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Research Paper / Makale

Optical Properties of Dilute Bismuth Semiconductor Alloys

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Abstract: The research on dilute bismuth containing III-V semiconductor alloys and its applications are studied. These alloys are obtained by incorporating a small amount of Bi in the host semiconductor. The presence of Bi reduced the energy bandgap of the alloys. The bandgap and optical properties of $InAs_{1-x}Bi_x$, $InP_{1-x}Bi_x$, and $InSb_{1-x}Bi_x$ alloy systems are investigated for optoelectronic devices. The optical properties of semiconductors are important to change the properties of device performance. The refractive index strongly depends on the direct bandgap of the semiconductor alloys. The bandgap of the In-V-Bi semiconductor layer can be engineered by means of adding bismuth into InAs, InP, InSb. In this work, the refractive indices and the optical parameters of the In-V-Bi alloys are investigated.

Keywords: InAsBi, InSbBi, InPBi, dilute bismide

Az Miktarda Bizmut Eklenen Yarıiletken Alaşımlarının Optik Özellikleri

Öz: Az miktarda bizmut (Bi) içeren III-V yarıiletken alaşımları üzerine yapılan araştırmalar ve optoelektronik uygulamaları son zamanlarda artmıştır. Bu alaşımlar, ev sahibi olarak seçilen yarıiletkene az miktarda Bi eklenerek elde edilirler. Bismut'un eklenmesi yarıiletken alaşımların enerji bant aralığını azaltır. Bu çalışmada optoelektronik cihazlarda kullanılan $InAs_{1-x}Bi_x$, $InP_{1-x}Bi_x$, ve $InSb_{1-x}Bi_x$ alaşım sistemlerinin bant aralığı ve optik özellikleri araştırılmıştır. Yarı iletkenlerin bu çalışmada incelenen optik özellikleri, cihaz performansının artırılması ve verimliliği için önemlidir. Kırılma indisi, yarı iletken alaşımların doğrudan bant aralığına bağlıdır. In-V-Bi yarı iletken elde etmek ve bant aralığını değiştirmek için ikili InAs, InP, InSb'ye az miktarda bizmut eklenerek geliştirilebilir. Bu çalışmada, önerilen In-V-Bi alaşımlarının kırılma indeksleri ve optik parametreleri araştırılmıştır.

Anahtar Kelimeler: InAsBi, InGsBi, InPBi, Bizmut

1. Introduction

In the last decades, there have been considerable interest in dilute bismide ternary alloys due to numerous potential applications in optoelectronic devices as detectors in the infrared range and solar cells. Semiconductor alloys made up of III-V group elements are commonly used to interact with light in novel optoelectronic devices and applications in many areas of modern technology with its special properties. The electronic energy bandgap of these alloys could be tailored for device applications by incorporating other III-V group elements. The dilute bismides are a novel class of III-V-Bi semiconductor alloys and their physical properties are still under investigation. Bi is the heaviest non-radioactive element [1]. The dilute bismide materials have large spin-orbit

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splitting energy and this allows the control of the effects of the Auger recombination for improving the temperature characteristic of novel devices.

Group III	Group V		Dilute Bismides
13 Al	15 P	Phosphide	InPBi
31 Ga	33 As	Arsenide	InAsBi
49 In	51 Sb	Antimonide	InSbBi
81 Tl	83 Bi	Bismide	

Figure 1. III-V-Bi group elements in the periodic table for compound semiconductor

The A^{III}-B^{V} compounds of the elements Al, Ga and In with the elements P, As and Sb have the (cubic) B3 type of structure [2]. Replacement of As, P and Sb by Bi in binaries change the crystal structure. The III-V bismide materials are a new family and novel research subject of optoelectronic materials. The research on III-V bismide starts with $InSb_{1-x}Bi_x$ material was grown on InSb substrates [3-5]. In 1990, Ma et al. and Fang et al. have demonstrated $InAs_{1-x}Bi_x$ used in the IR photodetectors on InAs substrates with Bi composition [6]. In these studies, the bandgap is reduced with the addition of a small amount of bismuth concentration. Bi is incorporated into III-Vs, Bi will form impurity levels close to the valence band and restructuring the host material [7]. The Bi interacts with the impurity level and splits the heavy and light hole energy bands. The bandgap of InP is 1.35 eV at room temperature and will be reduced by incorporating Bi to regulate the material bandgap [6, 8-12]. In $InP_{1-x}Bi_x$ alloy, the incorporated Bi atoms are believed to replace P atoms.

The bandgap of InBi with special properties and stable structure of PbO phase are very small [9]. The small amount of Bi acts as a surfactant in the growth process and does not reduce electron mobility [13, 14]. The smoother surface and mobility processes improving the optical properties of the materials. The indium (In) based dilute bismides are potential candidates for mid- and far-infrared optoelectronics applications [3, 15]. The super luminescence diodes of $InP_{1-x}Bi_x$ with the wavelength of 1.4–2.7 μm at room temperature are attractive in optical coherence tomography. In this paper, the properties of InSbBi, InAsBi, and InPBi are investigated.

2. Methods

The theoretical bandgap of dilute bismides are calculated and used to determine the optical parameters. The addition of a small amount of Bi into binary compounds InAs, InP, and InSb are used to grow their ternary alloys InAsBi, InPBi, and InSbBi. The bandgap of dilute bismides has been obtained by researchers by using different models and methods [16-18]. The InSbBi, and InAsBi are narrow band gap semiconductors and InPBi is another important member of the III–V-bismide family of medium band gap semiconductor alloys. The variation of bandgap energy versus the composition of Bi is given in Figure 2. As shown in the figure, the bandgap energy of alloys decreases nonlinearly with increasing Bi composition, and it remains a semiconductor. These results are good agreement with literature [16].

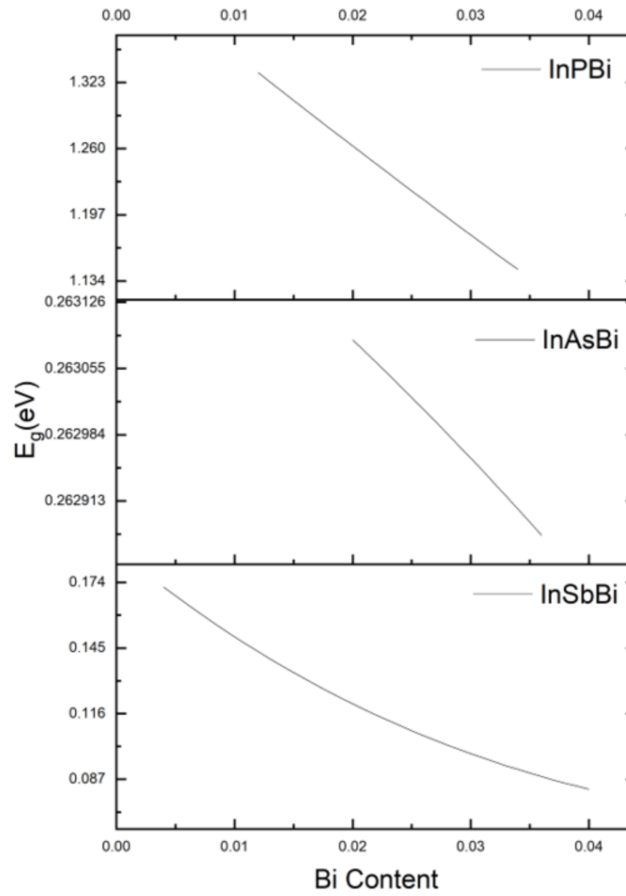

Figure 2. The calculated bandgap energies for Bi concentration incorporated III-V semiconductors.

The bandgap reduction of $InP_{1-x}Bi_x$ is due to the electronic states consist of Bi-6p states around the Fermi level. The InAsBi and InSbBi are narrow gap dilute bismides as shown in Figure 2. The small amount of Bi concentrations was chosen due to the rapid increase in the spin split-off band ($\Delta_{SO} > E_g$) with increasing Bi. The refractive index strongly depends on the bandgap of the materials. The characteristics and efficiencies of designed optoelectronic devices are mainly related to the refractive index difference between the layers. The refractive index, extinction coefficient, and absorption coefficient are strongly connected to the complex dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \tag{1}$$

The linear optical response of a system to the external electromagnetic field is illustrated using directly associated dielectric function. The dielectric function is the major parameter and used to determine optical parameters. The complex refractive index $n(\omega)$ is now given by

$$n(\omega) = n_{real}(\omega) + in_{Imaginary}(\omega) = \varepsilon(\omega)^{1/2} \tag{2}$$

where $n_{real}(\omega)$ is the real part of the refractive index and $n_{imaginary}(\omega)$ is the imaginary part and is called the extinction coefficient or the attenuation index. These optical constants are real and positive numbers. The absorption coefficient $\alpha(\omega)$ is a function of dielectric functions and the light wavelength in the vacuum. The ε_1 and ε_2 are calculated by using Adachi's methods in the entire range of photon energies. The peaks in these figures indicate the positions of critical points such as the fundamental absorption edge (E_0), interband critical energies (E_1 and $E_1+\Delta_{E1}$), and other related

energies of materials. The explanation of these contributions of energies and used equations are given in Reference [19].

3. Results and Discussion

The optical constants are necessary for analysing and designing new optical and photonic devices. The optical properties of the semiconductor alloys are obtained by determining the dielectric function ε(ω). The peaks of the optical dielectric functions are consistent with the electronic gap energies of the alloys . The imaginary part of the dielectric function is a function of the absorption spectrum calculated using material parameters related to given and transition energies [19].

Table 1. Parameters used in the calculation of optical dispersion relations.

Parameters	InAs	InSh	InP	InBi
E_0 (eV)	0.357	0.182	1.348	-1.63*
Δ_0(eV)	0.357	0.182	0.102	
E_1 (eV)	2.50	1.80	3.10	2.256
$E_1 + \Delta_1$ (eV)	2.78	2.30	3.25	
E_2 (eV)	4.45	3.9	4.7	4.89
E_g^{1D} (eV)	1.07	0.93	2.05	
A ($eV^{1.5}$)	0.61	0.19	6.57	
B_1	6.59	6.37	4.93	
B_{11} ($eV^{-0.5}$)	13.76	12.26	10.43	
Γ(eV)	0.21	0.16	0.10	
C	1.78	5.37	1.49	
Γ	0.108	0.318	0.094	
D	20.80	19.50	60.4	
$\varepsilon_{1,inf}$	2.80	3.10	1.60	

The used values are mostly taken from Reference [19] and *Reference [20, 21].

The interband transition energies have a role in optical properties. The used parameters were given in Table 1. The Vegard's law applied to calculate to determine some parameters.

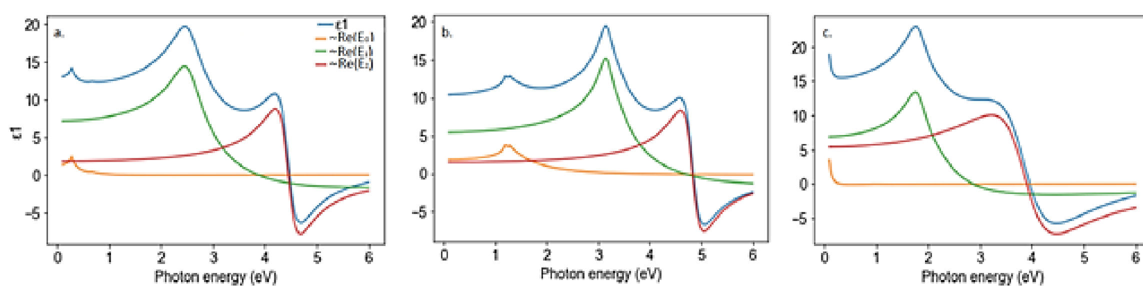

Figure 3. The contribution of transition energies of ε_1 for a. InAsBi, b. InPBi and c. InSbBi alloys at Bi composition of x=0.03.

The dielectric constant is a property of an electrical insulating material that provides a measure of its effect on a capacitor. The knowledge of its value is required to properly design and apply devices. The photon energy (frequency) dependent dielectric function in the spectral range upto 6.0 eV was calculated for Bi content of x=0.003. The peaks of three In based dilute bismides were given in the following figures. The peaks in the dielectric functions are due to excited interband transitions and have different points due to the selected type of dilute bismides.

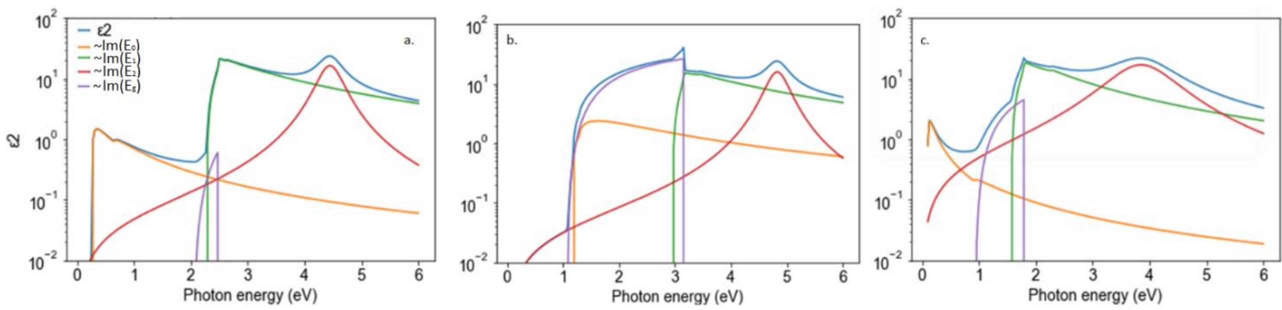

Figure 4. The contribution of transition energies of ε_2 for a. InAsBi, b. InPBi and c. InSbBi alloys at Bi composition of x=0.03.

The optical quantities of absorption coefficient α(ω), the real part of the dielectric function $\varepsilon_1(\omega)$, $\varepsilon_2(\omega)$ and the refractive index n(ω) for InAsBi, InSbBi and InPBi are plotted in Figure 3 - 5. The fundamental absorption edges shift towards higher energies. The peaks in the result shows the change energy gap. In the dispersion curve of the refractive index in Figure 5, there are two remarkable peaks located at calculated energies of 2.5 eV, 3.0 and 2.5 eV for InAsBi, InPbi and InSbBi, respectively. The result shows the same behaviour obtained for the alloys. The variation of the imaginary part of dielectric function $\varepsilon_2(\omega)$ of the alloys show that the critical points shift towards the higher energies in the order of Sb, As and P.

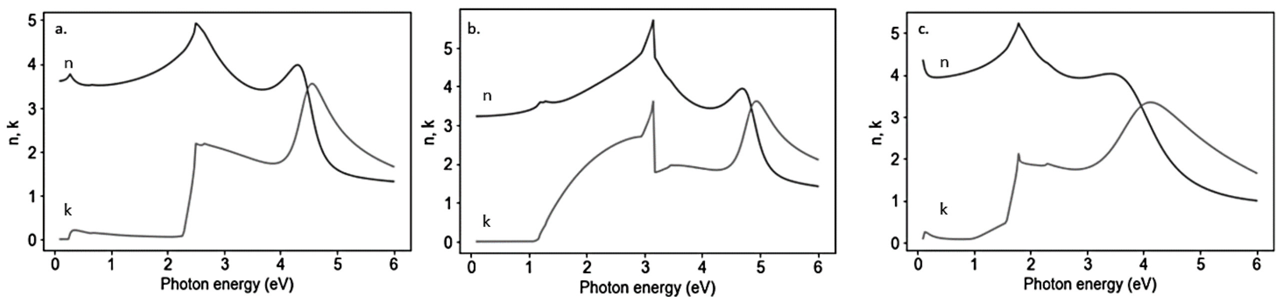

Figure 5. The calculated spectral dependence of n and k for a. InAsBi, b. InPBi and c. InSbBi alloys at Bi composition of x=0.03.

The calculated spectral dependence of n and k for InAsBi, InPBi, and InSbBi alloys at Bi composition of x=0.03. The refractive index at 700 nm of n_{InAs}= 3.8363, n_{InP}= 3.4876 and n_{InSb}= 4.8661 [22]. The strongest peak in the refractive index values occurs in the region near the E_1 edge. The interesting line shape of k is also presented in Figure 5.

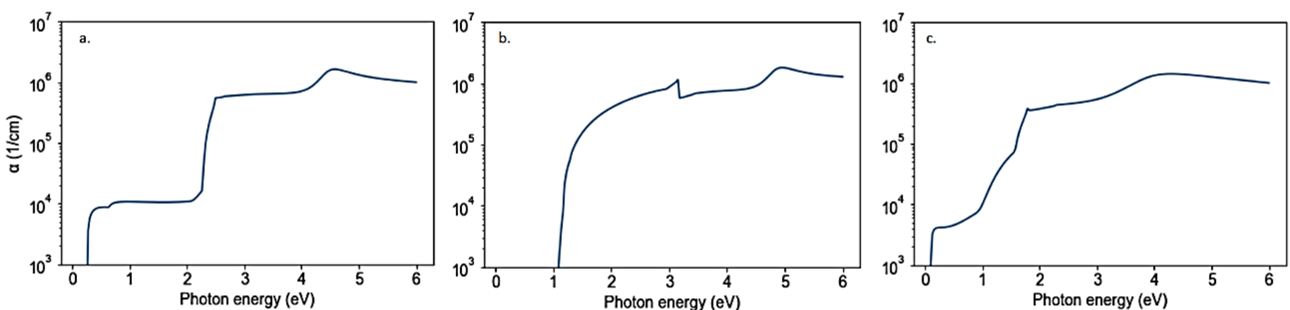

Figure 6. The calculated absorption coefficient (α)for a. InAsBi, b. InPBi and c. InSbBi alloys at Bi composition of x=0.03.

The absorption coefficient around the optical bandgap is proportional to $(E - E_g)^{1/2}$ where E is the photon energy for the interband transition. The optical parameters are determined from calculated dielectric parameters of ε_1 and ε_2.

4. Conclusion

The incorporation of Bi into the binaries results in a modification of the bandgap energy the host semiconductors in the valence band structure. Recent progresses on molecular beam epitaxy of novel III—Bi-V semiconductor alloys were easily growth. The calculated optical constants, the refractive index, extinction coefficient, and absorption coefficient, of some dilute bismides are demonstrated at photon energies up to 6.0 eV by using the Adachi's model. The bandgap energy decreased with increasing Bi content and used in the calculation of optical constants. The properties of III-V dilute bismides with temperature insensitive bandgap are very important for semiconductor devices. The understanding of the optical properties of In-V-Bi semiconductor alloys is necessary for designing practical optoelectronic devices for a wide range of applications for the optical communication window.

References

[1]. Alberi, K., J. Wu, W. Walukiewicz, K. Yu, O. Dubon, S. Watkins, et al., *Valence-band anticrossing in mismatched III-V semiconductor alloys.* Physical Review B,, 2007. **75**(4): p. 045203.

[2]. Meyer, R.T.W., J.J.A. Hofmans, and A.R. De Vroomen, *The de Haas-van Alphen effect in InBi.* Journal of Physics and Chemistry of Solids, 1974. **35**(3): p. 307-312.

[3]. Berding, M.A., A. Sher, A.B. Chen, and W. Miller, *Structural properties of bismuthbearing semiconductor alloys.* Journal of Applied Physics, 1988. **63**(1): p. 107-115.

[4]. D. P. Samajdar, T.D.D., S. Dhar, *Physics of Semiconductor Devices*. 2014, Cham: Springer.

[5]. Polak, M., P. Scharoch, and R. Kudrawiec, *First-principles calculations of bismuth induced changes in the band structure of dilute Ga–V–Bi and In–V–Bi alloys: chemical trends versus experimental data.* Semiconductor Science and Technology, 2015. **30**(9): p. 094001.

[6]. Zhang, X., P. Lu, L. Han, Z. Yu, J. Chen, and S. Wang, *Structural and electronic properties of InPBi alloys.* Modern Physics Letters B, 2014. **28**(17): p. 1450140.

[7]. Francoeur, S., M.-J. Seong, A. Mascarenhas, S. Tixier, M. Adamcyk, and T. Tiedje, *Band gap of GaAs1−xBix, 0< x < 3.6%.* Applied Physics Letters, 2003. **82**(22): p. 3874–3876.

[8]. X. Chen, W.S., D. Liang et al., Opt. Mater. Express 2018. **8**: p. 1184.

[9]. X. Zhang, P.L., L. Han et al., Mod. Phys. Lett. B 2014. **28**.

[10]. G.N. Wei, X.D., Q. Feng et al., Sci. China Phys. Mech. Astron. , 2017. **60**(047022).

[11]. Kopaczek, J., R. Kudrawiec, M. Polak, P. Scharoch, M. Birkett, T. Veal, et al., *Contactless electroreflectance and theoretical studies of band gap and spin-orbit splitting in InP1−xBix dilute bismide with x ≤ 0.034.* 0.034. Applied Physics Letters, 2014. **105**(22): p. 222104.

[12]. Köksal, K., B. Gönül, and M. Oduncuoğlu, *Critical layer thickness of GaIn(N)As(Sb) QWs on GaAs and InP substrates for (001) and (111) orientations.* The European Physical Journal B, 2009. **69**(2): p. 211-218.

[13]. Pan, W., P. Wang, X. Wu, K. Wang, J. Cui, L. Yue, et al., *Growth and material properties of InPBi thin films using gas source molecular beam epitaxy.* Journal of Alloys and Compounds, 2016: p. 777-783.

[14]. Naceur, H.B., T. Mzoughi, I. Moussa, L. Nguyen, A. Rebey, and B. El Jani, *Surfactant effect of bismuth in atmospheric pressure MOVPE growth of InAs layers on (100) GaAs substrates.* Physica E: Low-dimensional Systems and Nanostructures, 2010. **43**(1): p. 106-110.

[15]. Oduncuoğlu, M. and B. Gönül, *A theoretical comparison of the 1.3µm doped InxGa1−xNyAs1−y/GaAs quantum well lasers for different x/y concentrations.* Physica E: Low-dimensional Systems and Nanostructures, 2005. **27**(1): p. 253-261.
[16]. Linhart, W.M. and R. Kudrawiec, *Temperature dependence of band gaps in dilute bismides.* Semiconductor Science and Technology, 2018. **33**(7): p. 073001.
[17]. Sweeney, S.J., T.D. Eales, and I.P. Marko, *The physics of mid-infrared semiconductor materials and heterostructures*, in *Mid-infrared Optoelectronics*. 2020, Elsevier. p. 3-56.
[18]. Bushell, Z.L., et al., *Giant bowing of the band gap and spin-orbit splitting energy in GaP 1− x Bi x dilute bismide alloys.* 2019. **9**(1): p. 1-8.
[19]. Adachi, S., *Optical dispersion relations for GaP, GaAs, GaSb, InP, InAs, InSb, AlxGa1-xAs, and In1-xGax AsyP1-y* Journal of Applied Physics, 1989. **66**.
[20]. P. T. Webster, A.J.S., N. A. Riordan, C. Gogineni, H. Liang, A. R. Sharma, and S. R. Johnson, *Optical properties of InAsBi and optimal designs of lattice-matched and strainbalanced III-V semiconductor superlattices.* Journal of Applied Physics, 2016. **119**.
[21]. Vurgaftman I., M.J.R., Ram-Mohan L. R. , *Band parameters for III–V compound semiconductors and their alloys.* Journal of Applied Physics, 2001. **89**(11).
[22]. Aspnes, D.E. and A.J.P.r.B. Studna, *Dielectric functions and optical parameters of si, ge, gap, gaas, gasb, inp, inas, and insb from 1.5 to 6.0 ev.* 1983. **27**(2): p. 985.