

Theoretical Prediction of Some Physical Properties of $B_xAl_{1-x}Sb$ Ternary AlloysS. Daoud^{1,*}, P.K. Saini^{2,†}, H. Rekab-Djabri^{3,4,‡}¹ *Laboratoire Materiaux et Systemes Electroniques, Universite Mohamed Elbachir El Ibrahimi de Bordj Bou Arreridj, 34000 Bordj Bou Arreridj, Algeria*² *Department of Physics, Government College, Hansi, 125033 Haryana, India*³ *Laboratory of Micro and Nanophysics (LaMiN), Oran ENP, BP 1523, El M'Naouer, 31000 Oran, Algeria*⁴ *Faculty of Nature and Life Sciences and Earth Sciences, Akli Mohand-Oulhadj University, 10000 Bouira, Algeria*

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The present contribution aims to determine several significant properties of $B_xAl_{1-x}Sb$ ($0 \leq x \leq 1$) ternary semiconducting alloys. The nearest-neighbor distance, mass density, plasmon energy, bulk modulus, melting point, electronic polarizability, lattice energy density and microhardness as a function of boron concentration x were predicted using only the theoretical lattice constants reported in the literature. Except the bond-length and electronic polarizability, which decrease with increasing x , all other quantities increase gradually and monotonically with increasing boron content x . This suggests that when more boron atoms are incorporated into AlSb, the hardness of the material in question becomes more important. So, with the increase in x , the metallic characteristic of $B_xAl_{1-x}Sb$ decreases from Al–Sb bond to B–Sb bond, accompanied by an increase in the magnitude of these quantities. In order to test the incertitude of the method used in the present work, we compare our data for BSb and AlSb binary compounds. In general, our data for BSb and AlSb agree well with other values available in the literature. In addition, we think that there is no data reported in the literature on the different properties studied here for $B_xAl_{1-x}Sb$ ternary alloys.

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1. INTRODUCTION

Most binary III-V materials (AlP, AlSb, GaP, GaAs, GaSb, BSb, etc.) constitute one of the important classes of functional materials [1]. In recent years, III-V binary compounds and their alloys were studied intensively because of their potential application in high-frequency and high-power devices, light emitting diodes, optical communication systems, laser diodes, high efficiency solar cells, and sensors [2].

Under normal conditions (low pressures and room temperature), most of III-V compounds crystallize in zinc-blende (B3) phase [3]. Other materials, especially BN, AlN and GaN, crystallize in either cubic or hexagonal phases [3, 4]. The common and dominant feature of these two structures is the tetrahedral bonding to four atoms of the other elements. In B3 phase, these tetrahedra are arranged in a cubic-type configuration, while in wurtzite (B4) they are in a hexagonal-type [3].

The application of hydrostatic pressure to crystals often leads to a transformation from the most energetically stable phase to another, resulting in an increase in the hardness of the solid. Based on the first-principles full-potential linear augmented plane wave (FP-LAPW) approach within the density functional theory (DFT) framework, Salehi and co-authors [5] have studied several physical properties of binary antimonide compounds under hydrostatic pressures. Their results predict that the transition from B3 to B1 phase occurs at 48.5 GPa for BSb, 9.5 GPa for AlSb, 5.87 GPa for GaSb, and 3.15 GPa for InSb, respectively.

Using the plasma oscillations theory of solids, Ku-

mar and co-authors [6] have established several empirical relations for the calculation of the bulk modulus and microhardness H of group IV, II-VI, III-V, I-III-VI₂ and II-IV-V₂ semiconductors with tetrahedral structure. The maximum average deviation of 22.18 % has been found in the case of H of III-V materials.

Varshney et al. [7] have investigated the pressure-induced phase transition, elastic constants and thermal properties of BSb, AlSb, GaSb and InSb binary semiconducting compounds.

Using both the rigid ion model (RIM) and deformation bond approximation model (DBA), Shinde et al. [8] have studied the pressure-dependent phonon dispersion, phonon density of states, and mode Grüneisen parameters for some III-B semiconductors, while Fares and Bouarissa [9] have investigated the electron and positron band structures and some other properties of cubic zinc-blende $Al_xIn_{1-x}Sb$ ternary semiconducting alloys using a pseudopotential approach under the virtual crystal approximation (VCA).

Recently, the structural parameters and piezoelectric coefficients of BSb under compression have been studied using the pseudopotential plane wave method in the framework of the DFT and the density functional perturbation theory (DFPT) [10]. Interestingly, the synthesis of $B_xAl_{1-x}Sb$ ternary semiconducting alloys has not yet been reported. In the present paper, we determine several properties of $B_xAl_{1-x}Sb$ ternary semiconducting alloys. The lattice constants used here are taken from the work of Benchehima et al. [1] obtained from the local density approximation (LDA).

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2. THEORY

Experimentally, X-ray diffraction (XRD) and several other techniques are used to determine the structure and to measure the lattice parameters of any crystal. Using the lattice constant a of a cubic zinc-blende structure, the spacing between the neighboring atoms is equal to $a/\sqrt{2}$, while the chemical bond-length (called also the bond distance) d can be written as [4]:

$$d = (\sqrt{3}/4) a . \quad (1)$$

Because the standard errors of the lattice constants are usually small enough to make an insignificant contribution to errors in bond-length, they are usually not considered in the calculation.

The mass density ρ is related to the atomic arrangement and corresponding electron density map; it can be calculated as follows [4]:

$$\rho = 4M/NV, \quad (2)$$

where M is the molecular weight, N is the Avogadro constant, and V is the volume of the unit cell. In a cubic crystal, the volume of the unit cell V and the lattice constant a are related as $V = a^3$ [4].

The bulk modulus B is an important mechanical quantity. It is a measure of resistance of materials to volume variation (hydrostatic compression). Usually B increases with increasing pressure, and decreases with enhancing temperature. More empirical approaches have been developed to correlate the bulk modulus and other physical parameters (bond-length, melting point, microhardness, electronic susceptibility etc.) of materials. It is also related to the plasmon frequency, and through the Planck's equation to the plasmon energy $\hbar\omega_p$. For group III-V binary materials, the plasmon energy $\hbar\omega_p$ is given by the relation [11-13]

$$\hbar\omega_p = 28.8 \left(Z' \rho / W \right)^{1/2} \quad (3)$$

where Z' is the effective number of electrons taking part in plasma oscillations, ρ is the mass density, and W is the molecular weight.

For group IV, III-V, and II-VI semiconducting materials, the bulk modulus B is given as follows [14]:

$$B = \frac{N_c}{4} \frac{(1972 - 200I)}{d^{3.5}}, \quad (4)$$

where N_c is the average coordination number (for tetrahedral semiconducting materials $N_c = 4$), I is an empirical ionicity parameter, its numerical value is taken equal to $I = 0, 1$, and 2 for group IV, III-V, and II-VI semiconductors, respectively, and d is the bond-length parameter (expressed in Å). Although Eq. (4) was reported for group IV, III-V, and II-VI binary materials, it is quite reasonable that Eq. (4) can also be used to describe B for $B_xAl_{1-x}Sb$ ternary alloys.

3. DISCUSSION OF RESULTS

3.1 Structural Parameters and Plasmon Energy

Using the theoretical lattice constants obtained by Benchehima et al. [1], the dependences of the chemical bond-length d and the density ρ of cubic zinc-blende $B_xAl_{1-x}Sb$ ternary semiconducting alloys as a function of boron concentration x are plotted in Fig. 1. The crystal density ρ of AlSb was found to be 4.352 g/cm^3 , while that of BSb is equal to 6.281 g/cm^3 . Although our value of ρ for AlSb is slightly higher than the theoretical result (3.953 g/cm^3) reported by Salehi et al. [5], it is in good agreement with the experimental value 4.2775 g/cm^3 quoted by Adachi [4]. Our value of ρ for AlSb overestimates the experimental one reported by Adachi [4] by less than 1.75 %, while that (6.281 g/cm^3) of BSb underestimates the result (6.488 g/cm^3) reported by Daoud [10] by around 3.19 %. It can be noted that the value 3.953 g/cm^3 of ρ reported by Salehi and co-authors [5] for AlSb is not correct. By using the value 6.2230 Å of the equilibrium lattice parameter obtained by Salehi et al. [5], the correct value in Ref. [4] is 4.100 g/cm^3 , which is in general agreement with the experimental one 4.2775 g/cm^3 quoted in Ref. [4].

The bond distance d and the density ρ of $B_xAl_{1-x}Sb$ material in B3 structure as a function of boron concentration x are given by the following quadratic fits:

$$d = 2.645 - 0.2544x - 0.1406x^2, \quad (5)$$

$$\rho = 4.3520 + 0.5011x + 1.4009x^2, \quad (6)$$

where the bond distance d and the mass density ρ are expressed in Å and g/cm^3 , respectively.

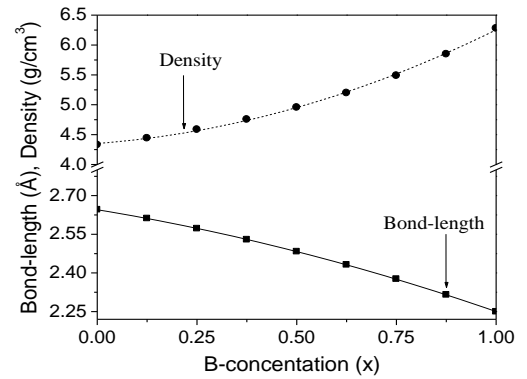


Fig. 1 – Variations of the bonding distance d and mass density ρ of $B_xAl_{1-x}Sb$ alloys with boron concentration x

By substituting our values of the mass density ρ into Eq. (3), the plasmon energy $\hbar\omega_p$ was calculated. The plasmon energy $\hbar\omega_p$ of AlSb and BSb was found to be 13.90 and 17.73 eV, respectively. Once $\hbar\omega_p$ is determined, we would like to compare our results with experiments or predict what an experiment would yield for $\hbar\omega_p$. Our computed values of $\hbar\omega_p$ are in very good agreement with other data existing in the literature [12, 13]. Our value (13.90 eV) of $\hbar\omega_p$ for AlSb overestimates the result (13.72 eV) reported by Kumar and co-authors [13] by around 1.31 %, while that (17.73 eV) of BSb overestimates the theoretical value (17.26 eV) reported by Bioud et al. [12] by about 2.72 %.

Fig. 2 presents the variation of $\hbar\omega_p$ for $B_xAl_{1-x}Sb$ material as a function of x . From the graph shown in Fig. 2, we can see that $\hbar\omega_p$ varies non-linearly with the

boron concentration x . The calculated plasmon energy $\hbar\omega_p$ follows an increasing quadratic function of boron content x , $\hbar\omega_p = 13.93 + 1.67x + 2.10x^2$.

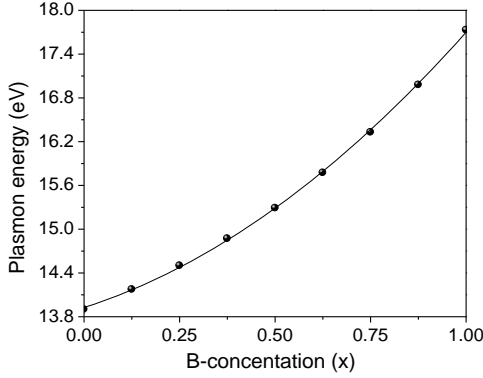


Fig. 2 – Variation of $\hbar\omega_p$ for $B_xAl_{1-x}Sb$ alloys as a function of x

3.2 Bulk Modulus and Melting Point

By substituting the calculated bond distance d into Eq. (4), the bulk modulus B has been evaluated. The value of B for AlSb is equal to 58.16 GPa, while that of BSb is 102.62 GPa. Our results of B for both AlSb and BSb binary compounds are in excellent agreement with the experimental and other theoretical values of the literature [4, 15]. Our obtained value (58.16 GPa) of B for AlSb underestimates the experimental one (58.2 GPa) reported by Adachi [4] by only around 0.07 %, while our data (102.62 GPa) for BSb underestimates the theoretical value (103 GPa) reported by Zaoui and El Haj Hassan [15] by around 0.37 %.

The composition dependence of the bulk modulus B for zinc-blende $B_xAl_{1-x}Sb$ with the data reported by Benchehima et al. [1] is illustrated in Fig. 3.

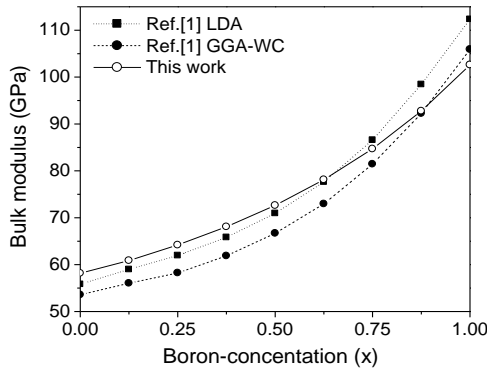


Fig. 3 – Variations of B for $B_xAl_{1-x}Sb$ alloys as a function of x

Note that B increases monotonically with increasing boron content x from 0 to 1. The increase in B with increasing x is expected from the decrease in the bond distance d (see Eq. (4)). We note a quadratic increase in B with the decrease in the bond distance from AlSb to BSb as shown in Fig. 3. This suggests that when more boron atoms are incorporated into AlSb, the hardness of the material in question becomes more important. For $B_xAl_{1-x}Sb$ alloys, with the increase in x (the decrease in the atomic number), the metallic characteristic decreases from Al–Sb bond to B–Sb bond, accompa-

nied by an increase in the magnitude of B . The best fit of our data on B for $B_xAl_{1-x}Sb$ as a function of x obeys the expression: $B = 58.68 + 12.25x + 31.02x^2$.

For several materials with a cubic structure, the melting point T_m correlates with the bulk modulus B by the following empirical expression [16]:

$$T_m = 607 + 9.3B, \quad (7)$$

where the bulk modulus B is expressed in GPa, while the melting point T_m is expressed in K.

The variation of T_m as a function of boron content x in $B_xAl_{1-x}Sb$ alloys is plotted in Fig. 4. We observe that T_m increases monotonically with increasing x . The fit of our data on T_m as a function of x obeys this quadratic expression: $T_m = 1152.76 + 113.96x + 288.46x^2$.

The melting point T_m of AlSb and BSb was found to be 1147.9 and 1561.4 K, respectively. Although our value of T_m for AlSb is slightly lower than the experimental one (1338 K) reported by Adachi [4], that (1561.4 K) of BSb is in general agreement with the theoretical ones 1500 and 1696±300 K reported by Bioud et al. [12] and Deligöz et al. [17], respectively.

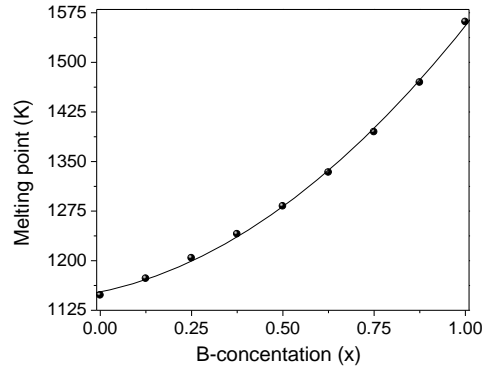


Fig. 4 – Dependence of T_m for $B_xAl_{1-x}Sb$ as a function of x

3.3 Electronic Polarizability and Lattice Energy Density

Polarizability is an important physical parameter, which is related to many other physical quantities, such as electro-optical effect, optical nonlinearity and dielectric properties [18]. If we know the bulk modulus B , molecular weight of the material M and its crystal density, it is usually possible to predict the electronic polarizability α_p as follows [19]:

$$\alpha_p = 0.395 \times 10^{-24} \left[\frac{(5.563 - 0.033B)^2 - 1}{(5.563 - 0.033B)^2 + 2} \right] \times \frac{M}{\rho} \quad (8)$$

The electronic polarizability α_p of AlSb is equal to 10.90 \AA^3 and that of BSb is 4.63 \AA^3 . Although our value of α_p for AlSb is slightly higher than the result 7.14 \AA^3 reported by Reddy et al. [19] and that (4.63 \AA^3) of BSb is slightly lower than the result 5.77 \AA^3 reported in Ref. [12], our value of α_p for AlSb is in good agreement with the value (9.65 \AA^3) reported by Moss [20].

Fig. 5 presents the variation of α_p for $B_xAl_{1-x}Sb$ as a function of x . We observe that the electronic polarizability α_p decreases monotonically with increasing x . The fit of our data regarding α_p as a function of x obeys the

following expression: $a_p = 10.87 - 3.57x - 2.60x^2$.

For many ANB^{8-N} crystals, Zhao et al. [18] have found an inverse proportionality between the lattice energy density U and the electronic polarizability a_p . The correlation between U and a_p is given as follows:

$$U = pa_p^q, \quad (9)$$

where U is expressed in 10^9 J.m^{-3} and a_p is expressed in \AA^3 , p and q are two constants which depend on the type of crystals. They are described from the view point of microscopic electronic structure by using some important bond parameters such as bond length and ionicity, the numerical values of p and q are 1835.503 and -0.938 , respectively, for III-V group [18].

Using the previous expression, the lattice energy density U of AlSb was found equal to $195.3 \cdot 10^9 \text{ J.m}^{-3}$ and that of BSb is around $436.4 \cdot 10^9 \text{ J.m}^{-3}$. The variation of U as a function of boron content x in $B_x\text{Al}_{1-x}\text{Sb}$ alloys is also presented in Fig. 5. The fit of our data on U as a function of x obeys the following polynomial expression: $U = 192.88 + 145.32x - 53.27x^2 + 348.14x^3$.

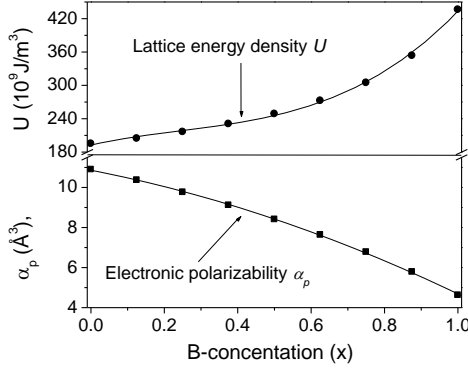


Fig. 5 – Variations of a_p and U for $B_x\text{Al}_{1-x}\text{Sb}$ as a function of x

A material with a higher lattice energy density implies a lower electronic polarizability. The lower electronic polarizability reflects the powerful chemical bonding in the crystal [18]. Hence, the distortion of the electron charge clouds of anions by the positive charge of the cation is not easy in BSb compared to the AlSb compound.

3.4 Microhardness

A hardness test can usually serve for the characterization of the mechanical behavior of solids. Although different techniques may be used to measure the microhardness H of semiconductors, generally, the most commonly employed is that of Knoop and Vickers methods. For groups II-VI and III-V semiconductors having tetrahedral structure, Bahadur and Mishra [11] have developed a simple empirical model based on the plasma oscillations theory of solids for the calculation of H which is expressed as follows:

$$H = \beta r_s^{-5.57}, \quad (10)$$

where β is a constant, its numerical value is 365.86 for III-V group compounds, and the electron density parameter r_s is expressed as follows [11]:

$$r_s = 1.388 a_0 (W / Z' \rho)^{1/2} \quad (11)$$

where a_0 is the Bohr radius, W is the molecular weight of the compound, Z' is the effective number of electrons taking part in plasma oscillations, and ρ is the density. The electron density parameter r_s and the bond-length d are also related by: $d = 1.173r_s$ [11].

Using the previous expressions, the microhardness H of AlSb was found equal to 3.94 GPa, while that of BSb was found to be 9.73 GPa. Our values of H are in excellent agreement with the values 4.0 and 9.80 GPa reported by Adachi [4] and Bioud et al. [12], respectively. The accord between our obtained values and those quoted in Ref. [4] and Ref. [12] is, respectively, within 1.5 % for AlSb and 0.72 % for BSb.

The evolution of H as a function of boron content x in $B_x\text{Al}_{1-x}\text{Sb}$ alloys is also plotted in Fig. 6. Like the bulk modulus, the microhardness H increases monotonically with increasing x . The behavior of H versus x indicates that the hardness of the material of interest becomes better when more boron atoms are added into AlSb. The fit of H for $B_x\text{Al}_{1-x}\text{Sb}$ alloys as a function of x obeys this expression: $H = 4.04 + 0.66x + 4.90x^2$.

For many semiconductors with a tetrahedral structure, the microhardness H and $\hbar\omega_p$ are related by [6]:

$$H = K_1 (\hbar\omega_p)^{7/3} - K_2, \quad (12)$$

where H and $\hbar\omega_p$ are expressed in GPa and eV, respectively, K_1 and K_2 are two constants, the numerical values of K_1 and K_2 are 0.0202 and 5.743, respectively, for III-V semiconducting materials.

By substituting our values of $\hbar\omega_p$ into Eq. (12), the microhardness H of AlSb was found at around 3.64 GPa, while that of BSb was found to be 10.81 GPa. The variation of H as a function of x in $B_x\text{Al}_{1-x}\text{Sb}$ alloys is also plotted in Fig. 6. The calculated microhardness H corresponds to an increasing quadratic function of boron concentration x , $H = 3.73 + 1.98x + 5.00x^2$.

For cubic group IV, II-VI and III-V semiconductors, the Knoop microhardness H and the bulk modulus B are related by the following expression [4]:

$$H = 0.16B - 5.74. \quad (13)$$

Using Eq. (13), the values of H for AlSb and BSb were found at around 3.57 and 10.68 GPa, respectively. These two values are in very good agreement with the results obtained from Eq. (10) and Eq. (12). The variation of H as a function of x in $B_x\text{Al}_{1-x}\text{Sb}$ alloys is also plotted in Fig. 6. The best quadratic fit of H for $B_x\text{Al}_{1-x}\text{Sb}$ as a function of boron content x obeys this expression: $H = 3.65 + 1.96x + 4.96x^2$.

4. CONCLUSIONS

Based only on the lattice constants reported in the literature, the present work aims to calculate several properties of $B_x\text{Al}_{1-x}\text{Sb}$ ternary alloys. Our investigation shows that the plasmon energy, bulk modulus, melting point, lattice energy density, and microhardness increase gradually and monotonically with increasing boron concentration x , while the bonding distance and electronic polarizability decrease with increasing x . The

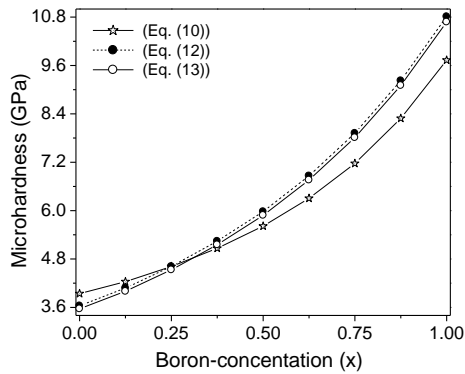


Fig. 6 – Dependence of H of $B_xAl_{1-x}Sb$ alloys as a function of x

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Теоретичне прогнозування деяких фізичних властивостей трикомпонентних сплавів $B_xAl_{1-x}Sb$

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Стаття спрямована на визначення кількох важливих властивостей трикомпонентних напівпровідникових сплавів $B_xAl_{1-x}Sb$ ($0 \leq x \leq 1$). Відстань до найближчого сусіда, масова густина, енергія плазмону, модуль об'ємної пружності, температура плавлення, електронна поляризація, густина енергії решітки та мікротвердість як функції концентрації бору x були передбачені з використанням лише теоретичних сталих решітки, про які повідомляється в літературі. За винятком довжини зв'язку та електронної поляризованості, які зменшуються із збільшенням x , усі інші величини збільшуються поступово та монотонно із збільшенням вмісту бору x . Це свідчить про те, що коли більше атомів бору включено до AlSb, твердість матеріалу, про який йде мова, стає більшою. Отже, із збільшенням x металева характеристика $B_xAl_{1-x}Sb$ зменшується від зв'язку Al-Sb до зв'язку B-Sb, що супроводжується збільшенням цих величин. Для того, щоб перевірити невизначеність методу, використаного в цій роботі, ми порівнюємо наші дані для бінарних сполук BSb та AlSb. Загалом, наші дані щодо BSb та AlSb добре узгоджуються з іншими значеннями, доступними в літературі. Крім того, ми вважаємо, що в літературі немає даних про різні властивості, що вивчаються тут для трикомпонентних сплавів $B_xAl_{1-x}Sb$.

Ключові слова: Сплави $B_xAl_{1-x}Sb$, Довжина зв'язку, Енергія плазмону, Електронна поляризація, Мікротвердість.