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TEMPERATURE DEPENDENCE OF THE MAIN PARAMETERS DETERMINING THE INTERBAND ABSORPTION SPECTRUM OF a-Si:H

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In this work, the temperature dependence of the interband optical absorption coefficient of hydrogenated amorphous silicon (a-Si:H) has been investigated both experimentally and theoretically. By fitting the values obtained from the optical absorption coefficient formula, the temperature dependence of the characteristic vibration energy of a-Si:H was studied using the Bose-Einstein and Varshni formulas.

Keywords: *Hydrogenated amorphous silicon; Interband optical absorption coefficient; Temperature; Characteristic vibration energy; Bose-Einstein formula; Varshni formula*
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INTRODUCTION

Currently, semiconductor materials, especially semiconductor-ferroelectric and amorphous semiconductor structures, are of great interest to researchers [1-3]. Based on theoretical and practical research on these structures, it has been possible to increase the thermal, optical, and energy efficiency of several diode structures [4-8].

Amorphous hydrogenated silicon *(a-Si:H)* has remained one of the most popular semiconductor electronics materials for many years due to its combination of low production costs, the ability to fabricate large-area devices, and a high optical absorption coefficient [9]. It is widely used in the production of thin-film solar cells, photosensitive sensors, and active matrices of liquid crystal displays [10-12]. One of the key characteristics determining the efficiency of optoelectronic devices based on *a-Si:H* is the mobility gap. The energy spectrum of amorphous materials is characterized by density-of-states "tails," making the optical properties of *a-Si:H* extremely sensitive to external influences, particularly temperature [13]. Analysis of the temperature dependence of interband absorption is crucial for predicting the performance of photovoltaic converters under real-world operating conditions, where temperature fluctuations are inevitable.

Typically, the empirical Varshni equation and the semi-empirical Bose–Einstein model, which takes into account the interaction of electrons with phonons, are used to describe the temperature dependence of the energy gap in semiconductors [14, 15]. However, the applicability of these models to amorphous structures requires a detailed comparison of theoretical calculations with experimental data over a wide temperature range. Furthermore, the proportionality coefficient in the interband absorption formula, which reflects the degree of disorder in the structure, can also be temperature-dependent, as is often observed in simplified models [16].

The aim of this work is to investigate the temperature dependence of the mobility gap width and proportionality coefficient in *a-Si:H* by fitting experimental absorption spectra to theoretical dependences. A comparative analysis of parameters obtained using the Bose-Einstein and Varshni models is also provided, clarifying the mechanisms by which thermal disorder influences the material's electronic structure.

In [13], experimentally determined values of the temperature dependence of the spectra of the interband absorption coefficient of amorphous hydrogenated silicon *a-Si:H* are presented (Fig. 1).

In the work [17] for the analytical form of the interband absorption spectrum, according to the Kubo-Greenwood formula and the Davis-Mott approximation method, the expression was obtained:

$$\alpha_2(\hbar\omega) = \frac{B}{4\hbar\omega E_g}\left[2(\hbar\omega - E_g)\sqrt{E_g\hbar\omega} - (E_g - \hbar\omega)^2 \, arctg\left(\frac{E_g - \hbar\omega}{2\sqrt{E_g\hbar\omega}}\right)\right] \tag{1}$$

where $B = N(\varepsilon_V)N(\varepsilon_C)\frac{8\pi^4 e^2\hbar^2 a}{nc(m^*)^2}\lim\limits_{\delta x \to 0}$, a is the average distance between semiconductor atoms, m^* is the effective mass of electrons in the allowed bands of *a-Si:H*, and E_g is the energy width of the mobility gap of *a-Si:H*. $N(\varepsilon_V)$ and

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$N(\varepsilon_C)$ are the effective values of the density of electron states at the boundaries of the valence band and conduction band, respectively.

RESEARCH METHODS AND RESULTS

From expression (1), it is evident that in order to calculate the interband absorption spectrum, it is necessary to determine the values of B and E_g included in it. According to the Tauc rule [15], the mobility gap energy could not be determined due to the limited number of experimental points. But these calculations showed that as the temperature increases, the mobility gap decreases. Therefore, considering B and Eg as fitting parameters, we use trial and error to fit the calculation results obtained by formula (1) to the experimental results shown in Fig. 1. To ensure consistency between the experimental and calculated results (curves in Fig. 1), the obtained values of the parameters B and E_g are presented in Table 1. The error of the experimental points and the calculation results does not exceed the permissible error of the experiment.

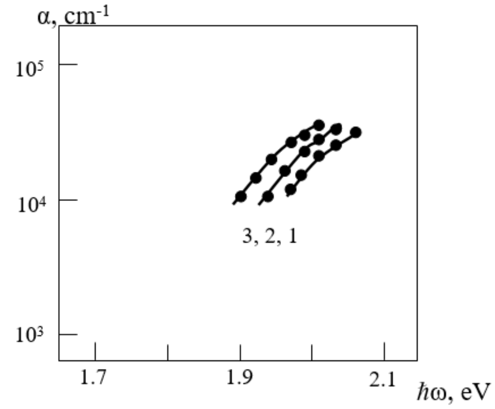

Figure 1. Experimental data from work [9]: 1 - T=12.7 K, 2 - T=151 K, 3 - T=293 K, and the results of calculations using formula (1) (solid curves). Points – experiment.

Table 1. Temperature dependence of the mobility gap width of unannealed a-Si:H and the proportionality coefficient (B) of formula (1).

No.	T	E_g, eV	B, cm^{-1}
1	12.7 K	1.861	$3.647*10^5$
2	151 K	1.841	$3.745*10^5$
3	293 K	1.793	$3.861*10^5$

In work [14], the Varshni empirical formula, which determines the dependence of the band gap of semiconductors (for amorphous semiconductors, the energy width of the mobility gap) on temperature, is presented in the following form: (Varshni's formula):

$$E_g = E_{g0} - \alpha T^2 / (T + \beta) \tag{2}$$

Here, E_{g0} is the width of the forbidden band at temperature T = 0 K, the empirical Varshni coefficients α are the temperature coefficient of the width of the mobility gap, β is a constant value.

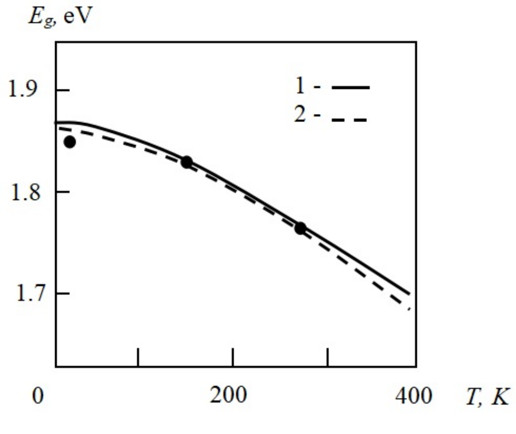

Figure 2. Dependence of the width of the mobility gap of amorphous hydrogenated silicon on temperature. Results obtained: 1 - according to the Varshni formula and 2 - according to the Bose-Einstein formula. Points - experimental data.

In work [18], the expression that determines the dependence of the band gap width of a semiconductor on temperature is presented in the following form (Bose-Einstein formula):

$$\Delta E_g(T) = 2\alpha_B / (\exp(\Theta./T) - 1) \tag{3}$$

Here, $\Delta E_g = E_{g0} - E_g$ is the change in the mobility gap width depending on temperature, $\boldsymbol{\alpha_B}$ is the temperature coefficient of the mobility band gap width, and Θ is the average phonon temperature.

In the work [19] for theoretical studies of the temperature dependence of the energy width of the mobility band of semiconductors *(MoS_2, $MjSe_2$, $MoTe_2$, WSe_2)* in the temperature range from 20 to 300 K using the Varshni (2) and Bose-Einstein (3) formulas. By fitting the experimental data to formula (2) for α and β, the average values obtained were $\alpha \approx (5.9 \cdot 10^{-4} - 4.4 \cdot 10^{-4})$ eV/K and for $\beta \approx (250 - 190)$ K.

Precisely, thus from formula (3) for α_B and Θ the values $\alpha_B \approx (6.8 \cdot 10^{-2} - 2.5 \cdot 10^{-2})$ eV and for $\Theta \approx (220\text{-}150)$ K were obtained.

In the work [20], the temperature dependence of the energy width of the mobility band of crystalline semiconductors such as (*GaAs, InP, ZnSe, Si*) was investigated using the present method. For the higher than the specified parameters, the following results were obtained for $\alpha \approx (1.02 \cdot 10^{-3} - 5.5 \cdot 10^{-4})$ eV/K and, for $\beta \approx (823\text{-}225)$ K and for $\alpha_B \approx (7.3 \cdot 10^{-2} - 5.7 \cdot 10^{-2})$ eV and for $\Theta \approx (260\text{-}240)$ K. Also, in the work [21] for InSe for these parameters, the values $\alpha \approx 4.6 \cdot 10^{-4}$ eV/K, $\beta \approx 279$ K, and for $\alpha_B \approx 2.06 \cdot 10^{-2}$ eV, $\Theta \approx 205$ K were obtained.

Calculations performed by substituting the energy mobility gap values for a-Si:H from Table 1 into formula (2) showed that at $\alpha = 4.95 \cdot 10^{-4}$ eV/K and $\beta = 438$ K, these values are in good agreement with formula (2). These results are presented in Fig. 2 (solid curve).

Calculations performed by substituting the mobility gap values from Table 1 into formula (3) showed that at $\boldsymbol{\alpha_B} = 3.61 \cdot 10^{-2}$ eV and $\Theta = 236$ K, these values are in good agreement with formula (3) (Fig. 2, dashed curve). From the above values, it is evident that the coefficients in formulas (2) and (3) do not differ significantly for crystalline and amorphous semiconductors.

Figure 3 shows the dependence of the value of the proportionality coefficient B from formula (1) on temperature. It is clear from the figure that as the temperature increases, the proportionality coefficient also increases.

Figure 4 shows the experimentally determined values of the spectra of the interband optical absorption coefficient of samples prepared using the same technology as amorphous hydrogenated silicon, with similar electrophysical properties, annealed for 30 minutes in the temperature range of 400–600 K, with a step of Δ25 K from 773 K to 898 K [9].

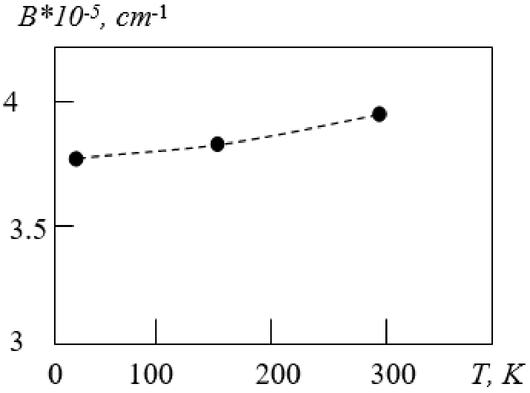

Figure 3. Dependence of the proportionality coefficient (B) in formula (1), written for the spectrum of the interband optical absorption coefficient of amorphous hydrogenated silicon, on temperature

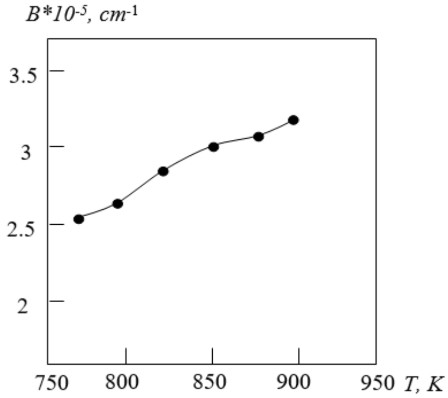

Figure 6. Dependence of the proportionality coefficient B from formula (1) on the temperature for annealed amorphous hydrogenated silicon

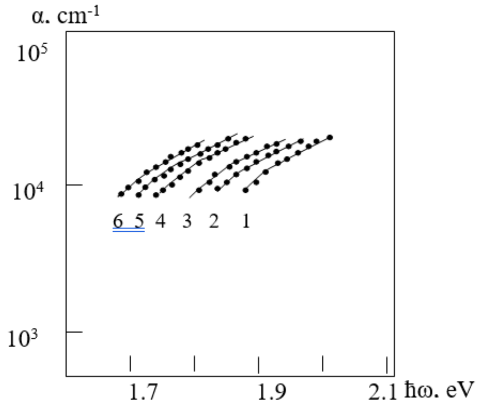

Figure 4. Experimental data from work [9]: 1 - T=773 K, 2 - T=798 K, 3 - T=823 K, 4 - T=848 K, 5 - T=873 K, 6 - T=898 K, and the results of calculations using formula (1) (solid curves). Points - experiment

The same figure also presents the results (curves) of calculations obtained using formula (1) by approximating the experimental data. Table 2 presents the values of $\boldsymbol{E_g}$ and $\boldsymbol{B}$ from formula (1), obtained as a result of these approximations, and shows their dependence on temperature. Figure 5 shows the results obtained using the Varshni and Bose-Einstein formulas for the dependence of $\boldsymbol{E_g}$ on temperature from Table 2.

The error in Fig. 5 and the other figures of experimental and calculated data does not exceed 8%. It was found that to calculate the mobility gap width of amorphous hydrogenated silicon using formula (2), the parameters of this formula should be equal to $\alpha=3.29\times10^{-4}$ eV/K and $\beta=135$ K. It was determined that to calculate the mobility gap width of a-Si:H using formula (3), the parameters should be equal to $\alpha_B=5.63\times10^{-2}$ eV and $\Theta=344$ K.

Table 2. Temperature dependence of the mobility gap width of annealed a-Si:H samples and the proportionality coefficient (B) of formula (1)

T, K	773	798	823	848	873	898
E_g, eV	1.673	1.659	1.651	1.642	1.634	1.626
$B{*}10^{-5}$, cm^{-1}	2.568	2.652	2.875	2.988	3.022	3.324

Figure 6 shows the dependence of the proportionality coefficient from Eq. (1) on temperature. For amorphous semiconductors, the value of B is equal to $B = N(\varepsilon_V)N(\varepsilon_C)\dfrac{8\pi^4 e^2\hbar^2 a}{nc(m^*)^2}$.

Here, it is known that the only free variable is the average distance a between the atoms of amorphous hydrogenated silicon. Figures 3 and 6 show that B increases with increasing temperature, which is associated with an increase in the vibrational frequency and amplitude of the atoms with increasing temperature, as a result of which the average distance between them also increases.

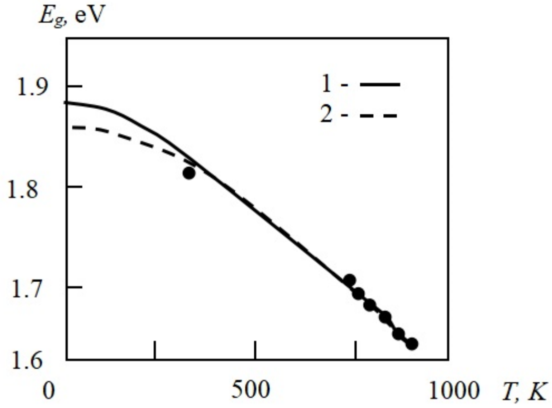

Figure 5. The mobility gap width of annealed amorphous hydrogenated silicon as a function of temperature. Results obtained using: 1 - the Varshni formula and 2 - the Bose-Einstein formula Points-experimental data

CONCLUSIONS

Thus, in this study, the temperature dependence of the interband absorption coefficient spectra of amorphous hydrogenated silicon was theoretically investigated. By comparing the experimentally determined interband absorption spectrum with the results obtained using the derived interband absorption formula, the mobility gap widths and proportionality coefficients in the formula were determined. It was shown that the determined temperature dependence of the mobility gap width is consistent with the Varshni and Bose-Einstein distributions. From the temperature dependence of the proportionality coefficient, it was established that the average distance between atoms in amorphous semiconductors increases with increasing temperature.

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ТЕМПЕРАТУРНА ЗАЛЕЖНІСТЬ ОСНОВНИХ ПАРАМЕТРІВ, ЩО ВИЗНАЧАЮТЬ СПЕКТР МІЖЗОННОГО ПОГЛИНАННЯ a-Si:H

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У даній роботі експериментально та теоретично досліджено температурну залежність коефіцієнта міжзонного оптичного поглинання гідрогенізованого аморфного кремнію (a-Si:H). Шляхом апроксимації значень, отриманих з формули коефіцієнта оптичного поглинання, температурну залежність характеристичної енергії коливань a-Si:H було досліджено за формулами Бозе-Ейнштейна та Варшні.

Ключові слова: *гідрогенізований аморфний кремній; коефіцієнт міжзонного оптичного поглинання; температура; характеристична енергія коливань; формула Бозе-Ейнштейна; формула Варшні*