

PROCEEDINGS OF SPIE

SPIDigitalLibrary.org/conference-proceedings-of-spie

Temperature dependence of the absorption edge of synthetic diamond

Kolesnik, E., Ripenko, V., Dzyadukh, S., Lipatov, E.

E. A. Kolesnik, V. S. Ripenko, S. M. Dzyadukh, E. I. Lipatov, "Temperature dependence of the absorption edge of synthetic diamond," Proc. SPIE 12086, XV International Conference on Pulsed Lasers and Laser Applications, 1208628 (2 December 2021); doi: 10.1117/12.2616516

SPIE.

Event: XV International Conference on Pulsed Lasers and Laser Applications, 2021, Tomsk, Russian Federation

Temperature dependence of the absorption edge of synthetic diamond

E.A. Kolesnik^{1,2}, V.S. Ripenko^{1,2}, S.M. Dzyadukh², E.I. Lipatov^{1,2}

¹Institute of High Current Electronics SB RAS, Tomsk, Russia;

²Tomsk State University, Tomsk, Russia

ABSTRACT

Using optical spectroscopy in the spectral range from 200 to 300 nm, the absorption edge and transmission spectra of 7 samples of synthetic diamond of IIa type in the temperature range from 12 K to 470 K was studied. Using numerical methods, the temperature dependences of optical absorption into the free exciton state were obtained for negative and positive phonon branches.

Keywords: synthetic diamond, optical spectroscopy, absorption edge, transmission spectra, band gap.

1. INTRODUCTION

Diamond is a wide-gap semiconductor with an indirect band gap $E_g \sim 5.49$ eV corresponding to the deep ultraviolet wavelength of 225 nm [1]. It is a cubic allotropic modification of carbon and its structure results in the strong covalent bonding between its atoms, which is the origin of its hardness. Diamonds have unique physical properties - the highest hardness and thermal conductivity of any bulk material.

In the optical absorption spectra, the following equation is valid:

$$hv_{h\omega} = E_g - E_x \pm h\omega \quad (1),$$

where $hv_{h\omega}$ - the maximum energy for the recombination radiation band, E_g - the band gap, E_x - the exciton binding energy, $h\omega$ - the photon energy.

2. EXPERIMENTAL, METHODS

Optical absorption spectroscopy was performed using an automated setup for nanoheterostructure admittance spectroscopy. The automated complex includes:

1. Janis CCS-400/204 closed-cycle non-optical helium cryostat (optionally installed in the form of quartz windows);
2. LakeShore 335 temperature controller (with individual calibration of one temperature sensor and the other with calibration for a series of sensors);
3. Turbomolecular vacuum post Pfeiffer Hi Cube Eco 80;
4. Personal computer with built-in National Instruments PCI-GPIB data acquisition board.

The use of the Janis CCS-400/204 closed-cycle helium cryostat in conjunction with the LakeShore 335 temperature controller allows cryostatting of the test sample in the range 10–475 K.

The setup for the optical transmission spectra measurements is shown in Figure 1.

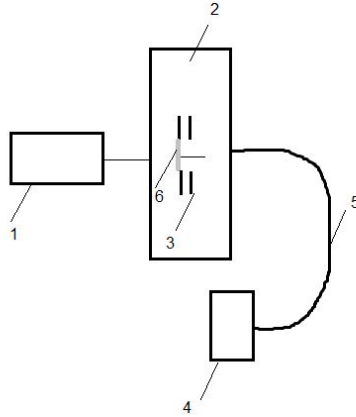


Figure 1 - The setup for the optical transmission spectra measurements

Where 1 - Light source; 2 - Vacuum chamber; 3 - Sample holder; 4 - Spectrometer; 5 - Optical fiber; 6 – Diamond.

The optical absorption spectra of 7 diamond samples were studied at different temperatures. The article presents the results for C5 diamond sample. With a change in temperature from 12 K to 470 K, the transmission spectra change. Figure 2 shows the temperature dependence of the transmission spectra of diamond.

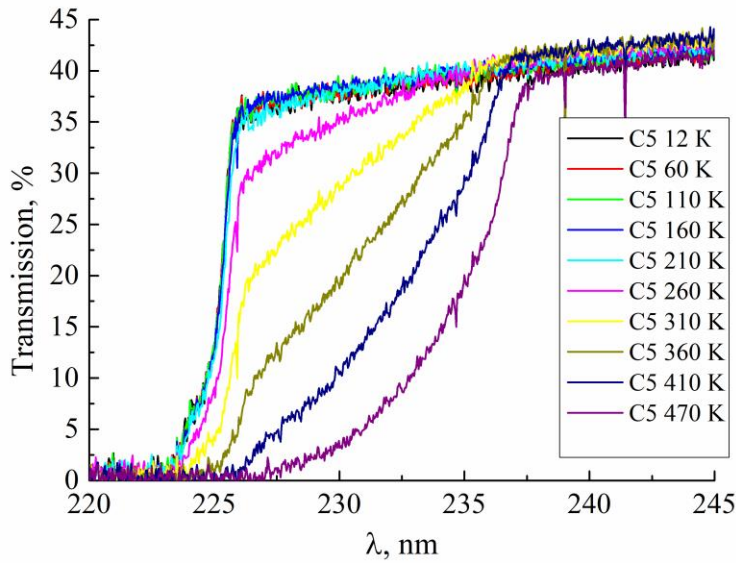


Figure 2 - Temperature dependence of the transmission spectra of diamond

The following formulas were used to calculate the absorption spectrum. The reflectance and refractive index are taken from the literature.

$$T(\lambda) = \frac{(1-r(\lambda))^2 \cdot e^{-\alpha(\lambda) \cdot d}}{1-r(\lambda)^2 \cdot e^{-2\alpha(\lambda) \cdot d}} \quad (2)$$

$$r(\lambda) = \frac{(1-n(\lambda))^2}{(1+n(\lambda))^2} \quad (3)$$

$$n(\lambda) = \sqrt{\frac{\lambda^2}{0.21413 \cdot \lambda^2 - 0.002678} + 1} \quad (4)$$

where T - the transmittance, r - the reflectance from one face, n - the refractive index of the medium, α - the absorption index, λ - wavelength.

Figure 3 shows the temperature dependence of the absorption spectra of the C5 sample.

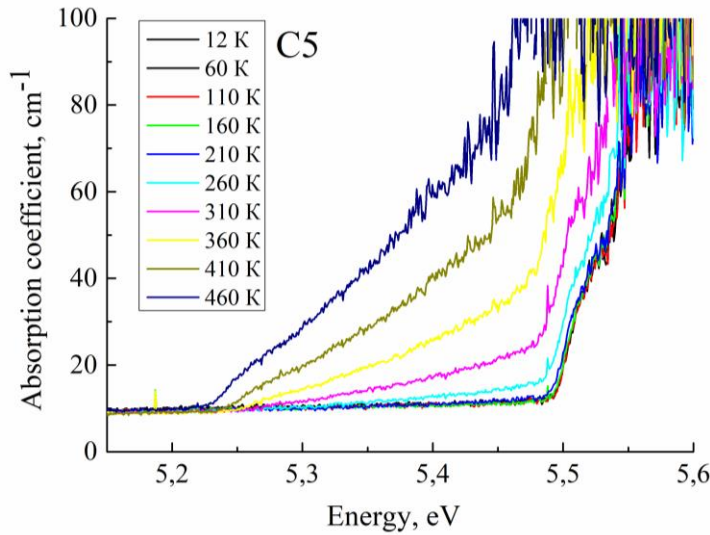


Figure 3 - Temperature dependence of the absorption coefficient for diamond

It is generally accepted that such changes in the absorption spectrum are associated with a change in the band gap. We think that such dependence can be obtained in another way - on the basis of the dependence of the inflection position in the absorption spectrum in the region of 225-226 nm by calculating the first derivative, where the first maximum of the derivative exactly corresponds to the inflection in the absorption spectrum (Figure 4). In this case, the dependence turns out to be similar to that in the article of the 1960s [2].

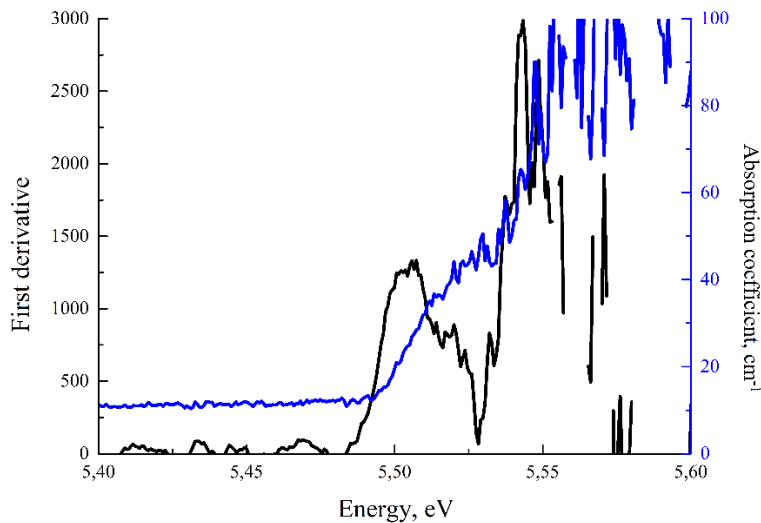


Figure 4 - First derivative of the absorption spectrum at 12 K and initial absorption spectrum

Figure 5 shows the temperature dependences of the inflection position in the C5 absorption spectra of the sample, there are results obtained in [2] and results obtained by us in the experiment.

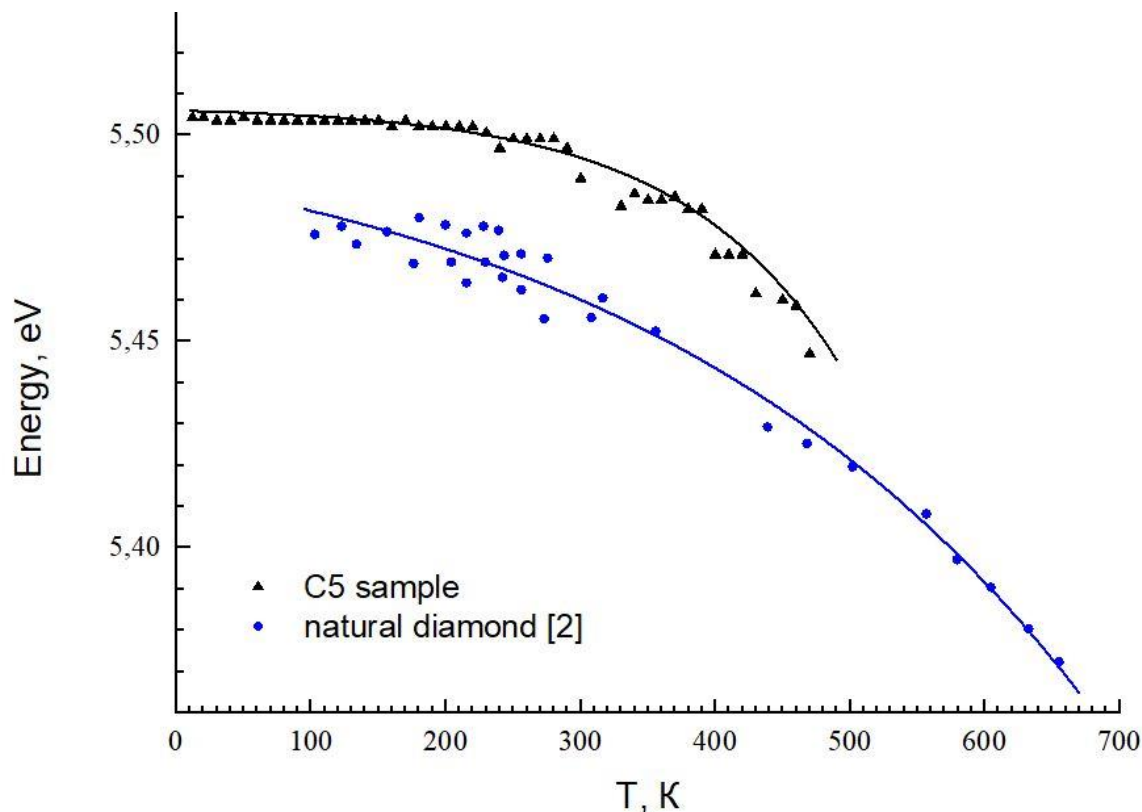


Figure 5 - Temperature dependence of the indirect energy band

The fundamental absorption edge is described by the formula 3 for absorption into the exciton state and interband transitions. According to this formula, the temperature dependence of the absorption edge of diamond is determined by absorption into the exciton state with both the absorption of phonons and the emission of a phonon. Interband absorption manifests itself even further into the short-wavelength region.

The following are the calculation results using the above formula. In this case, the band gap changes only slightly (Figure 6).

$$\alpha = \sum_p \left(\frac{n_B + 0.5 \pm 0.5}{h\nu} \cdot \left[\sum_i A_{p,i} \left(h\nu - (Eg - Ex_i \pm h\omega_p) \right)^{\frac{1}{2}} + B_p \left(h\nu - (Eg \pm h\omega_p) \right)^2 \right] \right) \quad (5)$$

$$n_B = \left(e^{\frac{h\omega_p}{k_B T}} - 1 \right)^{-1} \quad (6)$$

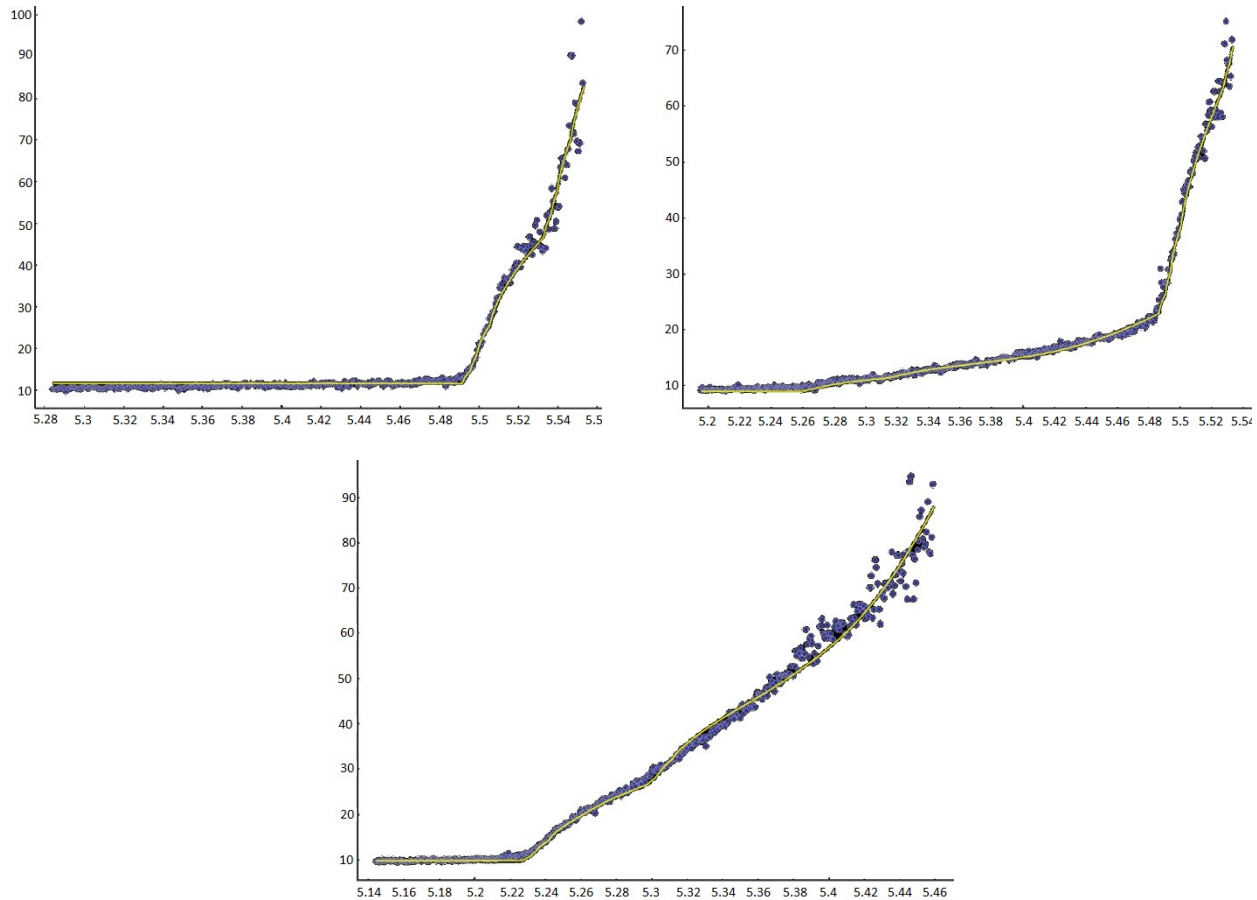


Figure 6- Temperature dependences of optical absorption in a split free exciton state (at 12 K, 300 K and 460 K)

3. CONCLUSIONS

It is shown that incorrect conclusions were found in the literature [2]. The temperature dependence of the fundamental absorption edge of diamond is caused by the temperature dependence of absorption into an exciton state with absorption of phonons. It is believed that changes in the absorption spectra are associated with a change in the band gap. Such a dependence can be obtained by calculating the first derivative, where the first maximum of the derivative exactly corresponds to the inflection in the spectrum (Figure 4). In this case, the dependence turns out to be similar to that in the article of the 1960s [2].

It is revealed that the band gap of diamond in the temperature range 80-400 K changes by 60 meV.

The study was carried out on the state order of the Ministry of Education and Science of Russia, project № 0721-2020-0048.

REFERENCES

- [1] Bokii G.B., Bezrukov G.N., Klyuev Yu.A., et al. Natural and synthetic diamonds / Ed. Shafranovsky I.I., Science, Moscow, 222 p. (1986) (in Russian).
- [2] Clark C.D., Dean P.J., Harris P.V. Intrinsic edge absorption in diamond / Proc. Roy. Soc (1963).