

The spectra of the main absorption of Bi₂Se₃

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Abstract:- Fundamental absorption spectrum in crystals with varying electron density, from minimum to maximum, it possible to determine the absolute value and position of extreme as the forbidden gap relative to each other and in the wavelength space of the Brillouin zone. The energy gap for direct and indirect inter-band transitions approximately equally dependent on the total concentration of donors and acceptors in the crystal Bi₂Se₃ in the range 10¹⁸ – 5x10¹⁹cm⁻³. From the main absorption spectra of heavily doped crystals with simple bands quantitative data on the number of equivalent ellipsoids in the zones can be obtained.

Keywords: -crystals, electron density, concentration, semiconductor, absorption

I. INTRODUCTION

Optical transitions from the valence band to the conduction band are possible only at levels located near and above the Fermi level. When introduced into the crystal of a large number of impurity centers of the energy levels corresponding to the impurity atoms are expanded to form an impurity band, which for small levels merges with the edge of the valence band, and the band gap is formed tail density of states and the Fermi level goes deep in the main zone.

$$g(E) = g_0(E)[f_v(E_v - E_F) - f_c(E_c - E_F)]$$

where f_v and f_c - occupation probabilities of single-electron states; $g_0(E)$ - the density of the final states without regard to their amusement.

From the main absorption spectra of heavily doped crystals with simple bands quantitative data on the number of equivalent ellipsoids in the zones can be obtained, i.e., on the location of the extreme points of the gap in the Brillouin zone. Fundamental absorption spectrum in crystals with varying electron density, from minimum to maximum, it possible to determine the absolute value and position of extreme as the forbidden gap relative to each other and in the wavelength space of the Brillouin zone [1-4].

Factors affecting the absorption in indirect transitions in heavily doped crystal, a scattering by impurities, which can inform the missing electron momentum he needs in indirect optical transitions [5]. For elastic scattering, the absorption coefficient is represented by the formula

$$\alpha(h\omega) = \frac{A_{dir} N_{dir}}{h\omega} (h\omega - E_{gl})^2$$

where N_{dir} - the concentration of impurity atoms, A_{dir} - a constant, E_{gl} - the width of the indirect gap for highly doped semiconductor selection rule does not make sense, because when the electron scattering by impurities significantly change its momentum.

The formula for the total absorption of highly-doped crystal for indirect transitions taking into account the scattering by impurities in the energy $h\omega > (E_g + 4kT)$ takes the form

$$\alpha = \frac{A_{dir} N_{dir} + A}{h\omega} (h\omega - E_{gl} - \frac{Ak\theta}{A_{dir} N_{dir} + A} th \frac{\theta}{2T})^2$$

which implies that the dependence $\sqrt{\alpha h\omega} = f(h\omega)$ is a straight line intersecting the axis of the energy at the point

$$h\omega = E_{gl} + \frac{Ak\theta}{A_{dir} N_{dir} + A} th \frac{\theta}{2T},$$

II. EXPERIMENTAL PROCEDURE

The position of which is shifted to shorter wavelengths with increasing concentration of impurities. Straight line depending also shifted towards lower energies with increasing concentration of impurities, and the slope increases.

The conduction band of the Bi₂Se₃ has two minima, and the absolute minimum, four degenerate in the absence of external fields, is 0.18 eV below the minimum in the center of the Brillouin zone, so the study of the optical absorption spectra of strongly basic Bi₂Se₃ allows investigating changes in the doping of both at the same time lows [6-8].

The results of studies of the effect of heavy doping on the structure of the optical absorption curve associated with the direct inter-band transitions at 77 K are shown in Figure 1. Samples Bi_2Se_3 were doped with antimony and arsenic to a concentration of 10^{13} to $1.5 \times 10^{18} \text{ cm}^{-3}$. The thickness of the free samples was approximately 10 μm . Because at 77K, all electrons are at an absolute minimum, the minimum at $k = 0$ electrons no effect Burstein - Moss absent. The figure shows that with increasing concentration of impurity centers exciting peak expanded, and then disappears. Absorption in $\hbar\omega > E_g$ with increasing concentration and decreases to a value characteristic of a pure crystal without Coulomb interaction of carriers. The critical impurity concentration, at which the exciting absorption features in the spectrum disappear, turns out to be 10^{16} cm^{-3} .

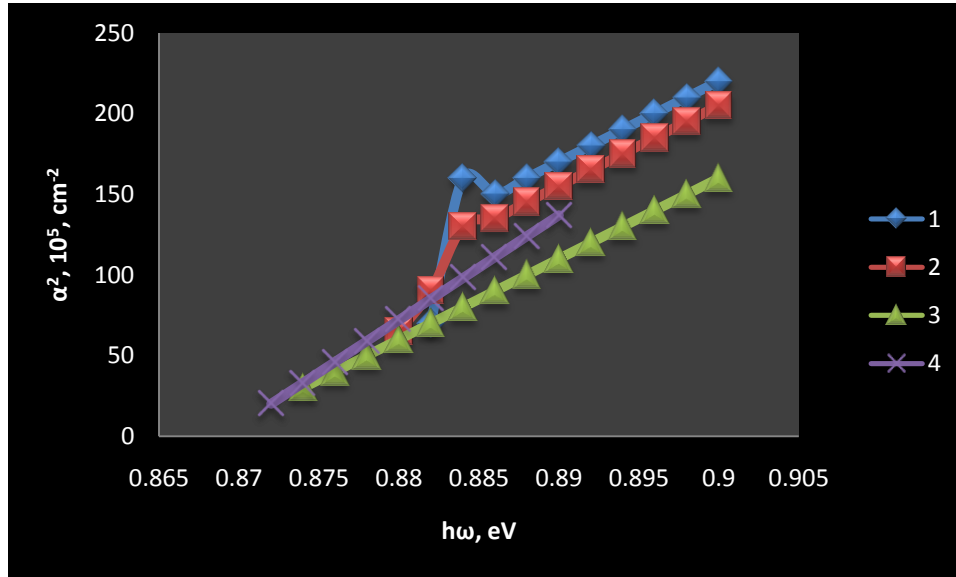


Fig. 1 The effect of the concentration of impurities in the structure Bi_2Se_3 of the fundamental absorption edge concentrations: 1- 10^{13} cm^{-3} ; 2- $8 \times 10^{15} \text{ cm}^{-3}$; 3- $2 \times 10^{18} \text{ cm}^{-3}$; 4- light injection Spectra corresponding $N_D = 2 \times 10^{17}$ and $1,5 \times 10^{18} \text{ cm}^{-3}$ are in good agreement with the formula

$$\alpha(\omega) = A \frac{\sqrt{\hbar\omega - E_g}}{\hbar\omega}$$

which does not account for the interaction of electrons and holes. The intersection points of these lines with the axis of energy correspond to the band gap. Figure 1 show that with increasing impurity concentration the energy band gap is reduced. When the concentration of impurities is $1,5 \times 10^{18} \text{ cm}^{-3}$, $\Delta E = -1,1 \times 10^{-2} \text{ cm}^{-3} \text{ eV}$ in agreement with the value calculated the formula $\Delta E = -2 \left(\frac{3}{\pi}\right)^{1/3} \frac{e^2 N^{1/3}}{\epsilon}$. Direct 4 of Figure 1 correspond to the case where the carriers injected into the light volume of the crystal [9].

Figure 2 shows the absorption spectra of the main samples Bi_2Se_3 at 4.2 K, more heavily doped with arsenic at a concentration of $5 \times 10^{18} \text{ cm}^{-3}$ to $4 \times 10^{19} \text{ cm}^{-3}$. It can be seen that the absorption edge associated with the direct interband transitions is shifted toward longer wavelengths.

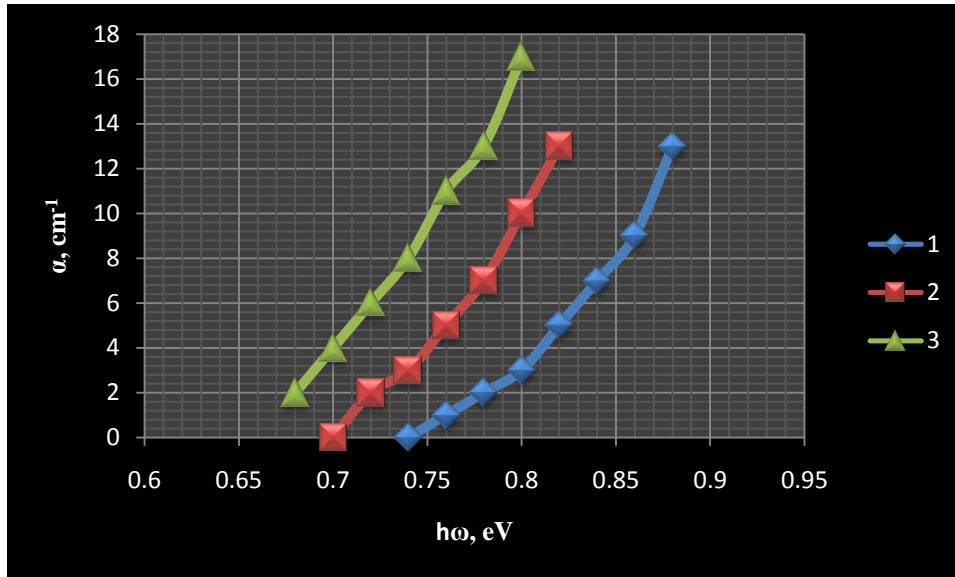


Fig. 2 The spectra of the fundamental absorption edge Bi_2Se_3 heavily doped with arsenic.

For a more detailed analysis of weak absorption, in Figure 3 the experimental data for samples Bi_2Se_3 with impurity atoms phosphorus, arsenic and gallium obtained at 80K, built to scale $\sqrt{\alpha(\omega)} \sim h\omega$. The same figure also shows the spectrum of a pure sample. The concentration of impurities in pure sample 10^{13}cm^{-3} (figure 3. 1). The impurity concentration of phosphorus atoms in the sample $2,4 \times 10^{18} - 4,3 \times 10^{19} \text{cm}^{-3}$ (figure 3. 2). The impurity concentration of arsenic and gallium atoms in the sample, respectively, equal to $2,9 \times 10^{19} \text{cm}^{-3}$; $1,8 \times 10^{19} \text{cm}^{-3}$ (figure 3. 3).

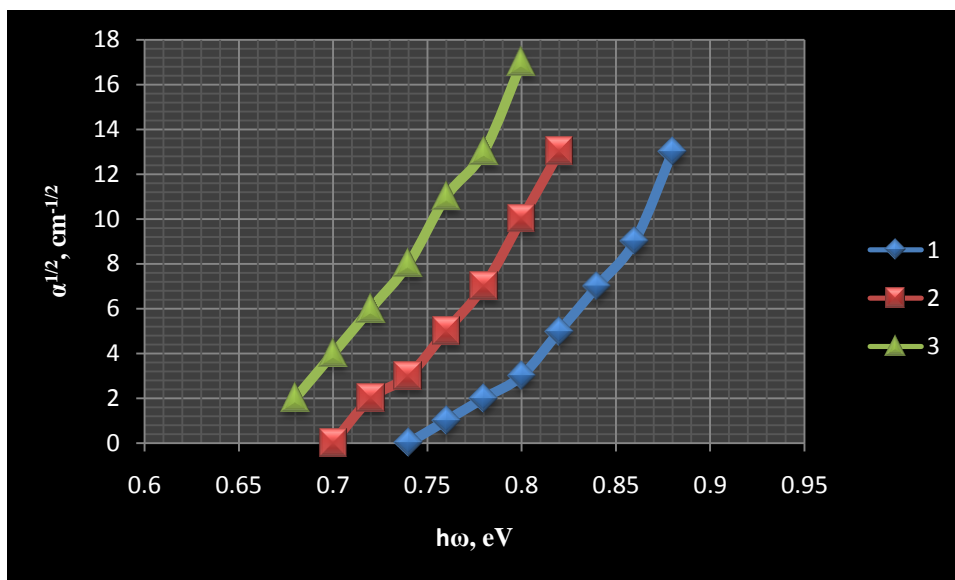


Fig. 3 The spectra of the fundamental absorption edge Bi_2Se_3 heavily doped with phosphorus, arsenic and gallium:
1 pure; 2- $2 \times 10^{19} \text{cm}^{-3} (\text{P})$; 3- $10^{19} \text{cm}^{-3} (\text{As+Ga})$

The figure shows two features: 1) absorption of highly doped uncompensated samples more sharply depends on the photon energy than pure sample; 2) absorption of all compensated samples begins at about the same photon energy, while at the beginning of the compensated sample absorption is shifted toward longer wavelengths. This indicates a significant reduction in band gap doped. For example, for sample 2 band gap decreased 80meV.

Reducing proportional to the cube root of the total concentration of impurity atoms and does not depend on the electron concentration.

$$\Delta E_g \sim \sqrt[3]{(N_D + N_A)}$$

III. CONCLUSION

Absorption of highly doped uncompensated samples more sharply depends on the photon energy than pure sample. Absorption of all compensated samples begins at about the same photon energy, while at the beginning of the compensated sample absorption is shifted toward longer wavelengths. The energy gap for direct and indirect inter-band transitions approximately equally dependent on the total concentration of donors and acceptors in the crystal Bi₂Se₃ in the range $10^{18} - 5 \times 10^{19} \text{ cm}^{-3}$.

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