European Journal of Molecular & Clinical Medicine
ISSN 2515-8260 Volume 08, Issue 01, 2021

Temperature change in the density of states and band gap of a semiconductor

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Abstract: ***In this work, the temperature dependence of the density of states is investigated using a mathematical model. The temperature broadening of the allowed bands in semiconductors is estimated. A convenient formula for calculating the temperature dependence of the bandgap of silicon is obtained using the approximation. Comparison of the experimental curve of the temperature dependence of the band gap and the curve according to the obtained formula for silicon showed agreement.***

Key words: band gap, thermodynamic density of states, mathematical model, energy band model, temperature dependence.

1. INTRODUCTION

When simulating the electrical properties of MIS structures and devices based on them, it is assumed that the dopant is uniformly distributed. However, this approximation is not always correct, since the redistribution of impurity atoms is possible as a result of various energy effects on semiconductor structures during their formation. In addition, the localized states can be affected by the thermal broadening of the allowed bands, which are estimated at room temperature. Thus, taking into account the well-known distribution law of electrically active impurities when calculating the density of surface states is an urgent problem and will make it possible to predict the parameters and characteristics of semiconductor devices based on MIS structures. A certain spectrum of the density of surface states carries information about the energy location of the impurity level in the band gap of the semiconductor. The concentration information is blurred due to the merging of the tail of the broadening of the energy levels of the allowed bands and the temperature broadening of the localized levels.
By modeling the temperature dependence of the density of surface states for a wide energy range, which includes the allowed and forbidden bands of a semiconductor, it becomes possible to obtain more accurate information about the nature of localized states at the semiconductor - insulator interface in MIS structures.

2. LITERATURE REVIEW

The resulting model [1] describing the process of ionization from the energy level E_0 in time t, all electrons with energy above E_1 the rest of the electrons with energies below E_1 remain in

their places. The model is a step function. In work [2,3] $\tau(E)$ as determining the lifetime of an electron, which strongly depends on the energy E is presented in the form

$$\tau(E) = \tau_0 \exp\left(\frac{E}{\kappa T}\right) \quad (1)$$

Here: τ_0 electron lifetime, *k*- Boltzmann constant, *T*- absolute temperature.

As a result, from (1.22) and (2.1) the following expression was obtained:

$$\rho(t,E,T) = 1 - \exp\left[-\exp\left(\frac{kT\ln\left(\frac{t}{\tau_0}\right) - E}{kT}\right)\right] \quad (2)$$

Let's denote the new variable E_0.

$$E_0(t,T) = kT\ln\left(\frac{t}{\tau_0}\right) \quad (3)$$

(3) represents the energy of an electron, which electrons with energies greater than E_0 ionized. In this expression, we note the peculiarity that E_0 depend on temperature and generation time. If we consider time as an ideal parameter, then for each value of the T-temperature it will be possible to choose the time t so that we consider the parameter E_0 as a separate parameter, independent of temperature. In other words, we can consider (3) as

$$E_0 = kT\ln\left(\frac{t}{\tau_0}\right) \quad (4)$$

Now formula (2) can be represented as [2]

$$\rho(E_0,E,T) = 1 - \exp\left[-\exp\left(\frac{E_0 - E}{kT}\right)\right] \quad (5)$$

Where E_0 - electron energy independent of temperature, which electrons with energies greater than E_0 ionized, *E*- electron energy, which energy levels are greater than E_0 filled (Fig. 1), *k*-Boltzmann constant, *T*- absolute temperature.

The derivative of the step function with respect to the argument gives the delta function. Derivative of function (6) with respect to energy E_0

$$\delta^*(E_0,E,T) = \frac{\partial\rho(E_0,E,T)}{\partial E_0} = \frac{1}{kT}\exp\left(\frac{1}{kT}(E-E_0) - \exp\left(\frac{1}{kT}(E-E_0)\right)\right) \quad (6)$$

(6) is a delta function for $T \to 0$ [2,3,5] and determines the presence of a level from which an electron with energy can be ionized E_0 or the presence of a level with energy *E* at which an electron can be ionized.

3. METHODS

The temperature dependence of the density of states for a wide energy range, which includes the allowed and forbidden bands of the semiconductor, were discussed in works. In the calculations, we used a mathematical model of the temperature dependence of the density of states in the following form [1-6]:

$$Ns_{\upsilon}(E_0,T)=2\cdot N_{0\upsilon}\cdot\int_{-\infty}^{E_{\upsilon}}(E_{\upsilon}-E)^{\frac{1}{2}}\delta(E_0,E,T)dE+2\cdot N_{0c}\cdot\int_{E_c}^{\infty}(E-E_c)^{\frac{1}{2}}\delta(E_0,E,T)dE \quad (7)$$

where $\delta(E_0,E,T)$ (6), $N_{0c}=4\pi\left(\frac{2m_n^*}{h^2}\right)^{\frac{3}{2}}$, $N_{0\upsilon}=4\pi\left(\frac{2m_p^*}{h^2}\right)^{\frac{3}{2}}$

since (6) is a delta function for $T\to 0$ and is obtained from the electron generation model using the Shockley – Readd statistics, by differentiating the expression (2) [1].

Formula (7) makes it possible to calculate the temperature broadening of the permissive zones of the pro-conductor. Therefore, we can write an equation to calculate the bandgap for different temperatures.

$$\begin{cases}Ns_v(E_{0v},T)=N_{0v}\\ Ns_c(E_{0c},T)=N_{0c}\end{cases} \quad (8)$$

where $N_{0v}=2\left(\frac{2\pi m_p kT}{h^2}\right)^{3/2}$ $N_{0c}=2\left(\frac{2\pi m_n kT}{h^2}\right)^{3/2}$

Let $Eg_0=E_c-E_v$, initial band gap of the material. For simplicity, we will assume that

$$E_{0v}=Eg_0-E_{0c} \quad (9)$$

That is, the broadening of the valence and conduction bands are the same. Then, to calculate the temperature dependence of the band gap, we will use the following expression:

$$Eg(T)=Eg_0-2E_{0v}(T) \quad (10)$$

It is enough for us to solve the equation

$$Ns_{\upsilon}(E_{0v},T)=N_{0v} \quad (11)$$

Equation (11) is integral transcendental and difficult for analytical calculation. For convenience, we will use an approximation. To begin with, in (6) the exponential function in the exponent to the second power and we obtain

$$\delta^*(E_0,E,T)=\frac{e^{-1}}{kT}\exp\left(-\left(\frac{E-E_0}{\sqrt{2}kT}\right)^2\right) \quad (12)$$

By subsequent approximation, we obtain:

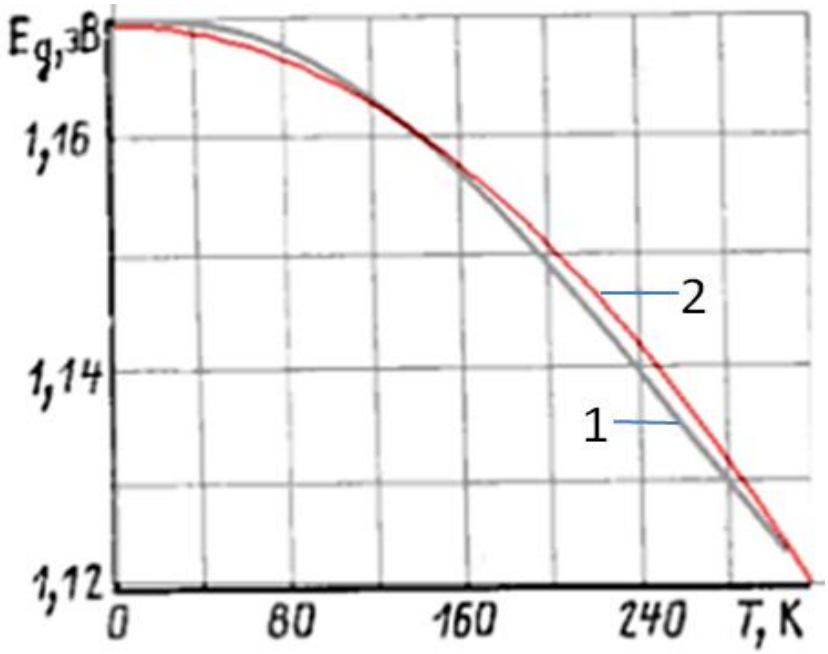
$$\delta_g(E_0,E,T)=\frac{e^{-1}}{kT}\left(1+\left(\frac{E-E_0}{\sqrt{2}kT}\right)^2\right)^{-1} \quad (13)$$

Using (13) in place of (6), we can calculate the integral by the analytical method. And the equation becomes solved by the analytical method. After calculations, we get the following expression in place (10):

$$Eg(T)=Eg_0-2\left(\frac{4\pi^2q^{-2}(kT)^2}{(kT+1)^2}-\frac{(kT+1)^2}{8e^{-1}\pi^2q^{-2}}\right) \quad (14)$$

For example, the temperature dependence of the band gap was studied in [7, 8]. Figure 1 compares model (10) and the experimental spectrum of the temperature dependence of the band gap of silicon from [5].

It can be seen from the figure that the model and experimental data are in agreement. The insignificant deviation is explained by the simplified condition (6). In fact, the broadening of the valence band and the conduction band are different.



line 1-experiment [13], line 2-model (10)

Fig. 1. The temperature dependence of the bandgap of silicon from [8] and the model (10).

4. DISCUSSION

The temperature dependence of the density of states can be used to study the temperature dependence of the semiconductor band gap $E_g(T)$. the density of surface states of a semiconductor, including the conduction and valence bands, The density of states in the bands is constant, and in the forbidden band in the energy range $E \in [E_v, E_c]$ no energy levels At low temperatures, the density of states has a clear boundary and a band gap $E_g = 1.1эВ$ for silicon. An increase in temperature changes $Ns(E,T)$ at $T = 300K$. The edges of the bands are blurred and there is no sharp transition from the allowed to the forbidden bands. In this case, due to the expansion of function (6) with increasing temperature, the edges of the expanded zones are shifted into the depth of the forbidden zone. As a result, the band gap E_g decreases with increasing temperature.

With an increase in temperature in the range of 10 ÷ 300K, the band gap E_g decreases from 1.1 eV to 1.0 eV. the experimental decrease in the band gap is approximately described by the following expression $E_g(T) = E_g(0) - \beta T$ (15)

The numerical value of β for various semiconductors varies in the range $4\cdot10^{-4}$-$5\cdot10^{-4}$ eV/K. Let us estimate the numerical value of the coefficient β using the results of the following formula

$$\beta = \frac{E_g(T_0) - E_g(T_1)}{T_1 - T_0} \qquad (16)$$

and for different temperature ranges for silicon

$T_0=50\ K, \quad T_1=500\ K, \quad \beta_{500}=3.9837\cdot10^4$

$T_0=50\ K, \quad T_1=300\ K, \quad \beta_{300}=3.980\cdot10^4$

Which agrees with the tabulated data for silicon $\beta_{Si}=4.\ 0\cdot10^4$

5. CONCLUSION

The band gap in semiconductors is sensitive to various external influences (deformation, pressure, temperature). the spectrum of the density of states strongly depends on temperature. This is due to the thermal broadening of energy states in the semiconductor band gap. Using the research results [1-5], one can study the effect of the thermal dependence of the band gap in semiconductors.

Temperature dependence of the band gap using the developed mathematical model. Temperature dependence of the density of states $Ns(E,T)$ can be used to study the temperature dependence of the semiconductor band gap $E_g(T)$.

The resulting formula (14) describes the band gap as a function of temperature. With the help of the formula, it becomes possible to dependence the band gap as a function of temperature. The model of thermal broadening of expanded zones made it possible to obtain this simple function.

The resulting model is in good agreement with classical theoretical and experimental results.

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