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# THE TEMPERATURE DEPENDENCE OF THE BAND GAP Si

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With the help of mathematical modeling of the thermal broadening of the energy levels studied the temperature dependence of the band gap semiconductors. In view of the temperature dependence of the effective mass of the density of states obtained graphs temperature dependence of the band gap. Investigated the effect of changes in the effective mass of charge carriers on the temperature dependence of the band gap semiconductors. The theoretical results of mathematical modeling are compared with experimental data for Si. The theoretical results satisfactorily explain the experimental results for Si.
**Keywords**: band gap, the effective density of states, the energy spectrum, the numerical simulation and experiment.

**О ТЕМПЕРАТУРНОЙ ЗАВИСИМОСТИ ШИРИНЫ ЗАПРЕЩЕННОЙ ЗОНЫ Si**

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С помощью математического моделирования процесса термического уширения энергетических уровней исследована температурная зависимость ширины запрещенной зоны полупроводников. С учетом температурной зависимости эффективной массы плотности состояний получены графики температурной зависимости ширины запрещенной зоны. Исследовано влияние изменения эффективной массы носителей зарядов на температурную зависимость ширины запрещенной зоны в полупроводниках. Теоретические результаты математического моделирования сравниваются с экспериментальными данными для Si. Результаты теории удовлетворительно объясняют экспериментальные результаты для Si.
**Ключевые слова:** ширина запрещенной зоны, эффективная масса плотности состояний, энергетический спектр, численный эксперимент и моделирование.

**ПРО ТЕМПЕРАТУРНУ ЗАЛЕЖНІСТЬ ШИРИНИ ЗАБОРОНЕНОЇ ЗОНИ Si**

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За допомогою математичного моделювання процесу термічного розширення енергетичних рівнів досліджена температурна залежність ширини забороненої зони напівпровідників. З урахуванням температурної залежності ефективної маси густини станів отримані графіки температурної залежності ширини забороненої зони. Досліджено вплив змінювання ефективної маси носіїв зарядів на температурну залежність ширини забороненої зони в напівпровідниках. Теоретичні результати математичного моделювання порівнюються з експериментальними даними для Si. Результати теорії задовільно пояснюють експериментальні результати для Si.
**Ключові слова:** ширина забороненої зони, ефективна маса густини станів, енергетичний спектр, чисельний експеримент і моделювання.

## INTRODUCTION

In [1 – 5] the temperature dependence of the density of states determined by relaxation spectroscopy of energy levels in semiconductors. It is shown that the surface state density is temperature dependent. The technique of determining the density of surface states. It is shown that due to the thermal broadening of the levels, the discrete spectrum with hanging temperature becomes a continuous energy spectrum. With the expansion of the energy spectrum of the density of states *GN* derivative function of the probability of energy required energy levels, it was shown that the magnitude of energy gap is temperature dependent. The temperature dependence of the band gap is determined by the temperature dependence of the density of the energy state of the conduction band and valence band of the semiconductor. Due to the thermal broadening of the density of states near the bottom of the conduction band and valence band is reduced band gap. In the calculation of the temperature dependence of the forbidden assumed for simplicity that the density of states in the areas of constant edge of the conduction band and valence band are sharp and have a stepped shape. In these studies it was assumed that the effective mass of the density of states does not depend on the temperature. However, as shown by experiments [6], the effective mass of the density of states depends on the temperature. These changes are effective mass changes the temperature dependence of the band-gap.

However, in the real state of the semiconductor density is a function of speed and energy band structure of the sample is determined. Moreover, the density of states is so general that it can be used even when there is no Brillouin zone and sharp boundaries of permitted and prohibited zones [7, 8].

Thus, for analysis of experimental results for comparison between theory and experiment is necessary to consider the specific form of the band structure of the semiconductor and the dependence of the effective mass of the charge carriers of the temperature.

The aim of this work is to study the temperature dependence of the band gap semiconductor with the band structure and temperature dependence of the effective mass of carriers and comparison of theory with experiment.

## THE TEMPERATURE DEPENDENCE OF THE DENSITY OF STATES

In determining the band gap values of the density of states corresponding to the energy band gap edges $E_c$ and $E_v$ denote by $N_k$ the temperature dependence of the density of states can be studied by expanding the density of states in a series of $GN(E_i, E, T)$-functions of the derivative of the ionization energy of discrete states. The expansion has the following form: [1 – 5]

$$N_s\left(E,T\right)=\sum_{i=1}^{n}N_{si}(E_i)GN\left(E_i,E,T\right). \quad (1)$$

This is derived in turn from the integral expression:

$$N\left(E_0,T\right)=\int_{E_v}^{E_c}N\left(E\right)\rho\left(E_0,E,T\right)dE \quad (2)$$

$N(E_0, T)$ – the number of electrons generated from quantum states with energy less than $E_0$, with a continuous distribution in energy levels. We apply this method of expansion for the density of states in the conduction band of the semiconductor. For a quadratic dispersion law for the density of states of the conduction band is given by [9]

$$N(E)=N_{n0}\sqrt{E-E_c}\ ,\ N_{n0}=4\pi\left(2m_n^*/h^2\right)^{3/2}. \quad (3)$$

Similarly, for the valence band

$$N(E)=N_{p0}\sqrt{E_p-E}\ ,\ N_{p0}=4\pi\left(2m_p^*/h^2\right)^{3/2}. \quad (4)$$

As in the theory of non-crystalline semiconductors [7, 8] to determine the allowed and forbidden energy bands, we use the concept of density of states. Formulation (3) and (4) into (2) we obtain a model that describes the temperature dependence of the density of states near the band edges. With this in mind, we expand $N_s(E, T)$ in a series of $GN(E_i, E, T)$-functions. In the following form:

for the conduction band:

$$N_{sn}\left(E,T\right)=\sum_{i=1}^{n}N_{n0}\sqrt{E_i-E_c}GN\left(E_i,E,T\right)\Delta E \quad \text{at } E>E_c; \quad (5)$$

for the valence band:

$$N_{sp}\left(E,T\right)=\sum_{i=1}^{n}N_{p0}\sqrt{E_p-E_i}GN\left(E_i,E,T\right)\Delta E \quad \text{at } E>E_v; \quad (6)$$

for the gap:

$$N_{ss}(E)=0 \ \text{ at } \ E_c>E>E_v,\ \ \Delta E=1/n. \quad (7)$$

The values of the density of states corresponding to the energy band gap edges $E_c$ and $E_v$ is denoted by $N_k$. Then the energy position of the edges of the gap are determined by solving the following transcendental equations

$$\sum_{i=1}^{n}N_{sn}(E_i)GN\left(E_i,E,T\right)\Delta E=N_k\,,$$

$$\sum_{i=1}^{n}N_{sp}(E_i)GN\left(E_i,E,T\right)\Delta E=N_k\,, \quad (8)$$

where $\Delta E=1/n$.

The solution of equation (8) determines the values at a given border gap $E_c(T)$ and $E_v(T)$, as a function of temperature $T$. $N_k$ parameter of the problem and is determined experimentally. Then the band gap

$E_g(T)$ at a given temperature is defined as the difference between the values of $E_c(T)$ and $E_v(T)$ (9). Here $E_c(T)$ energy of the bottom of the conduction band, $E_v(T)$ – the energy of the valence band. It follows that the method of determining the accuracy of the experiment and the important factors in determining the width of the gap. Indeed the band gap, determined by optical methods – "optical width" of the band gap can not match the value of the band gap, determined by the temperature dependence of the resistance of the semiconductor. One of the reasons is that different values for $N_k$ optical and electrical measuring techniques.

## THE TEMPERATURE DEPENDENCE OF THE BAND GAP AND TO COMPARE THEORY WITH EXPERIMENT

In [6] established that the Si effective mass density of states depends on the temperature. Fig. 1 shows the temperature dependence of the effective mass of the density of states in Si $m/m_0$ from [6]. Using the data of fig. 1 using the model calculated the change in the band gap as a function of temperature.

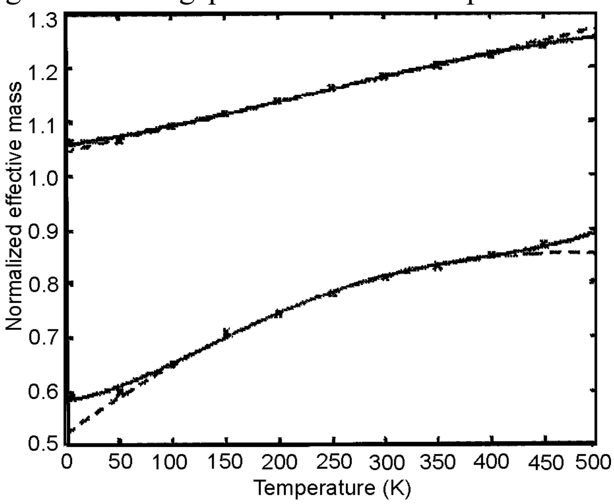


Fig. 1. The temperature dependence of the effective mass of the density of states in $m/m_0$ Si. [6]. ♦ – experiment [6]; — calculations for $m^*_n = m(T)$, $m^*_p = m(T)$; – – calculations for $m^*_n$ = const; $m^*_p$ = const.

Fig. 2 shows plots of the temperature dependence of the band gap of Si for the changes in the effective mass of the density of states taken from fig. 1 [6]. Fig. 2 shows that taking into account the temperature dependence of the effective mass significantly affect the results of the calculations.

Fig. 2 shows the results of the broken linear calculations and taking into account the temperature dependence of the electron effective mass. The same figure shows the theoretical linear continuous

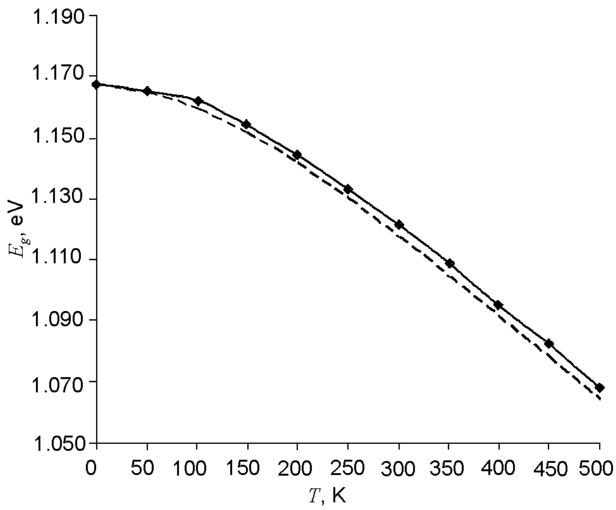


Fig. 2. Schedule - the temperature dependence of the band gap for Si. ♦ – experiment [6]; –– calculations for $m^*_n = m(T)$, $m^*_p = m(T)$; – – calculations for $m^*_n$ = const; $m^*_p$ = const.

temperature dependence of the band gap, taking into account the change in the effective mass of the electron and hole in the temperature range (0 K – 500 K). Experimental results for silicon taken from [6] are represented by dots. As can be seen from fig. 2 records the temperature dependence of the effective mass of electrons and holes are properly explain the temperature dependence of the band gap of silicon in the given temperature range. Thus, changes in the effective mass of the density of states with temperature can greatly affect the temperature dependence of the bandgap.

## CONCLUSION

In this temperature range (0 K; 500 K) mathematical modeling of the temperature dependence of the band gap is satisfactorily described by a parabolic dispersion law. Experimental results of changing bandgap silicon [6] within the precision of the measurements with the theoretical calculations. Comparison of theory and experiment shows that the thermal broadening of the energy levels described by a *GN*-function satisfactorily describes the process of the temperature dependence of the band gap in Si. The temperature dependence of the energy spectrum of the density of states of semiconductors, taking into account the temperature dependence of the effective mass of the density of states. The temperature dependence of the band gap for the changes in the effective mass of the density of states. With the help of numerical experiments show that at temperatures $T > 50$ K change in the effective mass of the density of states with increasing *T* a significant effect on the temperature dependence of the band gap.

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