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Simulation the effects of temperature and magnetic field on the density of surface states in semiconductor heterostructures

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Abstract
In this article, the physical properties of the surface of the CdS/Si(p) material under the influence of a magnetic field were studied . The dependence of the density of surface states of the p-type Si(p) semiconductor on the magnetic field and temperature has been studied. For the first time, a mathematical model has been developed to determine the temperature dependence of the density of surface states of a semiconductor under the influence of a strong magnetic field. Mathematical modeling of the processes was carried out using experimental values of the continuous energy spectrum of the density of surface states, obtained at various low temperatures and strong magnetic fields, whithin the band gap of silicon. The possibility of calculating discrete energy levels is demonstrated.

Keywords: density of surface states, magnetic field, heterostructure, deep levels, capacitance-voltage characteristic, mathematical modeling, temperature

1. Introduction

As is known, one of the pressing problems is the study of the electrical, optical and magnetic properties of the CdS/Si(p) semiconductor heterostructure , which is widely used as photoelectric converters. In particular, the formation of defects at the heterointerface CdS/Si(p) negatively affects the electrical properties of these semiconductor materials, and the density of surface states at deep energy levels leads to a deterioration in the photovoltaic efficiency of the heterostructure.

To date, several studies have been conducted to measure the density of surface states and determine its dependence on external factors. In particular, in [1-23], the density of surface states in semiconductor structures was determined by the capacitance-voltage (CV) method. At the same time, a method was proposed for calculating the densities of surface states in semiconductors based on the frequency dependence of the capacitance-voltage characteristic for states in which the charge of surface states depends on the applied constant reverse bias voltage [24-35]. But these works did not consider the influence of a magnetic field on the density of surface states at the semiconductor-insulator interface. And also, a perfect mathematical model has not been developed to determine the dependence of surface states on the magnetic field and temperature.

The main purpose of the work is to model the dependence of the densities of the surface states of a heterostructured CdS/Si(p) semiconductor on the magnetic field.

2. Model

2.1. Dependence of the maximum reverse bias voltage on a strong magnetic field in semiconductor heterostructures.

Since the bulk charge field of a CdS/Si(p) heterostructure semiconductor is mainly concentrated in Si(p), calculating the densities of silicon surface states up to the bandgap is sufficient. In this case, from the band diagram Si(p), presented in figure 1, one can trace the process of charge distribution at deep levels and, since the sample is p-type, the energy levels in surface states are filled with cavities, starting with E_V . According to the Fermi level rule, the energy levels of a heterojunction are filled with holes up to the quasi-Fermi level. However, energy levels above the quasi-Fermi levels are considered empty.

When determining the density of surface states, the capacitance -voltage (CV) method is used. When measuring the CV characteristic, the constant voltage corresponds to the reverse bias voltage of the heterostructure. The increase in the bending of the energy bands in figure 1 and the expansion

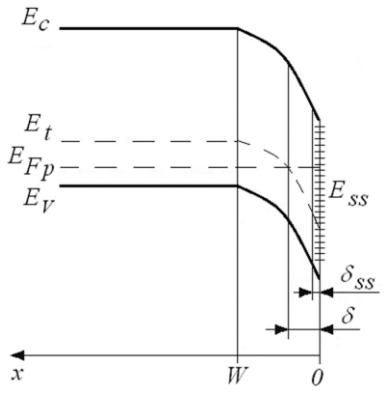


Figure 1. Band diagram of the base part of the CdS/Si(p) heterostructure at reverse bias, taking into account deep levels (E_{SS} - deep levels of surface states, E_t - discrete deep levels in the bulk of the base region) [1].

of the space charge region is directly proportional to the value of the reverse voltage. However, increasing the reverse voltage value causes deeper levels in surface states to become filled with holes. This will make it possible to control the quasi-Fermi levels. Si(p) is calculated starting from the valence field spin.

Deep energy levels at the interface of CdS and Si(p), that is, at the heterointerface, are associated with reverse voltage and are expressed as follows [1]

$$E_{SS} - E_V = q\ (\Phi - V), \tag{1}$$

where E_{SS} is the value of the deep energy level on the surface in the current state, q is the charge value, Φ is the effective value of the contact potential difference, V is the reverse voltage.

If we increase the value of the reverse voltage to the maximum degree, $V = V_{SS}^{max}$ this will lead to the quasi-Fermi levels reaching the conduction band Si(p). And this will be the reason that E_{SS} will be equal to E_C. In this case, E_C–*Si(p)* is the bottom of the conduction band. Therefore, $E_{SS} = E_C$, then equation (1) is written as

$$E_C - E_V = q\left(\Phi - V_{SS}^{max}\right), \tag{2}$$

Considering that $E_C - E_V = E_g$ (silicon band gap), the maximum reverse voltage can be determined from (2)

$$V_{SS}^{max} = \frac{\left|q\Phi - E_g\right|}{q}, \tag{3}$$

As a result of the influence of external factors on semiconductor structures, their properties will radically change. One of the main dynamic parameters of semiconductors is that the band gap is highly dependent on temperature, pressure, magnetic field and strain. In particular, the dependence of the band gap on the magnetic field and quantum well thickness was studied in [36-39]. The following analytical expression is derived for: $E_g^{2d}(B,T,d)$

$$E_g^{2d}(B,T,d) = E_g(0) - \frac{\alpha_1 T^2}{\alpha_2 + T} + \left(\hbar\omega_C^e\left(N_L^e + \frac{1}{2}\right) + \hbar\omega_C^p\left(N_L^p + \frac{1}{2}\right)\right) + \left(\frac{\pi^2\hbar^2}{2m_e d^2}n_e^2 + \frac{\pi^2\hbar^2}{2m_p d^2}n_p^2\right), \tag{4}$$

Here, $\hbar\omega_C^e = \hbar\frac{eB}{m_C^e}$, $\hbar\omega_C^p = \hbar\frac{eB}{m_C^p}$ are magnetic field energy; $E_g(0)$ - band gap at T = 0 K; α_1, α_2 - thermal coefficients in the empirical equation of Varshni; N_L^e, N_L^p - number of Landau levels in the conduction band and valence band; *d*- is the thickness of the quantum well; n_e, n_p – number of dimensional quanta in allowed zones; m_e, m_p are the effective masses of the electron and hole.

The physical processes occurring on the surface of the sample are similar to a quantum well . The reason for this is that the study is limited to two dimensions, both energy states in the plane and energy spectra in the quantum well. It follows from this that the object is a heterostructure or the quantum well condition is satisfied, equation (4) is applicable to the heterointerface of states . When *Si(p)* is exposed to a strong magnetic field at the heterointerface , according to equation (3), the value $E_g(B,T,d)$ at constant low temperature will increase slightly, and the maximum value of the reverse bias voltage will decrease to reduce V_{SS}^{max}. Considering that the heterostructure *CdS/Si(p)* does not have a quantum well, and also (3) and (4), the dependence of the maximum reverse bias voltage on the quantizing magnetic field can be found as follows

$$V_{SS}^{max}(B,T) = \frac{\left|q\Phi - \left(E_S(0) + \frac{\alpha_1 T^2}{\alpha_2 + T} + \hbar\frac{eB}{m_C^e}\left(N_L^e + \frac{1}{2}\right) + \hbar\frac{eB}{m_C^p}\left(N_L^p + \frac{1}{2}\right)\right)\right|}{q}, \tag{5}$$

In experiments, the density of surface states at room temperature (T=300 K) was calculated using the CV method. Taking into account deep energy levels, the effective value of the contact potential difference is equal to $\Phi = 0.11$ V [1], Varshni coefficients for silicon $\alpha_1 = 7.021{*}10^{-4}$; $\alpha_2 = 1108$ K; $E_g(0) = 1.17eV$ [40].

If consider $m_C^e = m_p^e = m_C^*$ and for the first Landau level, $N_L^e = N_L^p = 0$ then equation (5) can be written as:

$$V_{SS}^{max}(B,T) = \frac{\left|q\Phi - \left(E_S(0) - \frac{\alpha_1 T^2}{\alpha_2 + T} + \hbar\frac{eB}{m_C^*}\right)\right|}{q}, \tag{6}$$

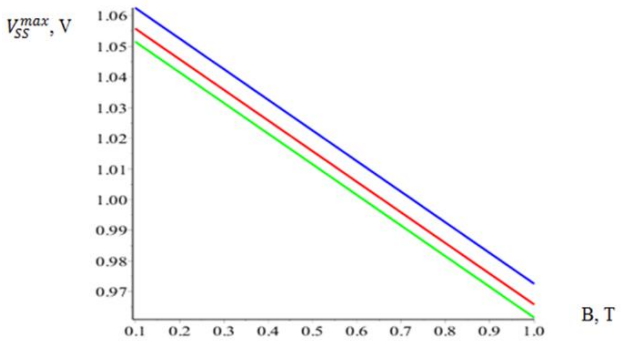


Figure 2. Graph of the dependence of the maximum voltage displacement V_{SS}^{max} on the magnetic field *B*.

Using these parameters, we will plot the dependence of the magnetic field induction *B* for a semiconductor with a heterostructure *CdS/Si(p)*, taking into account the value of the maximum bias voltage V_{SS}^{max} obtained by equation (6) (Figure 2).

2.2. Simulation effect of a strong magnetic field on the temperature dependence of the density of surface states in semiconductor heterostructures.

The low-frequency capacitance-voltage characteristics of a sharp pn junction diode can be described for a heterostructure semiconductor *CdS/Si(p)*. Then the low-frequency capacitance-voltage of the heterostructure is calculated using the following expression [1]

$$C_{\text{lf}} = \frac{dq_{\text{lf}}}{dV} = S\sqrt{\frac{\varepsilon\varepsilon_0 q\left(N_a + N_t\right)}{2\left(V_d - V - \Delta V_d\right)}}, \tag{7}$$

Here, q_{1f} is the ionic charge determines the low-frequency *CV* characteristics; N_a is the concentration of acceptor impurity; N_t is electron concentration at deep levels; V_d is contact potential difference; ΔV_d is the amount of reduction in the contact potential difference *CdS/Si(p)* due to the influence of deep levels. Then $V_d - \Delta V_d = \Phi$. In equation (7), the value of V will vary from 0 to V_{SS}^{max}.

Then, if we integrate (7) over V in the interval from 0 to V_{SS}^{max} and $V_{SS}^{max}\left(B,T\right)$ considering q_{lf} can be defined as follows

$$q_l f = q_{SS} = \int_0^{V_{SS}^{\max}(B,T)} C_{lf}(V)dV, \tag{8}$$

$$q_{SS} = \int_0^{V_{SS}^{max}(B,T)} S\sqrt{\frac{\varepsilon\varepsilon_0 q\left(N_a + N_t\right)}{2\left(\Phi - V\right)}}dV,$$

In addition, the amount of ionized charge on the surface depends on the acceptor concentration and the concentration of deep levels. This is calculated as follows.

$$q_{SS} = q\left(N_a + N_t\right)\delta S, \tag{9}$$

Where δ is the part of the space charge region in which recharging of deep level.

from figure 1. δ is defined as

$$W - \delta = \sqrt{\frac{\varepsilon\varepsilon_0 q\left(E_t - E_{F_p}\right)_W}{q^2 N_a}}, \tag{10}$$

In this case, the dependence of W on V has the following form [1]

$$W\left(V\right) = \frac{\varepsilon\varepsilon_0 S}{C\left(V\right)}, \tag{11}$$

Using (10) and (11), we find δ

$$\delta = \frac{\varepsilon\varepsilon_0 S}{C\left(V\right)} - \sqrt{\frac{\varepsilon\varepsilon_0 q\left(E_t - E_{F_p}\right)W}{q^2 N_a}}, \tag{12}$$

E_F for *Si(p)* relative to the valence band top is determined as follows [1]

$$E_{F_p} = E_V - kTln\left(\frac{N_a}{N_V}\right), \tag{13}$$

From (13) we get

$$E_{F_p} - E_V = kTln\left(\frac{N_V}{N_a}\right), \tag{14}$$

Let us connect E_t with (14)

$$E_t - E_{F_p} = E_t - E_V - kTln\left(\frac{N_V}{N_a}\right), \tag{15}$$

If we replace E_t on E_{SS} for surface states and use equation (1), we obtain

$$\left(E_{SS} - E_{F_p}\right) = q\left(\Phi - V\right) - kTln\left(\frac{N_V}{N_a}\right), \tag{16}$$

For surface states from (12), substituting (16) instead of $\left(E_t - E_{F_p}\right)$, we obtain the following expression

$$\delta_{SS} = \frac{\varepsilon\varepsilon_0 S}{C_{\text{lf}}\left(V\right)} - \sqrt{\frac{\varepsilon\varepsilon_0}{q^2 N_a}\left(q\left(\Phi - V\right) - kTln\left(\frac{N_V}{N_a}\right)\right)}, \tag{17}$$

The density of surface states N_{SS} at the heterointerface is related to the volume concentration at the deep level as follows

$$N_{SS} = N_t \delta_{SS}, \tag{18}$$

According to [1], δ_{SS} calculated based on the condition $V = V_{SS}^{max}$ and also taking into account $E_g\left(T\right) = E_g\left(0\right) - \frac{\alpha_1 T^2}{\alpha_2 + T}$, we calculate (17), then for $\delta_{SS}\left(B,T\right)$ let's get

$$\delta_{SS}(B)=\sqrt{\frac{2\varepsilon\varepsilon_0\left(E_g(T)+\hbar\frac{eB}{m_c^*}\right)}{q(N_a+N_t)}}- \tag{19}$$

$$\sqrt{\frac{\varepsilon\varepsilon_0}{q^2N_a}\left(q\left(E_g(T)+\hbar\frac{eB}{m_c^*}\right)-kTln\left(\frac{N_V}{N_a}\right)\right)},$$

Using (8), (9), (18) and (19), we find the dependence of the density of surface states on a strong magnetic field

$$N_{SS}^{(B)}=N_a\delta_{SS}^{(B)}-\frac{1}{qs}\int_0^{V_{SS}^{max}}C_{lf}(V)dV, \tag{20}$$

Thus, using (19) and (20), we determine the dependence of the density of surface states, determined by the *CV* method, on a strong magnetic field

$$N_{SS}(B)=$$

$$N_a\left(\sqrt{\frac{2\varepsilon\varepsilon_0}{q(N_a+N_t)}\left(E_g(T)+\hbar\frac{eB}{m_c^*}\right)}-\sqrt{\frac{2\varepsilon\varepsilon_0}{qN_a}\left(E_g(T)+\hbar\frac{eB}{m_c^*}\right)-kTln\left(\frac{N_V}{N_a}\right)}\right)- \tag{21}$$

$$-\sqrt{\frac{2\varepsilon\varepsilon_0(N_a+N_t)}{q}}*$$

$$\left(\sqrt{\Phi-\left(E_g(T)+\hbar\frac{eB}{m_c^*}\right)}-\sqrt{\Phi}\right),$$

If in this expression $B\to 0$, then the value of the density of surface states returns to the expression presented in [1]. This proves that our proposed mathematical model is correct from a theoretical point of view.

In the proposed mathematical model, $N_{SS}(B)$ cannot fully explain the temperature dependence of the densities of surface states according to equation (21). Because at low temperatures $N_{SS}(B)$ according to (21) practically does not change. That is, the value of α_1 is about 10^{-4} for all materials, while α_2 can only be obtained at higher temperatures, such as 100 K, according to [40]. Therefore,

$$\lim_{T\to 0}\left(E_g(0)-\frac{\alpha_1T^2}{\alpha_2+T}+\hbar\frac{eB}{m_c^*}\right)=E_g(0)+\hbar\frac{eB}{m_c^*}, \tag{22}$$

In addition, member $kTln\left(\frac{N_V}{N_a}\right)$ in equation (21), also has virtually no effect on the dynamics $N_{SS}(B)$ of the temperature dependence. To determine the temperature dependence of the density of surface states, the probability of thermal generation of charge carriers in deep energy levels (zones close to the center of the band gap) is used.

It is known that the probability of the time of release of surface states depends on the temperature and the nature of the center of the band gap. The probability of releasing the energy level E_{SS} at deep levels is determined by the equation [24,25,41]:

$$\rho(E_{SS})=1-exp\left(\frac{t}{\tau(E_{SS})}\right), \tag{23}$$

Here , $\tau(E_{SS})$ - electron release time from 0 to E_{SS} in deep energy levels . Of course, as the E_{SS} value increases, this will take longer. According to [42,43] (E_{SS}), the function strongly depends on E_{SS} and kT

$$\tau(E_{SS},T,t)=\tau_0exp\left(\frac{E_{SS}}{kT}\right), \tag{24}$$

Here, $\tau_0=\gamma_nN_C$ is a constant coefficient.

From (23) and (24) we determine $\rho(E_{SS},T,t)$

$$\rho(E_{SS},T,t)=1-exp\left(-\frac{t}{\tau_0}exp\left(\frac{E_{SS}}{kT}\right)\right), \tag{25}$$

(25) expresses the dependence of the probability of discharge of energy levels E_{SS} of charge carriers in the surface state on temperature.

It is known from the scientific literature that the dependence of the number of surface states on time is determined by the following expression [24,25]

$$N(t)=\int_{E_v}^{E_c}N_{SS}\rho(E_{SS},T,t)dE, \tag{26}$$

In expression (26), the value of N_{SS} is a quantity independent of energy, equal to the density of surface states calculated by the *CV* method in [1]. In addition, the $N_{SS}(B)$ we propose also returns to the N_{SS} specified in [1] when $B\to 0$. In this case, if we substitute (21) into (26) and consider it as an integral over the energy of surface states over a constant period of time (t=const), the number of surface states is determined as follows

$$N(E,B.T)=\int_{E_v}^{E_c}N_{SS}(B)\rho(E_{SS},T)dE_{SS}, \tag{27}$$

The product of the number of surface states $N(E,B)$ and the energy E_{SS} is called the energy density of surface states. In it, as a result of differentiation (27) by $E_{SS,}$ expression (27) will look like this

$$N_{SS}(E_{SS},B,T)=\frac{dN(E_{SS},B,T)}{dE_{SS}}$$

or

$$N_{SS}(E_{SS},B.T)=\sum_{N_L=0}^{N_i}N_{SSi}(B)\frac{d\rho(E_{SS},T)}{dE_{SS}}, \tag{28}$$

N_L – number of Landau levels

Equation (28) expresses the influence of a strong magnetic field on the temperature dependence of the density of energy surface states.

3. Discussion and results. Processing of experimental results

Now, based on the proposed model, the density of surface states under the influence of external factors can be applied to semiconductor structures.

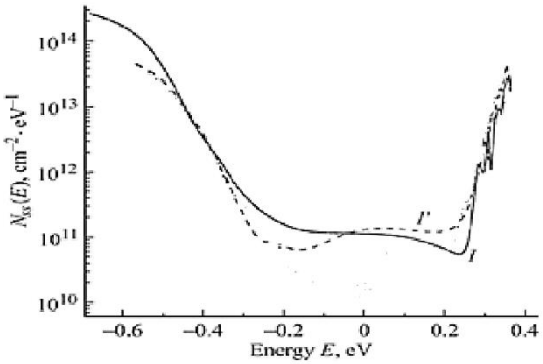
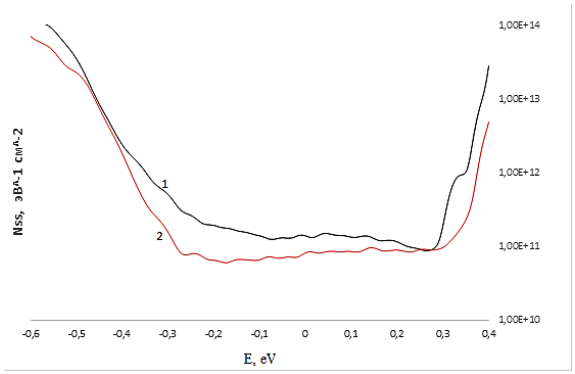


Figure 3. The influence of a magnetic field on the density of surface states in Bi-Si-Al structures (based on Si). 1- B=0 Tl, 1`- B =0.17 Tl, T=300 K [44].

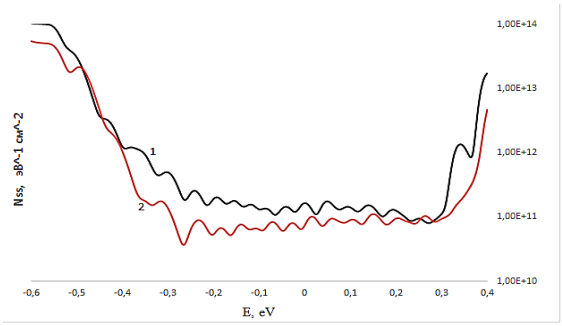


1- ***B =0 T, T =300 K,*** 2- ***B =0 .17 T, T =300 K***

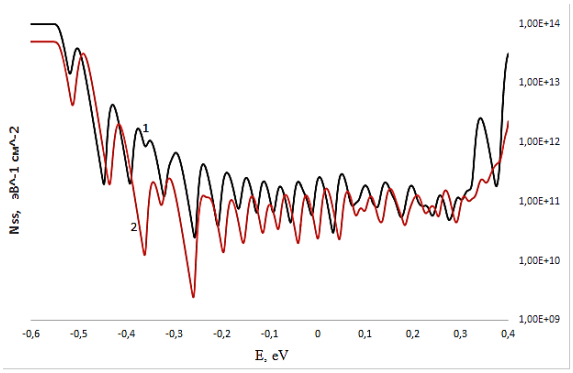
Figure 4. Modeling the influence of a magnetic field on the density of surface states in Bi-Si-Al structures (based on Si) at room temperature. Calculated using equation (28).

In particular, in [44-47], experimental results were obtained for the dependence of the influence of the density of surface states in metal-oxide-semiconductor structures on radiation and magnetic fields. That is, in [44], the effect of a magnetic field on the density of surface states of the Bi-Si-Al semiconductor structure at room temperature was determined (figure 3). In figure 3 shows graphs of N_{SS}(E) versus E, with magnetic fields B=0 and B=0.17 Tl. As can be seen from this figure, the experiment observed a displacement along the OY axis (N_{SS} axis) when exposed to a magnetic field. However, a mechanism to explain the reasons for the results of this experiment has not been developed.

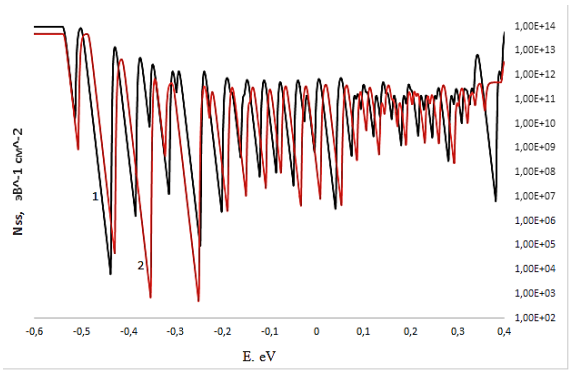
However, the mathematical model we proposed (equation 28) allows us to interpret the results of the experiment. For example, applying the physical parameters given in [44] to equation (28). That is, for the Bi-Si-Al structure (Si surface) $E_g(0) = 1.12eV$, B=0.17 Tl, T=300 K, Φ=0.11V. In figure 4 shows $N_{SS}(B,T)$, obtained by equation (28), depending on various magnetic fields. Comparing the graphs of experiment (figure 3) and theory (figure 4), we can say that the results are close to each other qualitatively, of course, when certain laws are fulfilled.



a) 1- ***B =0 T, T =200 K,*** 2- ***B =0 .17 T, T =200 K***



b) 1- ***B=0 T, T=50 K,*** 2- ***B=0 .17 T, T=50 K***



c) 1- ***B=0 T, T=10 K,*** 2- ***B=0 .17 T, T=10 K***

Figure 5. Modeling the temperature dependence of the density of surface states in the Bi-Si-Al structure (based on Si) under the influence of a magnetic field. Calculated using equation (28).

a) 1- B=0 T, T=200 K, 2- B=0 .17 T, T=200 K
b) 1- B=0 T, T=50 K, 2- B=0 .17 T, T=50 K
c) 1- B=0 T , T=10 K, 2- B=0 .17 T, T=10 K

Another advantage of the proposed model is that using equation (28) it is possible to calculate the experimental results at low temperatures and strong magnetic fields. In figure 5 shows the dependence $N_{SS}(E,B,T)$ on T for magnetic field induction values B=0 and B=0.17 Tl . As the temperature decreases, the continuous energy spectrum splits into discrete Landau levels.

4. Conclusions

The following conclusions were made during the study:

- For the first time, the dependence of the density of surface states on temperature and magnetic field for semiconductor heterostructural materials was theoretically explained.
- A new analytical expression is proposed for calculating the influence of a magnetic field on the density of surface states at the semiconductor-insulator interface.
- A mathematical model has been developed that determines the influence of a strong magnetic field on the temperature dependence of the density of surface states in semiconductor heterostructures.
- Based on the proposed model, the division of continuous energy spectra measured at room temperature and under the influence of a strong magnetic field into discrete levels at low temperatures is explained.

A physical mechanism has been developed for the shift of discrete energy levels into the band gap at different magnetic field values.

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