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Optical Response of $GaAs_{0.75}Sb_{0.25}$ Nanosheet for Dependent Pressure

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ABSTRACT

The study analyzed the optical response of $GaAs_{0.75}Sb_{0.25}$ nanosheet under high pressure. It is the generalized gradient approximation (GGA) within the framework of density functional theory (DFT) was employed by means of a simulation program, which is called CASTEP. Under different pressure (P = 0, 2, and 4 GPa). Geometry optimized parameters were calculated for the nanosheet. The optical data alter in accordance with high pressure. The increase of pressure in the nanosheet led to a rise in p = 4 GPa and a decline in p = 2 GPa of the optical energy band gap, the static dielectric constant $\varepsilon_1(0)$, and optical conductivity. The discussions of the real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ sections of the dielectric function, optical band gap energy, optical absorption, and optical conductivity were included.

KEYWORDS: GaAsSb; nanosheet; Optical response; high Pressure; DFT; GG.

الخلاصة

حللت في هذه الدراسة الاستجابة البصرية لصفيحة النانو $GaAs_{0.75}Sb_{0.25}$ تحت ضغط عالي. تم استخدام المبادئ الاساسية لطريقة الجهد الكاذب للموجة المستوية من خلال تعميم التقريب الانحداري (GGA) في إطار نظرية الكثافة الوظيفية (DFT) عن طريق برنامج المحاكاة ، والذي يسمى ب (CASTEP). تحت ضغوط مختلفة (٠، ٢، ٤) گيگا باسكال. تم حساب المعامل الهندسية المحسنة لصفيحة النانو. تتغير البيانات الضوئية وفقًا للضغط العالي. أدت زيادة الضغط في صفيحة النانو إلى ارتفاع في ٤ گيگا پاسكال وانخفاض في ٢ گيگا باسكال من فجوة نطاق الطاقة الضوئية، ثابت العزل الكهربائى والتوصيل البصري. تم تناول مناقشة الأقسام الحقيقية والخيالية، وظيفة العزل الكهربائي ،طاقة فجوة النطاق البصري ، الامتصاص البصري والتوصيل البصري.

INTRODUCTION

In the development of nanosheet alloys technologies, semiconductor compounds have attracted much attention because of their ability to tailor the optoelectronic performances, such as the physical properties with the alloy compositions. [1- 4]. The GaAsSb nanosheet and their solid solutions are useful in the fabrication of electronic devices. The GaAsxSb1$_{-x}$ alloys are interesting materials for optoelectronic applications because of the wide band gap energy range, from (0.87 to 1.55 eV), varying with the Sb content [5]. Although the high-pressure structural stability of the nanosheet alloys has been the topic of intense research for more than ten years the high-pressure phase diagrams of the GaAsSb nanosheet have not been completely understood. This is partially due to the specific sample-handling problems that arise in dealing with this alloy. Experimentally, all these compounds adopt the zinc-blende structure at low pressures. Before this work, we studied about $GaAs_{0.5}Sb_{0.5}$ electronic and optical responses by using DFT [6]. However, we studied mechanical properties of the Lead Sulfur Selenium under Pressure [7]. In addition, other work analysis theoretical and experimental about the elastic and optical performance of $GaAs_xSb_{1-x}$ alloys [8]. Nanosheet semiconductors provide the basis of the material for a number of well-established commercial technologies, as well as new cutting-edge classes of electronic and optoelectronic devices. Only a few examples include heterostructure bipolar transistors, light-emitting diodes, electro-optic photodetectors, and modulators [9]. The operating characteristics of these devices depend ultimately on the optical

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performance of the constituent materials, which are often combined in a quantum well-containing carriers confined to dimensions about a nanometer. Apparently, limitless flexibility is now available to the electronic device designer [10]. Nanosheet semiconductors are highly important technologically [11]. Semiconductors with predictable and reliable optical performances are necessary for mass production.

In particular, nanosheet compound is extremely efficient in generating light from converting light back into electricity. Therefore, they have been the key nanomaterials for solar cells and LEDs [12]. These are nearly about all optoelectronic systems and optical storage display technology. This nanosheet can be crystallized in the cubic zinc blende phase but for each nanomaterial, one or the other of those phases is calculated under pressure as fixed. The optical energy band gaps of the $GaAs_{0.25}Sb_{0.75}$ system range from 0.90 eV to 1.23 eV. A nanosheet will only detect light with photon energy smaller than the band gap energy, in other words, with a wavelength shorter than the cutoff wavelength associated with the optical band gap energy [13]. The operating structures of this nanosheet consist critically of the physical response of the constituent nanomaterial. This study was carried out to shed light on the future studies of scientists who experimentally prepare and test these nanosheet compounds, to help them in determining the change in amounts of additives in nanosheet with high pressure and to determine the accordance of theoretical studies with experiments works. The optical response of $GaAs_{0.25}Sb_{0.75}$ changes with high pressure, which directly affects various applications of nanosheet alloys based instruments nether the different working states. Using density functional theory with GGA approximation optical response of $GaAs_{1-x}Sb_x$ of the composition x =0.75 nanosheet have been focused at 0 – 4 GPa pressure. The geometry optimized structural and optical parameters for $GaAs_{0.25}Sb_{0.75}$ with pressures are listed.

THEORETICAL MODEL

The study has been done for the optical behavior of $GaAs_xSb_{1-x}$ of x =0.75 nanosheet by means of the DFT [14]. Calculation in this program is implemented via Kohn–Sham formation. (GGA) is made for electronic exchange-correlation potential energy, bring about by electron-ion interaction [15]. It is described as utilized pseudo-potential connotation. A cubic unit cell is constructed with (As/Sb). An 8-atom unit cell was applied, which matches 2×2×1 wurtzite unit cell concerning the size in the initial plan. Which was found by electron-ion interaction. The scheme which has been suggested by [16] was used to accept the optimized non-local pseudo-potential, in which orbitals including Ga ($3d^{10}4s^24p^1$), As ($3d^{10}\ 4s^2\ 4p^3$) and Sb ($4d^{10}\ 5s^2\ 5p^3$) worked role as valence electrons. A kinetic-energy cutoff of 980 eV was used in the plane waves, as the wave function was prolonged. While the k-points of 6×6×4 were applied for x = 0.75, the ratio between Ga, As and Sb atoms were identified for nanosheet, and it defined the geometrical arrangement of As–Sb atoms. Nanosheet compound with symmetry in the calculation was indicated for the systems to continue regularity and facility. The suspense was that for x= 0.75, cubic structure for the layered nanosheet. The geometry optimization was achieved for GaAsSb nanosheet for x = 0.75 compositions with symmetry P1. Figure 1 shows step optimum plot given only for pressure equal to 2 GPa for example. Structure parameters were calculated from symmetry directions. Calculations of band structures and determine the values of the optical energy band gap with changing pressure. The optical behaviors were fixed for GaAsSb nanosheet with high pressure. The dielectric equations $\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega)$ is applied for characterizing optical linear reply, resulting from the interaction of photons with electrons [17]. The exact side $\varepsilon_1(\omega)$ of dielectric equations was investigated using Kramer's–Kronig functions [18]. Some terms used to express dielectric functions [19, 20]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int_0^{\infty} \frac{\varepsilon_1(\omega')\omega' d\omega'}{\omega'^2 - \omega^2} \quad (1)$$

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int_0^{\infty} \frac{\varepsilon_1(\omega')\omega' d\omega'}{\omega'^2 - \omega^2} \quad (2)$$

$$\varepsilon_2(\omega) = \frac{Ve^2}{2\pi\hbar m^2\omega^2}\int d^3k \sum_{nn'} |\langle kn|p|kn'\rangle|^2 f(kn) \times [1 - f(kn')]\partial(E_{kn} - E_{kn'} - \hbar\omega) \quad (3)$$

While $\hbar\omega$ is incident photon energy p is the momentum $\frac{\hbar}{i}\frac{\partial}{\partial x}$, $|kn\rangle$ is the eigen-function with eigenvalue E_{kn}, $f(kn)$ and is Fermi distribution function.

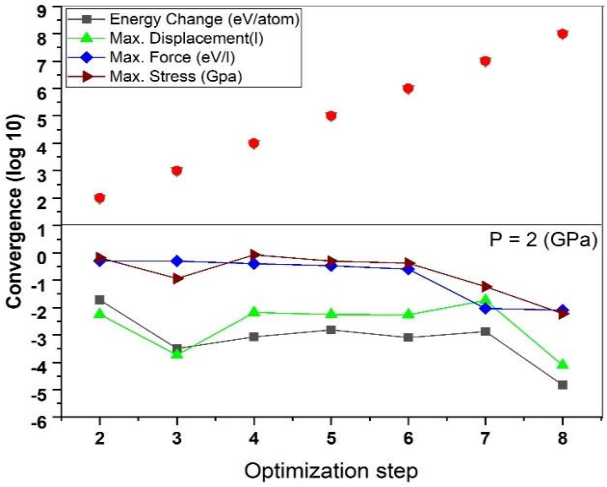

Figure 1. The optimization step convergence of nanosheet.

$$\alpha(\omega) = \sqrt{2\omega}\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right]^{1/2} \quad (4)$$

$$\sigma = \sigma_1 + i\sigma_2 = -i(\omega/4\pi)(\varepsilon - 1) \quad (5)$$

Using these relations of functions (1) – (4), real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ section of the dielectric functions, optical absorption $\alpha(\omega)$ and optical connectivity $\sigma(\omega)$ were calculated.

In general, the relationship between band gap and pressure can be expressed as

$$Eg\ (p) = Eg(0) + aP + bP^2 \quad (6)$$

where a and b are static pressure parameters. According to values of the band gap at 0, 2, and 4GPa, these can be calculated as a = 1.7 × 10–3 eV/GPa and b = –2.4 × 10–4 eV/GPa2. [21]. To verify the correctness of the results.

RESULTS AND DISCUSSIONS

Optical performance was calculated so as to reveal the response of $GaAs_{0.25}Sb_{0.75}$ with high pressure. The structural properties; structure stability through optimizations, lattice constant (a), minimum volume (V_0,) bulk modulus (B) and ground state energy (E_0) have been pointed out. It shows a functional correlation with the present work. Dielectric function (real and imaginary section), optical band gap energy, optical absorption, and optical conductivity have been discussed for optical response comprising the ductile or brittle nature of the nanosheet. The calculation of lattice constants of nanosheet with pressure at equilibrium was performed using minimizing lattice parameters of the crystal, and they indicated (596, 589 and 578 nm) for $GaAs_{1-x}Sb_x$ nanosheet for x = 0.75 correspondingly with pressure in the current study. Table 1 displays the achieved results.

Table 1. Structural properties of $GaAs_{0.25}Sb_{0.75}$ nanosheet.

No.	Properties	P = 0 (GPa)	P = 2 (GPa)	P = 4 (GPa)
1	a (nm)	596	589	578
2	V_0 (a.u^3)	243	239	221
3	B (GPa)	64.32	61.83	59.02
4	E_0 (eV×10^3)	-3.859	-3.867	-3.854

Figure 2 clarifies that as dielectric function (real section ε_1 (ω)) rises, the h□ goes up likewise out of the region between (1.44 and 2.28 eV). All of them can be named normal dispersion. Though strong absorption was displayed at (1.93–3.18 eV), it became explained in the optical absorption and conductivity graph under separate pressures.

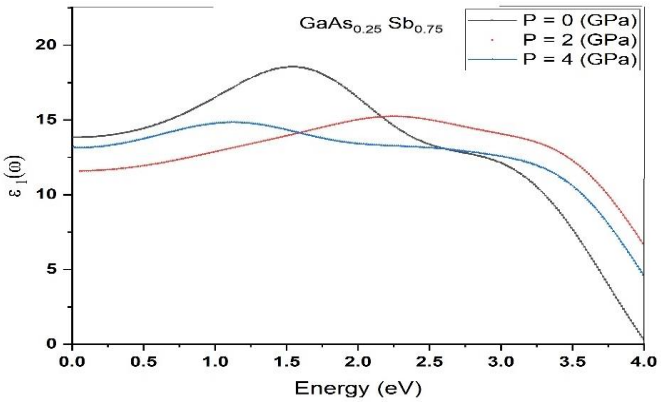

Figure 2. The real section of dielectric function.

For realizing of the optical energy band gap and optical transition of the nanosheet system, it is highly essential to explore the imaginary section of the dielectric function (imaginary section $\varepsilon_2(\omega)$) due to the significance of the section for optical response of GaAsSb nanosheet. It has been acknowledged that the interaction of a photon with the electrons in this system can be depicted in regard to time dependent perturbations of the ground electronic states. The photon energy is the base

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for the peak values of imaginary section of dielectric function Figure 3. These values agree with the electronic passages from valence band to transmission band (optical transitions), and they are explained to vary based on pressure [22].

The optical absorption series of the nanosheet system under pressure can be seen in Figure 4 (a). Scissor operation [23] was used to underestimate the optical band gap energy, but it is really uneasy to achieve the accurate optical energy band gap. This method is functioning for various organisms.

Figure 4 (b) refers to the calculation of values of absorption point, which are (48.13, 41.50 and 48.32 nm) with increasing pressure. On the other hand, Static dielectric constant $\varepsilon_1(0)$ of nanosheet are calculated which is displayed in Figure 3 (a), and the whole values are explained in table 2.

Optical conductivity of GaAsSb nanosheet is demonstrated in Figure 5. The nanosheet system dependence conductivity almost rises with pressure, and the development has an instant link with the optical band gap energy.

Table 2. Optical Band gap energy (E_g), optical absorption value $\alpha(0)$, statics dielectric constant $\varepsilon_1(0)$ and σ (ω) optical conductivity of $GaAs_{0.25}Sb_{0.75}$ nanosheet with pressure.

No.	Properties	P = 0 (GPa)	P = 2 (GPa)	P = 4 (GPa)
1	E_g (eV)	0.98	0.84	1.09
2	α (0) cm^{-1}	48.13	41.50	48.32
3	ε_1 (0)	13.85	11.57	13.11
4	σ (ω) Ω^{-1} m^{-1}	5.906	6.416	5.893

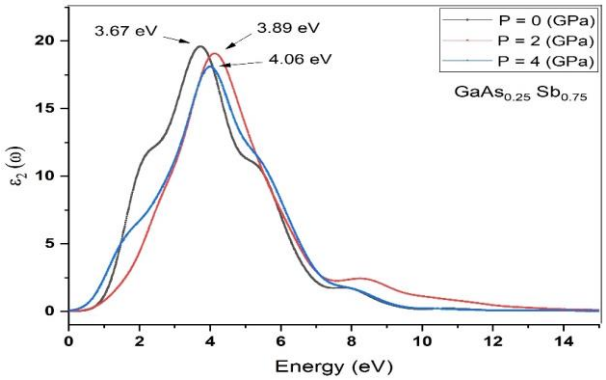

Figure 3. The imaginary section of dielectric function.

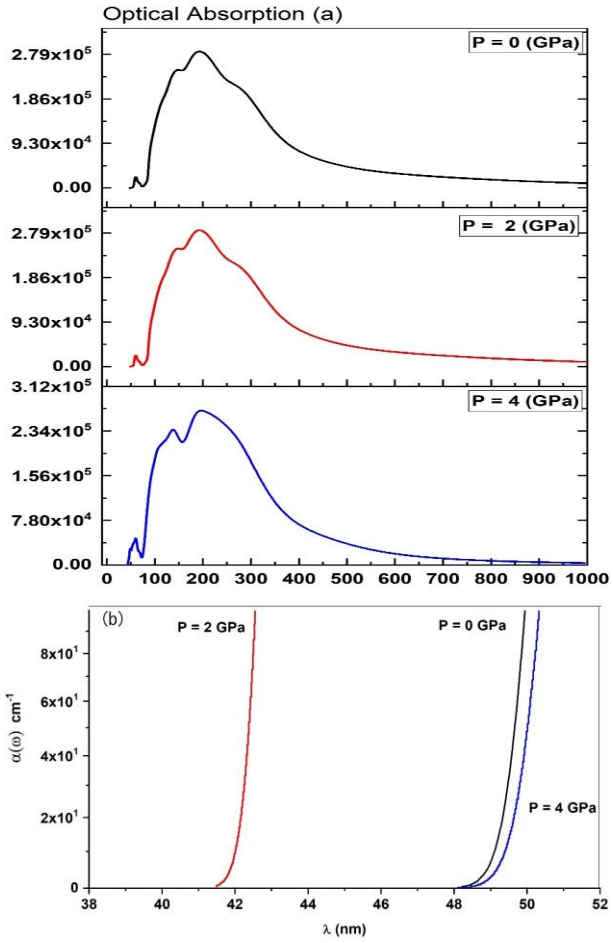

Figure 4. (a, b) the optical absorption of the nanosheet system.

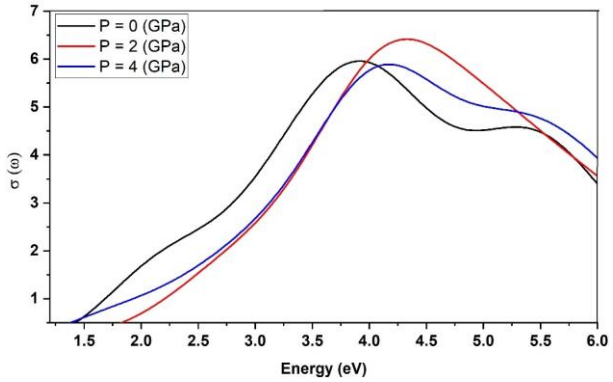

Figure 5. The optical conductivity of the nanosheet system.

CONCLUSIONS

In the final analysis, density functional theory was used to investigate the optical response of Gallium Arsenic Antimony for composition x=0.75. The study also pointed to the geometry optimized structural parameters for the nanosheet system with high pressure. The increase of pressure in the nanosheet led to a rise in p = 4 GPa and a decline in p = 2 GPa of the optical energy band gap and the static dielectric constant $\varepsilon_1(0)$. Then the calculation of

the starting values of optical absorption and conductivity for naonsheet was processed. The data were comprised of P=2 and 4 GPa, and it becomes a dependable reference for some studies which will be conducted. Electronic devices and applications take advantage from Optical performance of the nanosheet with pressure increasing. Moreover, it can be utilized as a favorable source in contemporary technology.

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