CALCULATION OF SILICON BAND GAP BY MEANS OF FERMI-DIRAC INTEGRALS

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Summary. The article by mathematical simulation using quantum statistics and Fermi-Dirac integrals investigated narrowing band gap of silicon. As well as its dependence on the temperature and carrier density effects on the change in the carrier density in the conduction band. Particular attention is paid to the determination of the equilibrium concentration of charge carriers in the conduction band and the influence of the narrowing of the band gap on it. The narrowing values of the band gap, calculated using the theoretical model, are compared with the experimental results.

1 INTRODUCTION

The wide use of silicon in numerous technological applications, such as the creation of nanoparticles and nanostructures [1,2], metamaterials [3], the modification of the surface of semiconductors by laser pulses, which has aroused special interest in bio- [4] and IT-technologies [5,6] causes interest in the properties of this semiconductor. Studies of the melting mechanisms of semiconductors and the properties of high-density electron-hole plasma remain topical. Numerous experiments [7-12] have shown that in the process of melting in silicon, covalent bonds are destroyed, with a change in the short-range order, accompanied by a sharp increase in the concentration of conduction electrons and leading to the transition of silicon to the metallic state. However, the role and influence of one of the most important fundamental characteristics of silicon of the band gap on the processes associated with the phase transition and in the region of higher temperatures have remained uncovered both experimentally and theoretically.

The notion of a band gap arose within the framework of quantum theory [13-18] in connection with the need to explain the differences in the physical properties of metals and semiconductors in solid state physics. The most important property of both metals and semiconductors is electrical conductivity and its characteristic - carrier concentration. In determining the carrier concentration necessary to describe all the properties of semiconductors, the width (energy) of the band gap E_g is of great importance, since it is the most important characteristic of the energy structure of semiconductors. For use in mathematical modeling, the band gap should be represented in the form of a temperature dependence $E_g(T)$ (or baric $E_g(P)$). In accordance with the concepts of quantum theory, when a crystal is formed from individual atoms, the interatomic distances decrease, and due to the action of the Pauli principle, allowed bands arise in which electrons can be located. The allowed bands are characterized by the density of electronic states. The most "deep" allowed bands, i.e. energy bands formed by the electrons of the deep-lying shells are the same for all substances. The uppermost of them - the valence band E_v in semiconductors is completely

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filled with electrons at zero absolute temperature (T=0 °K). The next allowed zone behind it is not filled with electrons at the same temperature. This band is called the conduction band E_c. The allowed bands of a crystal are separated by band gaps, the density of electronic states in which is zero. The band gap largely determines the nature of the chemical bond in the material. To characterize the filling of electronic bands we introduce the concept of Fermi energy (level) E_F, which separates on the energy scale the filled electronic states of the crystal from free ones at zero absolute temperature. Depending on the position of the Fermi level the allowed bands of the crystal can be filled completely or partially by electrons, or remain unfilled. The location of the Fermi level E_F with respect to the edges of these zones determines the electronic nature and physical properties of the crystal. Indeed, the valence electrons of the crystal in the filled bands are bound and do not participate in the conductivity. Electrons can participate in electronic conduction, becoming free, only if they are in an unfilled zone [16]. Accordingly, substances in which the valence band is partially filled, or the conduction band and the valence band overlap, are metals. Substances in which the valence and conduction bands do not overlap at zero absolute temperature (T=0 °K) are semiconductors or dielectrics [15, 16, 17, 18]. Semiconductors and dielectrics differ in the value of E_g. Conditionally, dielectrics include substances with a band gap E_g>2-3 eV (1 eV= 1.6021×10-12 Erg = 1.6021 × 10-19 J), to semiconductors with a bandgap E_g <2-3 eV. Wide-band (1.0 eV <Eg <2-3 eV) and narrow-gap (Eg <0.1 - 0.2 eV) semiconductors are distinguished by the width of band gap. Substances with Eg≈0 are attributed to gapless semiconductors, substances with $E_g \leq 0$ (band overlap) to semimetals, the Fermi level in these substances is located deep in the conduction bands or in the valence band [13, 16, 17, 18].

For semiconductors, including silicon, were carried out experiments to determine the width of the band gap [19-24], which for Si was determined in the temperature range from 4.2 °K to 800 °K. Experimental studies have shown that the narrowing of the band gap depends not only on temperature [19-22], but also on carrier concentration [23-24]. However, a number of limitations of the experimental approach do not make it possible to obtain the necessary characteristics in the melting temperature range and, therefore, theoretical studies are required to determine the band gap and the carrier concentration over a wide temperature range.

In this paper, mathematical modeling will be used - a recognized tool for theoretical studies of problems accompanying the use of silicon in numerous technological applications [25-30]. In the conditions of temperature increase, the band gap $E_g(T)$ narrows, the carrier concentration reaches high values of $N(T) \approx 10^{18}$ cm^{-3} and higher, which is confirmed by experimental studies [7-12], the electron gas degenerates, the values of $Eg(T)$, $EF(T)$, $N(T)$ become interdependent, the classical Maxwell-Boltzmann statistics becomes unjust, which greatly complicates the calculation of all quantities. To solve this problem, the use of Fermi-Dirac quantum statistics becomes fundamental. Therefore, the basis of mathematical modeling is the use of quantum statistics and Fermi-Dirac integrals (F-D) to take into account the degeneracy of the electron gas.

This article is devoted to the study of the behavior of the band gap with increasing temperature and carrier concentration and its role in processes associated with a phase transition in the region of the equilibrium melting temperature of silicon and higher temperatures. Particular attention is paid to the determination of the equilibrium concentration of charge carriers in the conduction band and the impact on it of narrowing the band gap. We consider silicon with intrinsic conductivity under conditions of thermodynamic equilibrium and electroneutrality in the temperature range 300 °K <T <1.5×Tm.

2 QUANTUM APPROACH

In the mathematical modeling of the band gap of silicon, using the statistics of electron gas, the central place is occupied by the law of the distribution of charge carriers over energy states.

In semiconductors, unlike metals, the number of charge carriers and their mobility depend on temperature, defects and the presence of impurities. Under thermodynamic equilibrium conditions at a temperature $T=T_{lat}=T_e$ (T_{lat} is the lattice temperature, T_e is the electron temperature), the probability of the electron filling the state with energy E is determined by the Fermi-Dirac distribution law using the Fermi level E_F

$$f(\mathrm{E},\mathrm{T}) = \frac{1}{\left(1+\exp\left(\frac{E-E_F}{k_B T}\right)\right)} \tag{1}$$

where k_B - Boltzmann constant. At low temperatures, the valence band of the semiconductor is completely occupied and, according to the Pauli principle, charge carriers cannot move inside the valence band. In connection with this, at low temperatures in semiconductors the concentration of conduction electrons is so small that they behave like a gas of noninteracting particles, the Fermi energy exceeds the electron energy $(E-E_F)<0$ and the electron gas is nondegenerate. In this case (1) reduces to the Maxwell-Boltzmann distribution function

$$f(\mathrm{E},\mathrm{T}) = \exp\left(\frac{E_F-E}{k_B T_e}\right) \tag{2}$$

To move free carriers from the valence band to unoccupied conduction band, an additional finite energy is required and it exceeds the energy of the band gap, which for silicon E_g=1.17 eV for at T = 0 °K [13]. With increasing temperature, hot electrons give off energy to the lattice, while the width of band gap decreases, and the concentration of free charge carriers in the conduction band increases, determined by the processes of generation and recombination of electrons from the conduction band and holes from the valence band, which occur continuously and in parallel, the electron gas degenerates and $(E-E_F)> 0$. In a state of thermodynamic equilibrium, these opposite processes must coincide in speed, both in the whole and in each region of the spectrum. Such a detailed equilibrium exists when the phonon energy is converted into the energy of electrons and back and in any other process of energy transformation that can occur in a solid. From the principle of detailed balance it follows that there is a unique electron energy distribution characterized by a single Fermi level E_F for a material of a given composition at a given temperature T.

As we can see, the distribution function has the necessary minimum information for describing the processes taking place inside a solid body with an acceptable accuracy.

By integrating the distribution function of the carriers (1), one can obtain many characteristics of the electron gas. Therefore, in determining the properties of silicon in an arbitrary degeneracy range from the classical Boltzmann limit to the degenerate Fermi-Dirac, including the weak degeneracy range ($E\sim E_F$), a large role is played by the Fermi-Dirac integrals

$$\mathcal{F}_j(\eta_c) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\varepsilon^j}{1+exp(\varepsilon-\eta_c)} d\varepsilon \tag{3}$$

where $\Gamma(x)$ is the gamma function, j is the index of the Fermi-Dirac integral, c=e for electrons and c=h for holes, ε is the reduced electron energy (hole), the reduced Fermi level for electrons

$$\eta_e = \frac{E_F - E_C}{k_B T} \tag{4}$$

for holes

$$\eta_h = \frac{E_V - E_F}{k_B T}. \tag{5}$$

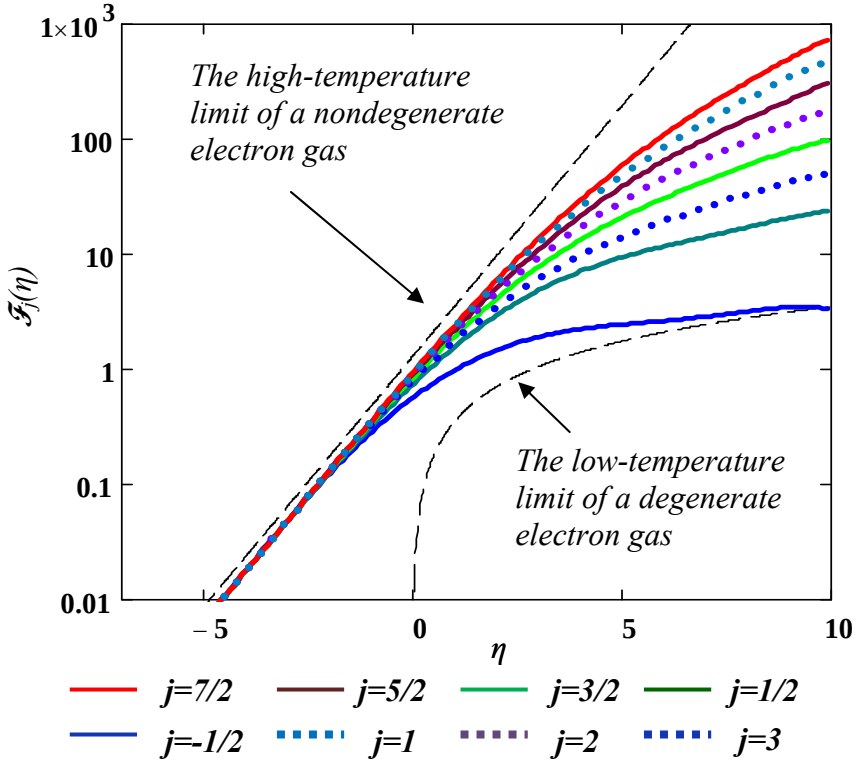

Fig. 1. Approximating functions of Fermi-Dirac integrals $\mathcal{F}_j(\eta)$ of order j.

To determine the carrier concentration and the band gap of semiconductors we use F-D integral with the index j=1/2. The integral (3) with the exception of an integral with order $j=0$, cannot be calculated analytically. This involves a variety of methods for approximate calculation and approximation of Fermi integrals [30], among them: expansion in series [31-33], numerical quadratures [33-35], recurrence relations and interpolation of tabulated values [36-38], piecewise polynomials and rational functions [39-41]. In [42,43] Fermi-Dirac integrals of orders j=-1/2, 1/2, 1, 3/2, 2, 5/2, 3 and 7/2, continuous analytic expressions that unique for each order were obtained in a wide range of degeneracy -10 ≤η≤ 10. The

approximating function of F-D integral with order j=1/2 from [42,43] will be used to calculate the properties of the electron gas of silicon.

Figure 1 shows the dependences of the Fermi-Dirac function of integers j and half-integral *j/2* orders, for different values of η. The dotted lines in the figure show the high-temperature limit for the nondegenerate ($\eta<0$) and low-temperature limit for the degenerate ($\eta>0$) electron gas. It is seen that the use of approximating functions makes it possible to carry out a smooth, continuous transition from the domain of nondegeneracy to the degeneracy region, which is very important for obtaining smooth functional dependences of the properties of the electron gas of silicon.

3 CALCULATION OF THE BAND GAP OF SILICON

The band gap of silicon E_g, like other semiconductors, depends on external parameters such as temperature, pressure, electric, magnetic, gravitational fields, and others [13-18]. With increasing temperature and an increase in the concentration of charge carriers, the energy of band gap tends to decrease [12, 13, 19-24].

Narrowing of the band gap for wide-gap semiconductors was studied by optical methods and by photoluminescence spectroscopy. The experimental data give an idea of narrowing of the band gap in the range of carrier concentrations from 4×10^8 -10^{20} cm^{-3} and temperatures of 20-300 K [19, 23-24]. In [10], it was suggested that the width of the forbidden band at the melting temperature T_m abruptly becomes zero.

In this paper, it is of interest to investigate the influence of the band gap of silicon on processes associated with the phase transition and in the region of higher temperatures. It is known that upon melting silicon acquires metallic properties, so the width of the forbidden band in the vicinity of the melting temperature should become close to or equal to zero. These arguments form the basis of our assumption about the observance at the equilibrium melting temperature of the condition

$$E_g(T_m)\approx 0, \text{ при } T_m = 1687°\text{K} \qquad (6)$$

Let us consider the basic mechanisms that affect the temperature dependence of the width of the band gap.

The first mechanism is associated with the expansion of the lattice when the temperature rises causing displacement of position relatively the conduction band and the valence band. The second mechanism is associated with the enhancement of electron-lattice interaction with an increase in temperature [44-50]. In low-temperature region these effects make a significant contribution to the change in the energy of the band gap. The temperature dependence of the width of the band gap at low temperature is nonlinear. In high-temperature region according to estimates made in Ref. [48], the contribution of these mechanisms is approximately 20-25% of total change in the energy of the band gap and temperature dependence is linear

$$T << \theta, \quad \Delta E_g \infty T^2; \quad T >> \theta, \quad \Delta E_g \infty T \quad , \qquad (7)$$

where θ is the Debye temperature (for Si θ = 640 °K).

At present, empirical and semiempirical dependences are used to describe the temperature changes in the band gap E_g (T) [44-51]. They usually use linear coefficients (for example, temperature coefficient [48] - $\alpha_T = -\frac{\partial E_g}{\partial T}$ and baric [56] - $\alpha_P \approx -\frac{\partial E_g}{\partial P}$, here T and P are the

absolute temperature and hydrostatic pressure). The most common is the Varshni approximation [48], which describes well first two mechanisms of narrowing of the band gap

$$E_g(T) = E_{g,0} - \frac{\alpha T^2}{T+\beta} \tag{8}$$

where $E_{g,0}$ is the band gap at 0 °K, α and β are constants that have been evaluated experimentally and for silicon are: α=7.021×10-4 eV/T, β=1108K. The constant β is comparable with the Debye temperature with a coefficient ≈2.5 for silicon [48]. At high temperatures T>>β, it follows from (8), that $\alpha \approx -\frac{\partial E_g}{\partial T}$, so it is temperature coefficient of the width of band gap.

The third mechanism of narrowing of band gap is related to the effects of collective interactions and operates at sufficiently high carrier concentrations and degeneracy of the electron gas. The most significant contribution to narrowing the width of the band gap is due to the exchange interaction which leads to an empirical dependence of the form $\Delta E_g \sim \gamma \times N(T)^{1/3}$, where γ is a parameter that has the behavior of a fitting to this experiment. In [51-55], the parameter γ is defined in the range $1\times10^{-8} \div 7.3\times10^{-8}$ eV×cm.

Thermal and quantum mechanisms are taken into account in the relation of [26], which represents the modification of (8)

$$E_g(T,N) = E_{g,0} - \frac{\alpha T^2}{T+\beta} - \gamma \cdot N^{1/3}(T) \tag{9}$$

where α, β are the constants that coincide with the corresponding constants from (8), the constant γ=1.5×10^{-8} eV×cm, $N(T)$ is the concentration of charge carriers in the conduction band, and T is the temperature. In this paper, two values of the fitting parameter γ were chosen. The first - $\gamma = 8.35\times10^{-8}$ eV×cm - was chosen from the condition that the width of the band gap should be zero at equilibrium melting point $E_g(T_m)=0$. The second value - γ=4.2×10^{-8} eV×cm was chosen as a half of first one.

4 CARRIER CONCENTRATION AND FERMI LEVEL

In metals the carrier concentration is constant and can be characterized by a definite value of the electrochemical potential (Fermi energy), the value of which can be obtained from the experimental data [17]. In semimetals which have a band gap $E_g \leq 0$, the Fermi level is located in conduction band or in valence band, and the carrier concentration is about 10^{18}-10^{20} cm^{-3}, several orders of magnitude lower than typical for metals of 1022 cm-3. With increasing temperature, the number of carriers in semimetals increases, and the electrical conductivity increases [18].

In semiconductors, unlike metals, the carrier concentration and their mobility depends on the temperature and on the presence of defects and impurities. For any semiconductor, the most important characteristic is the concentration of electrons N_e in the conduction band or holes N_h in the valence band. For an intrinsic semiconductor that does not contain impurities, the equality of the concentrations $N_e=N_h$ is observed.

The temperature dependences of the carrier concentrations in the conduction band and holes in the valence band are determined by integrating the distribution function of the carriers (1)

$$N_e(T) = N_C \mathcal{F}_{1/2}(\eta_e) \tag{10}$$

$$N_h(T) = N_V \mathcal{F}_{1/2}(\eta_h) \tag{11}$$

where $\mathcal{F}_{1/2}(\eta_e), \mathcal{F}_{1/2}(\eta_h)$ - the Fermi-Dirac integrals (3) of order j=1/2 for electrons and holes, η_e and η_h are the reduced Fermi energy $E_F(T)$ for electrons (4) and holes (5), N_C and N_V are the density of states in the conduction band and valence band

$$N_C = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2}, \; N_V = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} \tag{12}$$

where $m_e = M^{2/3}\left(m_l \cdot m_t^2\right)^{1/3}$ - the effective mass of the density of states of electrons in the conduction band, taking into account the contribution from the total set of ellipsoids M - the number of equivalent energy minima in the conduction band (for silicon M=6) [14, 18], m_l, m_t are respectively longitudinal and transverse masses, m_h is the effective mass of the density of states of holes in the valence band.

Since in thermodynamic equilibrium the probability of filling all electronic states with any energy can be expressed using a single normalization parameter-the Fermi level E_F, then the temperature dependence of $E_F(T)$ is necessary to determine the carrier concentration and other properties of silicon. The position of the Fermi level is determined from the condition of electroneutrality.

Taking into account (10) and (11), the electroneutrality condition takes the form

$$N_C \cdot \mathcal{F}_{1/2}(\eta_e) = N_V \cdot \mathcal{F}_{1/2}(\eta_h) \tag{13}$$

Equation (13) is greatly simplified when approximating expressions are used for integrals $\mathcal{F}_{1/2}(\eta_e), \mathcal{F}_{1/2}(\eta_h)$ [27, 28]

$$\mathcal{F}_{1/2}(\eta_c) = \exp\left(\sum_{i=0}^{7} a_i \eta_c^i\right)_{c=e,h} \tag{14}$$

where a_i - coefficients of the polynomial [42,43]. The use of a continuous analytic expression approximating F-D integral allows us to calculate carrier concentrations and energy of the Fermi level with an arbitrary degeneracy degree of the electron gas.

Taking (14) into account, equation (13) takes the form

$$N_C \cdot exp\left(\sum_{i=0}^{7} a_i \eta_e^i\right) = N_V \cdot exp\left(\sum_{i=0}^{7} a_i \eta_h^i\right) \tag{15}$$

Formulated equations (9) - (15) represent a mathematical description of the interrelated variables $E_F(T)$, $N(T)$, $E_g(T,N)$ that vary with temperature, the derivation of which in this paper was carried out from a numerical solution of equations using a computational procedure consisting of 2 nested iteration cycles. At one step in temperature $[T_i, T_{i+1}]$, the sequence of

calculations looks like this. In the inner cycle, the energy of the Fermi level $E_F(T_{i+1})$ is determined from the condition of electroneutrality (15) of the intrinsic semiconductor using the iterative Newton method [57]. In the outer cycle, taking into account the new value $E_F(T_{i+1})$, the values are determined by the simple iteration method. The procedure is repeated until complete convergence.

The results of the calculations are shown in Figures 2-6.

5 MODELING RESULTS

Figure 2 shows the temperature dependences of the band gap calculated for the Fermi-Dirac distribution (9) with both values of the parameter γ (curves 1, 2) and for the Maxwell-Boltzmann distribution (curve 3). In the temperature range from 300 ° K to θ, where the influence of quantum mechanisms is weak, the width of band gap is equally well approximated by all the dependences and completely coincide with the experiment [22]. Above the Debye temperature, the contribution of collective interaction mechanisms to the width of the forbidden band becomes appreciable, which is reflected in the behavior of the dependences. The width of the forbidden band, calculated with the Maxwell-Boltzmann statistics (curve 3), depends only on the temperature remains positive longer than others. The condition $E_g(T)=0$ for this dependence is satisfied at T=2400K, and at the melting point - $E_g(T_m)$=0.5 eV. The dependences calculated with Fermi-Dirac statistics (curves 1, 2), which take into account the effect of temperature and carrier concentration, narrow more strongly. For the value of parameter $\gamma=4.2\times10^{-8}$ eV×cm, $E_g(T)=0$ at T=2000 K, $E_g(T_m)$=0.248 eV. For the value of parameter $\gamma=8.35\times10^{-8}$ eV×cm, the width of band gap at temperature $T>Tm$ becomes negative.

Figure 3 gives a clear picture of the shape and velocity of the narrowing of the band gap $E_g(T,N)$ and the position of the Fermi energy level $E_F(T)$, calculated with quantum statistics, relative to the edges of the valence $E_V(T)$ and conduction $E_C(T)$ bands and intrinsic Fermi level located in the middle of the band gap. With increasing temperature the Fermi energy $E_F(T)$ deviates from its own level toward the edge of the valence band $E_V(T)$, which is determined by lower effective mass of the density of states of the valence band. For silicon, the ratio of the effective masses of the electron and hole states is m_{de}/m_{dh}=1.89. Because of this, the degeneracy of the hole gas ($\eta_h=0$) occurs earlier than the degeneracy of the electron gas ($\eta_e=0$) (Fig. 5).

Beginning with T=1000K the carrier concentration and the width of the forbidden band, calculated with quantum and classical statistics begin to differ: for Fermi-Dirac – $N(T)=1.5\times10^{18}$ cm^{-3}, for Maxwell-Boltzmann - $N(T)=9.1\times10^{17}$ cm^{-3}, $E_g(T,N)$=0.81 eV. Obtained data corresponds to appearance of a weak degeneracy, to which the values $\eta_h\approx-4$ correspond (Fig. 5).

The region of strong degeneracy arises when the curves $E_F(T)$ and $E_V(T)$ (Figure 3), which corresponds to $\eta_h=0$ and to the values T=1600K, $N(T)=1.1\times10^{20}$ cm^{-3} (Fig. 4), $E_g(T,N)$=0.083 eV for Fermi-Dirac distribution and $N_{M\text{-}B}(T)=3.8\times10^{19}$ cm^{-3} (Fig. 4), $E_g(T)$=0.48 eV for Maxwell-Boltzmann.

The same picture, with a certain shift to higher temperatures, is observed with degeneracy of the electron gas. Weak degeneracy: $\eta_e\approx-4$, T=1090K (Fig.5), $N(T)=4.5\times10^{18}$ cm^{-3}, $E_g(T,N)$=0.61 eV (Fig. 3, 4), strong degeneracy: $\eta_e\approx-0$ (Fig.5), T=1920K, $E_g(T,N)$=-0.28 eV (Fig. 3, 4).

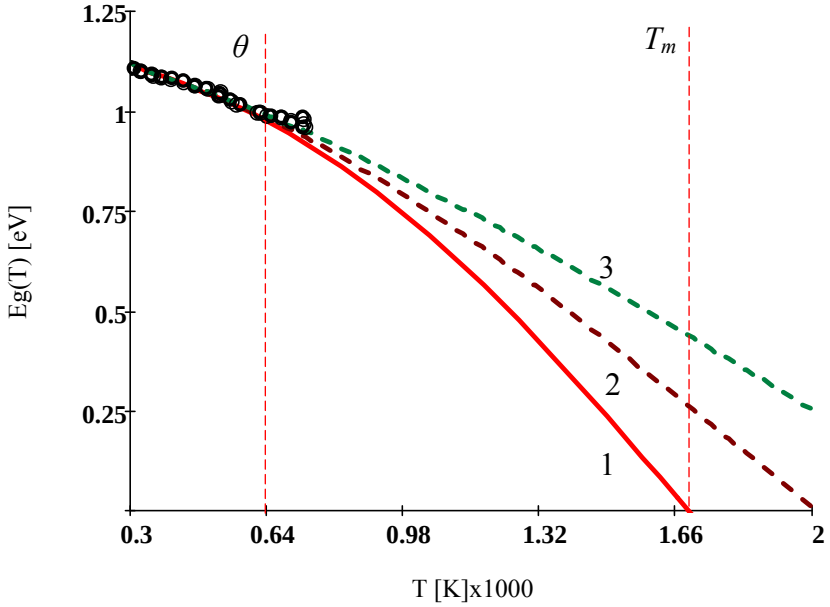

Fig. 2. Temperature dependence of the width of band gap of silicon. The calculation was carried out using: 1 - quantum statistics with $\gamma=8.35\times10^{-8}$ in (10); 2 - quantum statistics with $\gamma=4.2\times10^{-8}$ in (10); 3 - Maxwell-Boltzmann statistics and Varshni relation [48]. Experimental data are marked by unpainted circles [22].

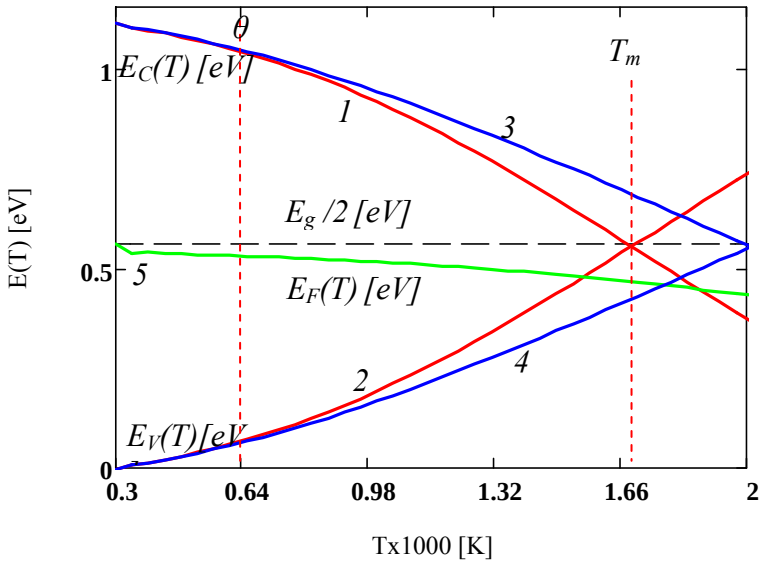

Fig. 3. Temperature dependence of edges of the conduction band $E_C(T)$ and the valence band for various degrees of narrowing of band gap: (1), (2) - $\gamma=8.35\times10^{-8}$ eV×cm, (3), (4) - $\gamma=4.2\times10^{-8}$ eV×cm; (5) is the temperature dependence of Fermi energy $E_F(T)$.

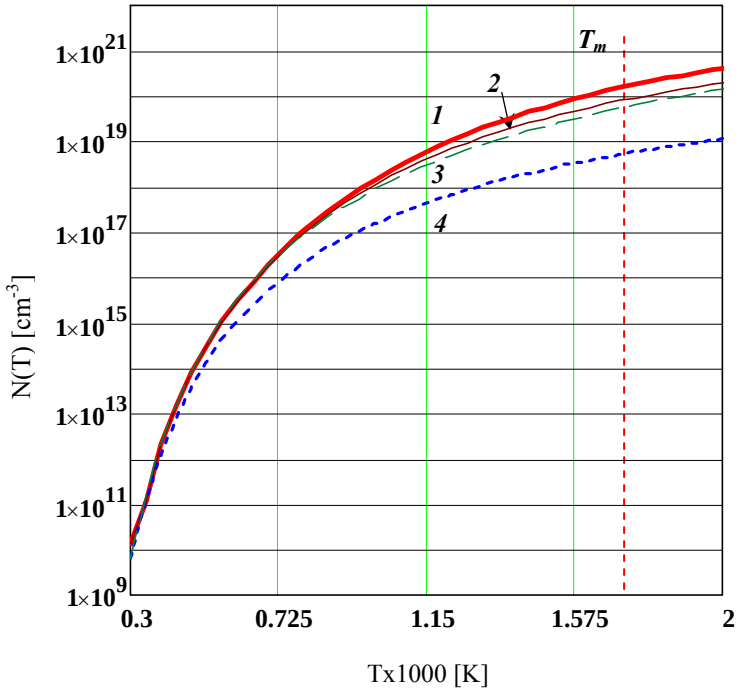

Fig. 4. The temperature dependences of the carrier concentration calculated using the Fermi-Dirac statistics (1) - γ = 8.35 × 10-8 eV × cm, (2) γ = 4.2 × 10-8 eV × cm; and Maxwell-Boltzmann (3) - the temperature dependence, (4) - the constant Eg = 1.12 eV.

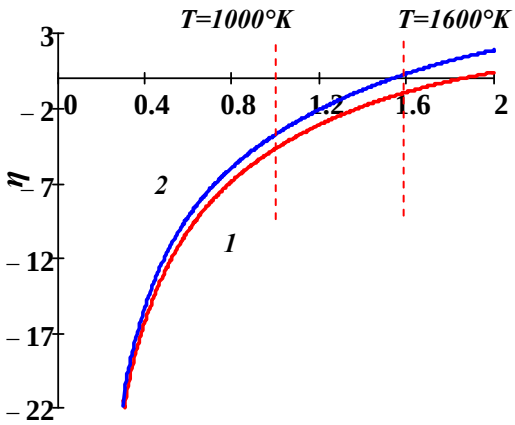

Fig. 5. Temperature dependences of the electron (1) and hole (2) reduced levels of the Fermi energy.

At the equilibrium melting temperature $T=T_m$=1687K in the variant with quantum statistics and fitting parameter $\gamma=8.35\times10^{-8}$ eV×cm the width of the forbidden band vanishes $E_g(T,N)=0$ with the carrier density $N(T)=1.7\times10^{20}$ cm^{-3}.

With further heating up to T=2000K, the width of the forbidden band becomes negative, and the carrier concentration continues to increase, (Fig. 3, 4) $N(T)=4.2\times10^{20}$ cm^{-3}, $E_g(T,N)$=-0.38 eV. With the Maxwell-Boltzmann statistics (Figure 2), the width of the forbidden band still remains positive, and the concentration is much lower than in the Fermi-Dirac statistics: $E_g(T,N)$=0.24 (Fig. 2), $N_{M\text{-}B}=1.4\times10^{20}$ cm^{-3} (Fig. 4).

As the fitting parameter decreases by a factor of 2 $\gamma=4.2\times10^{-8}$ eV×cm, the width of the forbidden band vanishes $E_g(T,N)$=0 (Fig. 3) at a temperature T=2000K with a concentration $N(T)=2.05\times10^{20}$ cm^{-3} (Fig. 4).

6 CONCLUSIONS

- Under the conditions of thermodynamic equilibrium, the degeneracy of charge carriers in silicon with intrinsic conductivity begins at a temperature which is considerably below the equilibrium melting point. This requires the use of quantum statistics and Fermi-Dirac integrals calculation technique when determining the properties of solid-state silicon.
- The width of the band gap and its variation is one of the most important fundamental characteristics of silicon, which affects substantially on the concentration of electrons and holes and, therefore, all properties and characteristics of a solid-state semiconductor.
- Concentrations of both types of carriers indicate their strong degeneracy in the temperature range T=1600÷2500K. Taking into accoun quantum effects allow one to vanish the width of the forbidden band at the point of equilibrium melting point or its vicinity. However, the concentrations are in the range $N(T)=4.2\times10^{20}\div 10^{21}$ cm^{-3}, which is typical for semimetals with a negative band gap [18], but several orders of magnitude lower than the values typical for metals $10^{22}\div 10^{23}$ cm^{-3}.
- The thermodynamic equilibrium melting of pure crystalline silicon occurs in two stages. First, the melt acquires the properties of a semimetal with growing with a temperature number of carriers, and then reaching a certain temperature T>Tm~3000K, the molten silicon acquires metallic properties with a constant concentration of electrons and holes.
- The above analysis is very important for a better understanding of the processes of nonequilibrium heating and melting of pure crystalline silicon, for example by ultrashort femtosecond laser pulses [7]. Under the condition $\hbar\omega_L > E_g(T)$, where $\hbar\omega_L$ is the energy of the quantum of laser radiation, in solid silicon due to photoeffects, the electron and hole concentrations can reached the values $N(T)\approx10^{22}$ cm^{-3} without the lattice reaching the melting temperature, but with the achievement of metal properties. In the physical literature, this phenomenon was called pre-melting or softening of the lattice up to the melting. However, these concepts are given without proper quantitative characteristics.
- The acquisition of metallic properties by a semiconductor (silicon) depends on specific situation, in particular, related to the certain mode of action, and can occur before melting, at the moment of melting or after the melting.

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