qU}{kT}\right). \tag{19}$$

The graph of expression (19) on a logarithmic scale is as follows in Fig. 9.

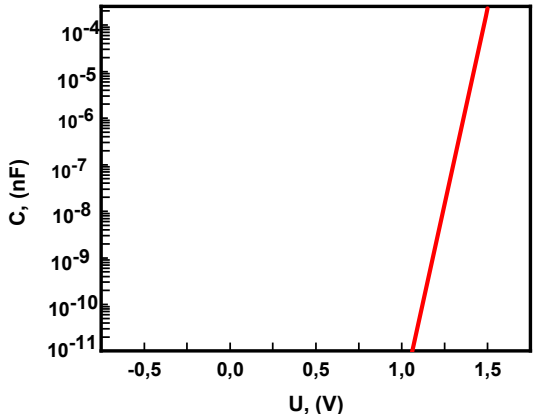

Fig. 9 – Diffusion capacitance of a single-layer SL MoS_2 two-dimensional 2D diode as a function of voltage.

The comparison of diffusion capacitances of three-dimensional 3D and two-dimensional 2D transitions can be seen in Fig. 10.

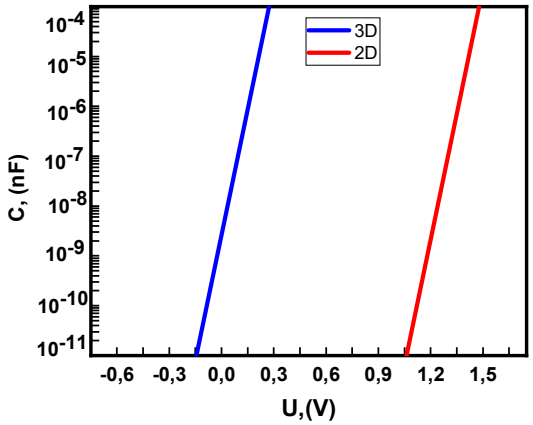

Fig. 10 – Diffusion capacitance of three-dimensional 3D and two-dimensional 2D junction diodes as a function of voltage.

Where the diffusion capacitance of single-layer SL MoS_2 two-dimensional 2D diode is larger than the diffusion capacitance of Si three-dimensional 3D diode.

3. CONCLUSIONS

When observing, it was revealed that, under the influence of a strong electromagnetic field, the Fermi level of two-dimensional semiconductors 2D is divided into quasi-Fermi levels. In addition, the quasi-Fermi levels of the minority

carriers in the regions and change more strongly than the quasi-Fermi levels of the majority current carriers. Therefore, it is possible to determine the EMF from the change in the quasi-Fermi levels of the majority and minor charge carriers. That is, the EMF of a single-layer SL MoS_2 two-dimensional 2D diode can be found from the difference in the heights of the potential barrier.

Under the influence of large values of intensity, it was noticed that the quasi-Fermi levels can vary in large values. In addition, the quasi-Fermi levels of minority current carriers in the regions and change more strongly than the quasi-Fermi levels of the main current carriers. Therefore, it is possible to determine the photo-EMF under the deformation effect by the difference in the EMF formed by the change in the quasi-Fermi levels of the main and minor charge carriers under the deformation effect for certain intensities.

The change in the current-voltage characteristic of a two-dimensional 2D junction diode depending on the wavelength of light is theoretically considered, and the qualitative correspondence of the obtained result to the experimental results [1] is shown.

Theoretically, it has been shown that the differential conductance of a two-dimensional 2D junction is greater than that of a three-dimensional 3D junction, which shows that a two-dimensional 2D junction is more efficient than a three-dimensional 3D junction.

Consider that the diffusion capacitance of a single-layer SL MoS_2 two-dimensional 2D diode will be larger than the diffusion capacitance of a three-dimensional 3D Si diode.

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