ENERGY SPECTRA OF STRONGLY LIGERIZED SEMICONDUCTORS AND SEMICONDUCTOR COMPOUNDS

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Abstract*. In this work, the temperature dependence of discrete energy states in the silicon band gap was analyzed using a mathematical model of the band gap width of semiconductors depending on the alloying level and the density of states spectrum.*

Keywords*: mathematical model, discrete states, spectrum, semiconductor compounds, temperature, concentration.*

Adding a small number of inputs to the semiconductor crystal lattice does not change the width of the band gap and does not affect the energy spectrum of electrons. Discrete cases appear only in the forbidden zone. If the amount of input is large enough, the energy spectra and band gap of the crystal will change. In strongly ligated semiconductors, the interaction of charge carriers with access atoms is of great importance. Absorption of light with a frequency lower than the cutoff is undoubtedly due to the presence of a tail of the density of states in the forbidden zone. The concentration of full states in the tail of the density of states varies depending on the material and the sample, and often their number is quite large, up to 1019-1020 cm-3. In weak ligation, the electron interacts with one atom of the input. The impact energy is the same for all electrons. In strong ligation, the potential energy of an electron depends on the location of several entrances at once. The energy of charge carriers remains a random quantity. The case of further increasing the concentration of impurities is that the electrons localized in different atoms of the impurity overlap the wave functions, and the impurity state spreads over the zone. This effect is referred to as the quantum expansion of the state. The expansion of these discrete states leads to a narrowing of the forbidden zone. One of the main factors determining energy gaps is the critical value of the concentration of energy states. If the critical concentration Nk is equal to the density of energy states Ns=Nk, then the energy field with a concentration smaller than Nk determines the field of forbidden states. And vice versa, if the energy field with a concentration greater than Nk determines the field of non-forbidden states. $Ns(E) = Nk$ condition defines the band gap boundary, the conduction band bottom Ec and the valence band ceiling Ec. In this case, the temperature dependence of the forbidden zone is determined by the temperature dependence of the density of states. Using the mathematical model of the spectrum of the density of states, the temperature dependence of the discrete energy states in the forbidden zone of silicon was analyzed. We apply this model to the given problem. If we assume that the absorption coefficient is proportional to the density of states, then the density of states in the former forbidden zone is 104 times lower than the density of states in the conduction and valence zones (1022-1020). A new zone in the region Ns=1018-1019 is Eg<0.9 (0.4<Eg<0.9 eV). This value of the density of states gives an absorption coefficient of a~1-10 cm-2. Thus, the band gap and absorption coefficient can be controlled by ligation. Using the above model, T=300 K, Eg=1.21 e.V. We construct the spectrum of the density of states for ligated silicon, taking into account the balls of the experiment (Fig. 1).

As can be seen from the figure, a large concentration of inputs gives a sufficiently large number of states defined by the clusters created by the input states. The states in the forbidden zone are created by a random distribution of the inputs. The absorption coefficient α is proportional to the full number of states. The formation of clusters can better explain the absorption coefficient of strongly ligated semiconductors with deep levels. Figure 2 shows the density of integral states (number of full states) calculated using the model. It should be noted that the graph of the full number of cases obtained by the model is in Figure 2 and the graph of the full number of experimental cases is sufficiently close.

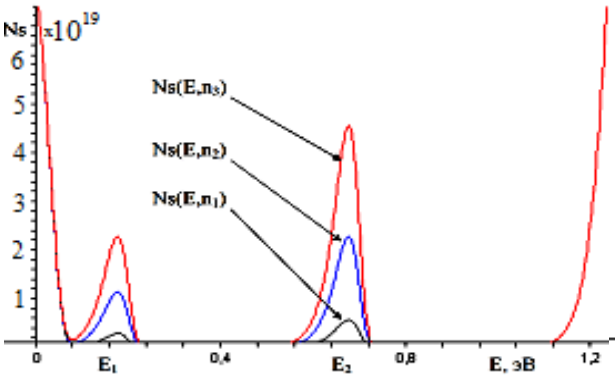


Figure 1. density of states model, level of n1<n2<n3

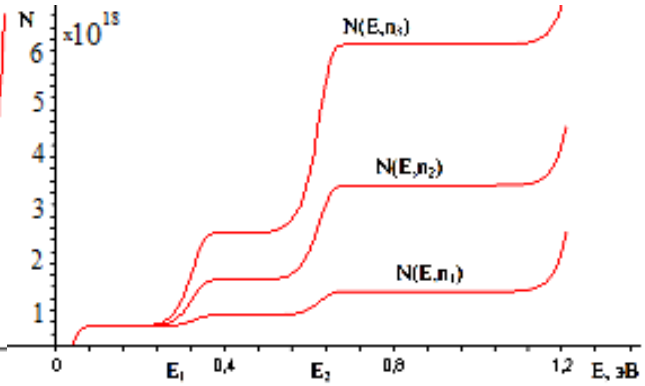


Figure 2. the total number of legalization. cases calculated using the model, degree of legibility n1<n2<n3

Taking into account these cases, it can be concluded that the absorption in the range of 0.5-0.9 eV for silicon is determined by the state of entrances in the forbidden zone. Impedance states can significantly reduce the bandgap of a semiconductor.

For the study of semiconductor compounds, a temperature dependence spectrum model of energy states was built, taking into account the concentration in the mixture. This model was implemented by adding additional terms to the previously used model.

$$Ns(E_0,T) = 2\cdot N_\upsilon \cdot \int_{-\infty}^{E_\upsilon} (E_\upsilon - E)^{\frac{1}{2}} GN(E_0,E,T)dE + \\ + \sum_{i=1}^{n} N_{si} GN(E,E_0,T) + 2\cdot N_c \cdot \int_{E_c}^{\infty} (E - E_c)^{\frac{1}{2}} GN(E_0,E,T)dE \quad (1)$$

Formula (2) has the following form after appropriate changes.

$$Ns(E) = Ns_c^{Si}(E) + Ns_c^{Ge}(E) + Ns_s^{Si}(E) + Ns_s^{Ge}(E) + Ns_\upsilon^{Si}(E) + Ns_\upsilon^{Ge}(E) \quad (2)$$

In this: E_υ^{Ge} and E_υ^{Si} on the relative energetic axis for 0, E_g^{Si} – *Si* forbidden zone width, E_g^{Ge} – *Ge* the width of the forbidden zone. $Ns_\upsilon^{Si}(E)$- *Si*, $Ns_\upsilon^{Ge}(E)$- *Ge* density of states for the valence band:

$$Ns_\upsilon^{Si}(E) = x\cdot \sum_{i=1}^{n} N_\upsilon^{Si} \cdot \sqrt{0-E_i} \cdot GN(E_i,E,T)\ E_i = -\frac{1}{n}, E \le 0 \ (3)$$

$$Ns_\upsilon^{Ge}(E) = (1-x)\cdot \sum_{i=1}^{n} N_\upsilon^{Ge} \cdot \sqrt{0-E_i} \cdot GN(E_i,E,T)\ E_i = -\frac{1}{n}, E \le 0 \ (4)$$

$Ns_c^{Si}(E)$- *Si*, $Ns_c^{Ge}(E)$- *Ge*:

$$Ns_c^{Si}(E) = x \cdot \sum_{i=1}^{n} N_c^{Si} \cdot \sqrt{E_i - E_g^{Si}} \cdot GN(E_i, E, T)\, E_i = \frac{1}{n}, E \geq E_g^{Si} \quad (5)$$

$$Ns_c^{Ge}(E) = (1-x) \cdot \sum_{i=1}^{n} N_c^{Ge} \cdot \sqrt{E_i - E_g^{Ge}} \cdot GN(E_i, E, T)\, E_i = \frac{1}{n}, E \geq E_g^{Ge} \quad (6)$$

$Ns_s^{Si}(E)$- *Si*, $Ns_s^{Ge}(E)$- *Ge* density of states for the forbidden zone:

$$Ns_s^{Si}(E) = \sum_{i=1}^{n} Ns_i^{Si} \cdot GN(E_i, E, T)\; E_i = \frac{1}{n}, 0 \leq E \leq E_g^{Si} \quad (7)$$

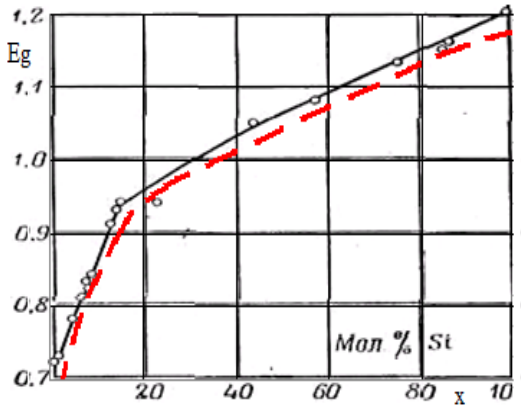
$$Ns_s^{Ge}(E) = \sum_{i=1}^{n} Ns_i^{Ge} \cdot GN(E_i, E, T)\, E_i = \frac{1}{n}, 0 \leq E \leq E_g^{Ge} \quad (8)$$

In this $$GN(E_i, E, T) = \frac{1}{kT} \exp\left[\frac{E - E_i}{kT} - \exp\left(\frac{E - E_i}{kT}\right)\right] \quad (9)$$

Ei can take values in the valence, forbidden, and conduction bands. Nsi is the concentration of energy states, E-state energy, T-temperature, respectively, for Ei energies. k - Boltzmann's constant.

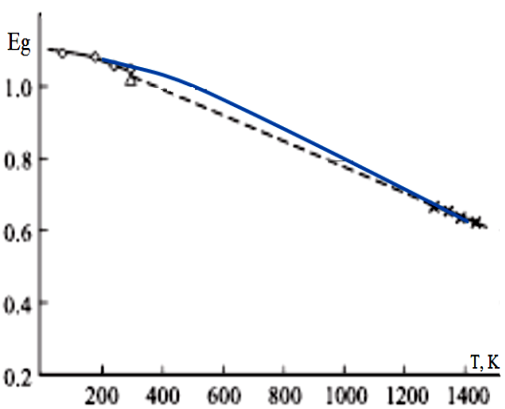
With the help of this model, theoretical and experimental results are compared, the spectrum of the density of states and the width of the forbidden zone for Si_XGe_{1-X} as a function of concentration (Fig. 3). and $Si_{0.15}Ge_{0.85}$ forbidden band width is studied as a function of temperature (Fig. 4).

Graphs comparing theoretical and experimental results are presented in figures 3 and 4. In conclusion, the created model can open the door of wide possibilities in the study of energy spectra of Si_xGe_{1-x} mixture.



—— experiment, – – model

Figure 3. Si_xGe_{1-x} a graph of the link to the forbidden zone and the concentration



o Δ x –experiment, ─ model

Figure 4. $Si_{0.15}Ge_{0.85}$ graph of the binding of the forbidden zone to the temperature

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