

Temperature Dependence of the Density of States and the Change in the Band Gap in Semiconductors

Nosir Sharibayev, Jasurbek Mirzayev



Abstract: The temperature dependence of the density of energy states in semiconductors has been studied. Strong doping with impurities with deep levels broadens the conduction band and the valence band. This enhances the absorption of light below the red border. Consequently, a possible change in the width of the forbidden zone. In this paper, using the mathematical model, temperature dependence of the density spectrum of states, changes in the band gap are shown by analyzing the density spectrum of energy states, an explanation of the anomalous temperature dependence in acceleration semiconductors is proposed, the effects of doping with a high concentration on the band gap of the semiconductor are investigated. Explained absorption in the range of 0.6-0.9 eV for silicon.

Keywords: density of states, energy gaps, doping, impurity, forbidden semiconductor zone, control of energy bands, accelerated semiconductor.

I. INTRODUCTION

The introduction of impurities into the crystal lattice at low concentrations does not change the band gap of the semiconductor and does not affect the energy spectrum of the electrons. Only appear discrete levels in the forbidden zone. When the concentration of impurities becomes large enough, the energy spectrum and the band gap of the crystal change. [1]

In heavily doped semiconductors, the interaction of charge carriers with impurity atoms plays a special role. The absorption of light with a frequency of lower threshold $\omega = Eg/h$ naturally associated with the presence of the tail of the density of states in the forbidden zone. The total concentration of the levels on the tails varies from substance to substance and from sample to sample and often turn out to be quite large up to $10^{19}-10^{20} \text{ cm}^{-3}$.

The values of light absorption coefficient at $h\omega < Eg$ depends on the degree of doping. Mainly, the deepest levels on the density of values state hosts can participate here. $\alpha(\omega)$ at $\omega < Eg/h$ may be small. The observed values of the absorption coefficient is the result of some averaging over the coordinates of impurity atoms (the totality of these coordinates is referred to as impurity concentration). Because of the random distribution, the concentration of impurities in different parts of the sample is different. When the measurement is performed, averaging over configurations is performed [2].

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With weak doping, the electron interacts with a single impurity atom. The interaction energy is the same for all electrons. With strong doping, the potential energy of an electron depends on the positions of several impurities at once. Energy carriers become random variables. With a further increase in the concentration of impurities, the overlap of the wave functions of electrons localized on various impurity atoms becomes noticeable and the impurity level is blurred into the band. This effect is referred to as quantum level broadening. [3]. These broadening of discrete levels lead to a decrease in the band gap.

II. MATERIALS AND METHODS

The purpose of this work is to study the thermal dependence of the band gap of a semiconductor doped with high concentration of impurities.

a. Model of the temperature dependence of the density spectrum of states.

Thermal broadening of the energy levels in the allowed zones and in the band gap of the crystal also leads to temperature changes in the width of the energy gaps. At low temperatures, thermal blurring of energy levels is weak and the gap between the levels changes differently depending on temperature. The expansion or contraction of the band gap depends on many factors. One of the main factors determining the width of the energy gap is the critical value of the concentration of energy states. When critical concentration N_k is equal to the density of energy states $N_s = N_k$, region of energy with less concentration than N_k , $N_s(E) < N_k$ defines the area of forbidden states. And vice versa, when the area is energized with greater concentration than N_k , $N_s(E) > N_k$ energy of allowed states. Conditions $N_s(E) = N_k$ determines the edge of the forbidden zone, the bottom of the conduction band E_c , and the valence band ceiling E_v . With this approach, the temperature dependence of the forbidden zone is determined by the temperature dependence of the density of states.

A mathematical model of the density spectrum of states was constructed in [4,5, 6]. With the help of which, the temperature dependence of discrete energy levels in the forbidden zone of silicon was analyzed. Consider this model for this problem. Expand the density spectrum of energy states, $N_s(E_0, T)$ by $GN(E_0, E_i, T)$.

$$N_s(E_0, T) = \sum_{i=1}^n N_{s_i}(E_i)GN(E_0, E_i, T) \quad (1)$$



where:

$$GN(E_0, E_i, T) = \frac{1}{kT} \exp\left(\frac{1}{kT}(E_i - E_0) - \exp\left(\frac{1}{kT}(E_i - E_0)\right)\right) \quad (2)$$

$GN(E_0, E_i, T)$ - derivative of the probability of ionization of electrons from the energy level in energy and determines the presence of the energy state.

E_1 - can run through the entire valence, the forbidden band and the conduction band. N_s - concentration of energy states appropriate for energy E_i , E_0 - energy of states available, T-temperature. k is the Boltzmann constant.

Depending on the behavior of the function $N_s(E_0, T)$ and critical concentration values N_k The temperature dependence of the energy gaps can be different (Fig. 1). At concentration N_{k0} the band gap is weakly dependent on temperature. In particular, at a concentration below some

N_{k0} with increasing temperature, the band gap should decrease. The maximum value of the width of the forbidden zone has at $T \rightarrow 0$. In most semiconductors, the band gap decreases with increasing temperature. This corresponds to the cases $N_k < N_{k0}$.

III. DISCUSSION

At high critical concentrations $N_k > N_{k0}$ with increasing temperature, the band gap increases. Most semiconductors $N_k < N_{k0}$, critical concentration less N_{k0} for example, Si, Ge, GaAs, etc. However, in some semiconductors, for example, PbS, PbTe, and others. lead holcogenides increase in the band gap with increasing temperature, i.e. critical concentration is large enough $N_k > N_{k0}$. Therefore, with increasing temperature, the width of the forbidden zone increases.

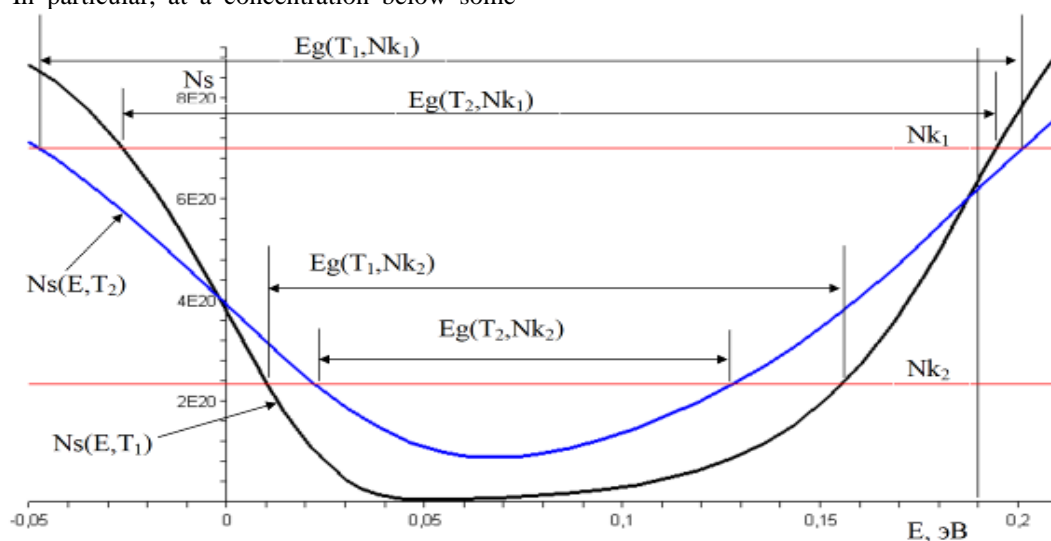


Fig.1. The spectrum of the density of energy states of acceleration semiconductors constructed according to the mathematical model (1) . N_{k1}, N_{k2} -critical concentration. $T_1 < T_2$ temperature.

Increases or decreases in the band gap with increasing temperature can be explained by thermal expansion. It is necessary to compare the thermal expansion of a crystal with the thermal broadening of discrete states in quantum wells (square points). Here, the coefficient of thermal expansion determines the temperature dependence of the width of the forbidden zone. Lead Holcogenides $l = l_0(1 + \gamma T)$ γ - the value is negative $E = E_0 + \alpha T$ α - positively.

Thus, the temperature dependence of the width of the energy gaps can be explained by thermal broadening of the states of the conduction band and the valence band and of states in the band gap of a semiconductor.

a. Comparison with experiment

In the work [7], monochromatic light is absorbed at frequencies below the threshold. The strong doping of silicon with the red boundary for photon energy decreased from 1.2 eV. up to 0.6 eV. Consequently, doping with impurities by deep levels broadens the conduction band and the valence band. This enhances the absorption of light below the red border.

An increase in absorption in the frequency range below the red boundary indicates a decrease in the width of the

forbidden band. However, the absorption coefficient in the region of 0.6 eV-0.9 eV, approximately $\alpha \sim 1-10 \text{ cm}^{-1}$ and by 3-4 orders of magnitude less than in the region of the intrinsic absorption of pure silicon. As can be seen from Figure 2 at the same time. If we assume that the absorption coefficients are proportional to the density of states (combined density of states), then the density of states in the former forbidden band is 104 orders of magnitude lower than the density of states of the conduction band and the valence band ($10^{22}-10^{20}$).

IV. RESULTS

In the new zone in the range of values $Eg < 0.9 \text{ eV}$ $N_s = 10^{18}-10^{19}$ ($0.4 < Eg < 0.9 \text{ eV}$). These values of the density of states gives the absorption coefficients $\alpha \sim 1-10 \text{ cm}^{-2}$. Thus, with the help of doping you can control the width of the forbidden zone and the absorption coefficient. On fig.2.a. The density of states of the magnitude was determined from measurements of the absorption coefficient [7]. On fig.2.b. The variant of energy dependence in eV is shown. The graph marks the total number of concentration levels.



Using the derivative of the number of concentration levels of the energy density of states of Fig.2.c. in energy from the graphical relation, we obtained the graph

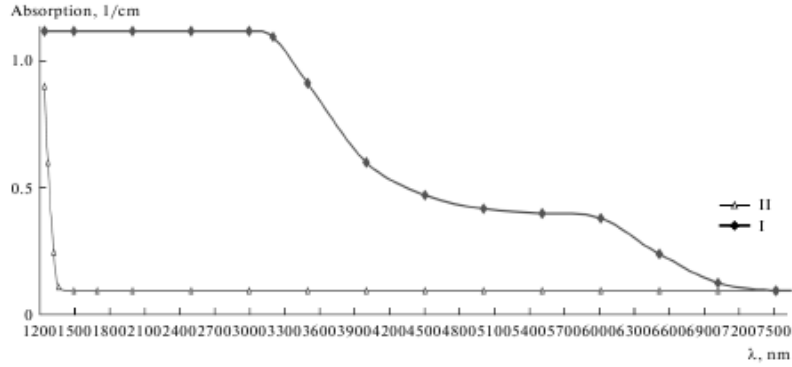


Рис. 2. а)

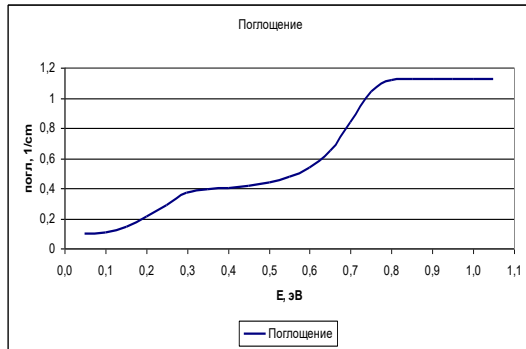


Fig. 2. b)

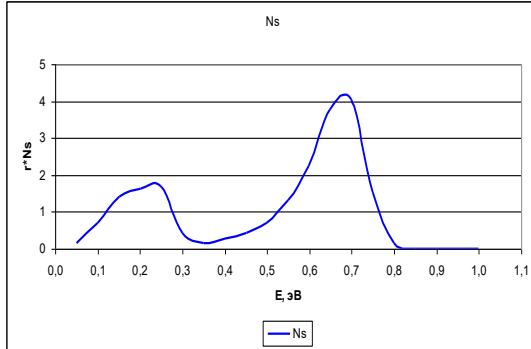


Fig. 2. c)

Fig.2. Graph of light absorption of doped silicon from [7].
a) relative to the wavelength, b) relative to the wave energy in eV.
c) The density of states obtained by calculating the energy derivative of the graph

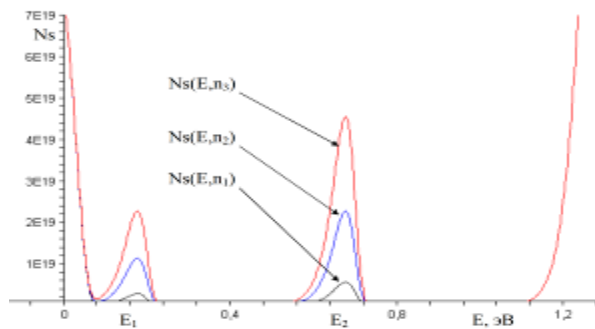


fig. 3. a)

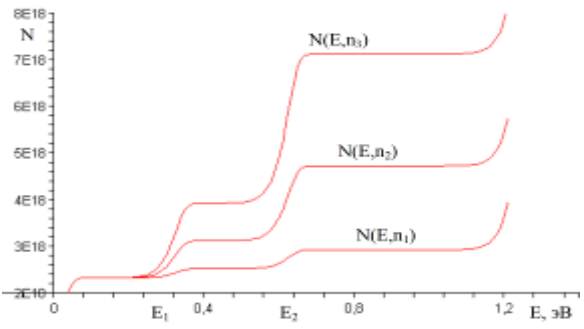


fig. 3. b)

Fig.3. a) The density of states obtained by the model. $n_1 < n_2 < n_3$ -degree of doping.
b) the total number of states calculated by the model. $n_1 < n_2 < n_3$ -degree of doping.

Using the above model (1) we construct the density spectrum of states for doped silicon taking into account the experimental conditions, $T = 300$ K, $E_g = 1.21$ e.V. It can be seen from the figure that a high concentration of impurities provides sufficient large amounts of levels determined by clusters formed by impurity levels.

The levels in the forbidden zone are created by the random distribution of impurities. The absorption coefficient α is proportional to the total number of states. It is possible that the formation of clusters is more suitable for explaining the absorption coefficient of heavily doped semiconductors with deep levels. In Figure 3.b. shows the integral density of states (the total number of states) calculated by the model.

It should be noted that the obtained graph of the total number of states using the model in Fig. 3.b and the experimental graph of the total number of states in Fig. 2.b are comparable.

V. CONCLUSION

With a sufficiently large amount of impurity concentration, discrete levels form an impurity zone. With increasing temperature, the lattice vibrations increase. This leads to new configurations of the arrangement of atoms in the crystal lattice with different deviations. Changes in the configuration of atoms in the lattice leads to changes in the energy states of the electrons.

Changes in energy states occur randomly, in proportion to the appearance of a corresponding configuration of impurity atoms and a lattice. This leads to different energy levels. For each configuration of atoms, its own energy of impurity states and its edge of the conduction band and the edges of the valence band correspond.



Given this circumstance, it can be concluded that the concentration of energy states in the vicinity of the allowed zones is unpredictable. The presence of energy states in the vicinity of the resolved zones in higher concentrations with the merging of the temperature broadening of the allowed zones leads to the effect of a change in the material forbidden zone. The absorption in the range of 0.5–0.9 eV for silicon is due to impurity states in the band gap. Impurity states can greatly reduce the band gap of a semiconductor.

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