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Short Communication

Main Temperature Dependent Parameters of the Exponential Absorption Spectrum of a-Si: H

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Abstract

In this work, the temperature dependence of the key parameters determining the exponential optical absorption coefficient spectra of hydrogenated amorphous silicon (a-Si: H) has been investigated. The study is based on both experimentally obtained values and the results derived from theoretical calculations of the exponential absorption spectrum. Using these results, the temperature dependence of the main parameters governing the exponential absorption spectrum of a-Si: H has been analyzed.

Keywords: Hydrogenated amorphous silicon (a-Si: H); Exponential optical absorption coefficient spectra; Temperature; Energy width of the mobility gap; Parameters determining the curvature of the exponential tails of the valence and conduction bands

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Introduction

In the work [1], experimentally determined values of the temperature dependence of the spectra of interband and exponential optical absorption coefficients of amorphous hydrogenated silicon (a-Si: H) are presented (Figure 1). The same figure shows the experimentally determined values of the temperature dependence of the spectra of the interband and exponential optical absorption coefficients for a-Si: H films obtained using the same technology but subjected to annealing for 30 minutes in the temperature range of 400-600 °C. It is shown that the Urbach focus for exponential absorption spectra is located at the point $E_g \approx 2.2$eV and $\alpha \approx 1.5*10^6 sm^{-1}$.

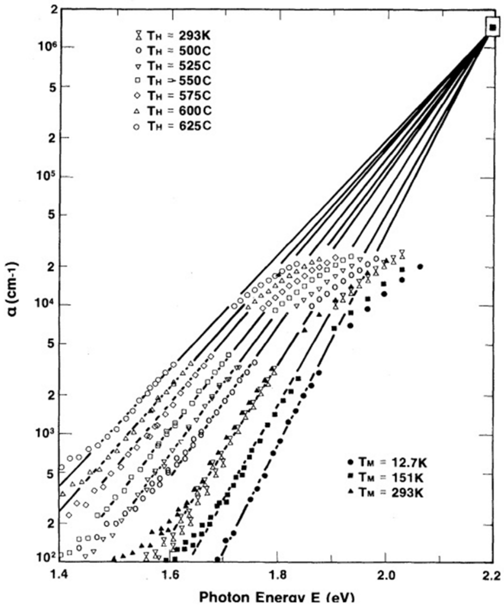

Figure 1: Temperature dependence of experimentally determined interband and exponential absorption spectra of unannealed and annealed a-Si: H in [1].

In work [2], the following expression was obtained for the exponential absorption spectrum using the theoretical method of the Davis-Mott approximation from the Kubo-Greenwood formula:

$$\alpha_2(\hbar\omega) = \frac{B}{(\beta_2-\beta_1)\hbar\omega}\exp(\beta_1(\hbar\omega - E_g)\,[1-\exp(\beta_2-\beta_1)(\hbar\omega - E_g)] \quad (1)$$

In work [3], the following expression was obtained for the interband absorption spectrum using a theoretical method based on the Davis-Mott approximation from the Kubo-Greenwood formula:

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

In formulas (1) and (2), $B = N(\varepsilon_V)N(\varepsilon_C)\frac{8\pi e^2\hbar^2 a}{m_0 c}$ is the proportionality coefficient independent of the energy of absorbed photons, where N(εV) and N(εC) are the effective values of the density of electron states in the valence band and conduction band, respectively, e is the electron charge, m is the effective mass of electrons in the allowed bands, n_0 is the refractive index of amorphous hydrogenated silicon, c is the speed of light, a is the a-Si: H average distance between atoms, E_g is the energy width of the a-Si: H mobility gap, β_1 and β_2 are the parameters determining the curvature of the exponential tails of the valence band and conduction band, respectively. The symbol (*) in this table denotes annealed samples.

Results and Discussion

To calculate the interband absorption spectrum from expression (2), it is necessary to determine the parameters B and E_g in this formula. Considering B and E_g in formula (2) as fitting parameters, we fit the calculated results obtained from this formula to the experimental data taken for the interband absorption spectrum, presented in Figure 1. The agreement between the experimental and calculated results from formula (2) (Figure 2, lines) for B and E_g is presented in Table 1.

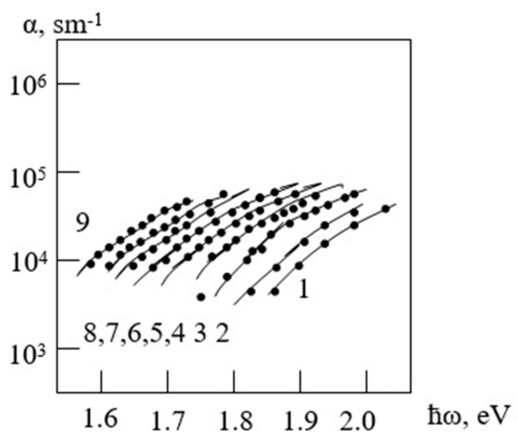

Figure 2: Temperature dependence of the interband absorption spectrum. Points are the experiment, lines are the results obtained from formula (2). Not annealed a-Si: H, 1-T=12.7K, 2-T=151K, 3- T-293K, Annealed a-Si: H 4-T=773K, 5-T=798K, 6-T=823K, 7-T= 848K, 8-T=873K, 9-T=898K.

To determine the values of β_1 and β_2, which are considered as fitting parameters, in formula (1), the values for B and E_g are obtained from Table 1, the obtained results of fitting to the experimental data are presented in Figure 3, and the values of β_1 and β_2 in Table 2. Figures 4 & 5 show the dependences of β_1 and β_2 on temperature for unannealed and annealed a-Si: H samples.

Table 1:

№	T, K	E_g, eV	B*10^{-5}, sm^{-1}
1	12.7	1.861	3.647
2	151	1.841	3.745
3	293	1.793	3.861
4	773*	1.673	2.568
5	798*	1.659	2.652
6	823*	1.651	2.875
7	848*	1.642	2.988
8	873*	1.634	3.022
9	898*	1.626	3.324

Table 2:

№	T, K	β_1, eV^{-1}	β_2, eV^{-1}
1	12.7	50.6	53.7
2	151	39.8	40.9
3	293	37.7	39.2
4	773*	61.7	64.9
5	798*	49.1	52.8
6	823*	43.6	47.5
7	848*	37.3	39.1
8	873*	31.7	34.9
9	898*	28.4	31.3

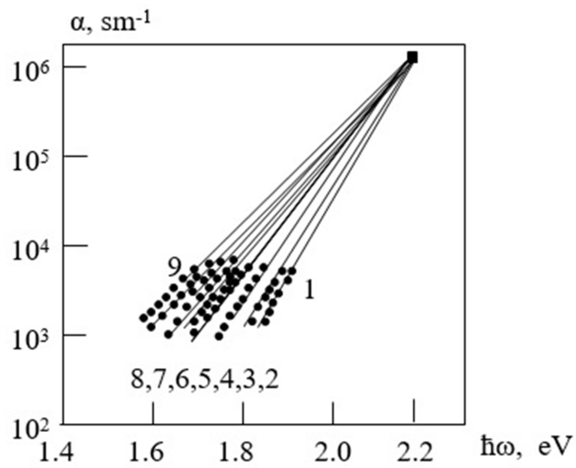

Figure 3: Temperature dependence of the exponential absorption spectrum. Points are the experiment, lines are the results of calculations using formula (1). The square point is the Urbach focus. Not annealed a-Si: H, 1-T=12.7K, 2-T=151K, 3- T=293K, Annealed a-Si: H 4-T=773K, 5-T=798K, 6-T=823K, 7-T= 848K, 8-T=873K.

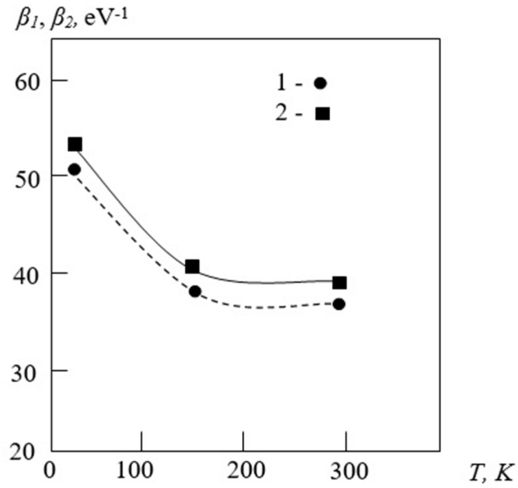

Figure 4: Temperature dependence of the parameters determining the curvature of the exponential tails of the conduction and valence bands of unannealed a-Si: H: 1 - β_2 for the tail of the conduction band; 2 - β_1 for the valence band.

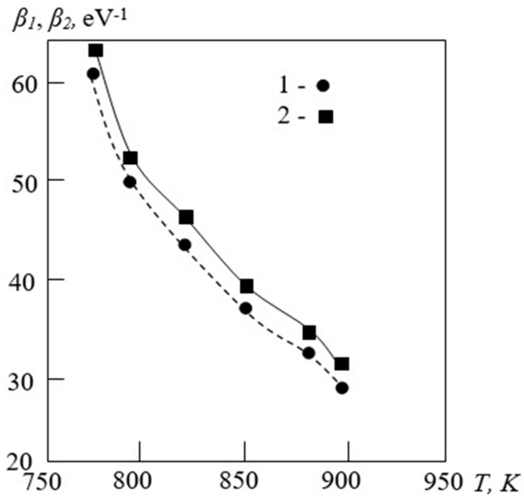

Figure 5: Temperature dependence of the parameters determining the curvature of the exponential tails of the conduction and valence bands of annealed a-Si: H: 1 - β_2 for the tail of the conduction band; 2 - β_1 for the valence band.

The determined values of these parameters are presented in Table 2.

The table shows that with increasing temperature, the exponential tails of the valence and conduction bands increase. After annealing the a-Si: H samples, the exponential tails of the valence and conduction bands also continue to increase. Moreover, for newly fabricated a-Si: H samples, the β_1 and β_2 values are strongly correlated at low temperatures. As the temperature increases, this dependence weakens. During annealing of the a-Si: H samples, the β_1 and β_2 values increase.

Conclusion

Thus, in this work, the temperature dependence of the main parameters that determine the optical absorption spectra of amorphous hydrogenated silicon was studied using a theoretical method. It was found that the exponential tails of the valence and conduction bands increase with increasing temperature. It was also found that the exponential tails of the valence and conduction bands of annealed a-Si: H samples increase with increasing temperature.

It was shown that the β_1 and β_2 values in unannealed a-Si: H samples exhibit a strong dependence at low temperatures. This dependence was shown to weaken as temperature increases. The Urbach focus for annealed and unannealed a-Si: H samples were found to be at E_g = 2.2eV and $\alpha = 1.5\times10^{6}$sm^{-1}. Annealing of a-Si: H samples lead to an increase in the β_1 and β_2 values.

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