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Research paper

Plasmon energy and microhardness of $B_xAl_{1-x}Sb$ alloys: semi-empirical prediction

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Abstract

Based on the reflective index reported in the literature, the present work aims to investigate the plasmon energy, the microhardness and the homopolar band gap energy of $B_xAl_{1-x}Sb$ ternary semiconducting alloys as a function of boron concentration x in the range 0 –1. We found that both the plasmon energy and the microhardness of $B_xAl_{1-x}Sb$ alloys change gradually but not monotonically with increasing of boron concentration x from 0 to 1, while the homopolar band gap energy increases monotonically with enhancing of x.

We emphasize that a boron concentration x dependent plasmon energy and microhardness between 0 and 1 is extremely unusual behavior for $B_xAl_{1-x}Sb$ alloys. Normally, both plasmon energy and the microhardness monotonically increase with increasing boron concentration x as it was mentioned in the literature. The plasmon energy of AlSb and BSb was found to be 16.14 and 15.58 eV, respectively. Our value (16.14 eV) of the plasmon energy for AlSb compound is higher than the result (13.8 eV) reported by Böer and Pohl. The minimum of the plasmon energy was found to be 14.4 eV for both $B_{0.5}Al_{0.5}Sb$ and $B_{0.625}Al_{0.375}Sb$ alloys.

The microhardness of AlSb was found at around 7.56 GPa, while that of BSb was found to be 6.51 GPa. Similar to the plasmon energy, the minimum value of the microhardness was found to be 4.45 GPa for both $B_{0.5}Al_{0.5}Sb$ and $B_{0.625}Al_{0.375}Sb$ alloys.

Keywords: *A^NB^{8-N} Semiconductors; Reflective Index; Plasmon Energy; Microhardness; $B_xAl_{1-x}Sb$ Alloys.*

1. Introduction

Because of their technical and scientific importance for optoelectronic device applications, recently A^NB^{8-N} tetrahedrally coordinated semiconducting materials have been extensively studied [1-13]. When several possible atomic configurations are considered, the solid crystallizes in a modification that maximizes the number of atoms in a given volume [2]. This configuration represents the state of lowest potential energy of the crystal, which is the most stable one [2]. Most of A^NB^{8-N} binary semiconducting compounds have the zinc-blende crystallographic structure [3-6]. Kr. Pathak et al. [7] have investigated the composition effect on bond hardness and microhardness of semiconductors alloys. They found that the value of both bond hardness and microhardness tend to increase (decrease) with decrease (increase) in ionic size of the doped ion relative to the host ion.

Daoud [8] has studied the correlation between the Debye temperature and the lattice thermal conductivity in II-VI and III-V semiconductors. In both families of semiconductors, He found that the lattice thermal conductivity correlates proportionally and linearly with the Debye temperature.

Using full potential linearized augmented plane wave (FP-LAPW) approach, Benchehima et al. [9] have studied the structural parameters, electronic band structures, densities of states and optical properties of the ordered $B_xAl_{1-x}Sb$ at different boron concentrations x.

Mezouar et al.[10] have predicted theoretically some interesting mechanical properties of $B_xAl_{1-x}Sb$ ternary semiconducting alloys. They found that all other physical quantities of $B_xAl_{1-x}Sb$ alloys change gradually and monotonically with increasing of boron concentration x in the range 0-1.

Using different empirical expressions, Daoud et al.[11] have calculated several physical parameters of $B_xAl_{1-x}Sb$ ternary semiconducting alloys. They mentioned also that all the nearest-neighbor distance, the mass density, the plasmon energy, the bulk modulus, the melting point, the electronic polarizability, the lattice energy density and the microhardness of $B_xAl_{1-x}Sb$ alloys change also gradually and monotonically with increasing of B concentration x. Some other works [14-18] studied mechanical, thermal, electronic and thermodynamic properties A^NB^{8-N} materials.

Based on the reflective index n values reported by Benchehima et al. [9], in the present work we predict the plasmon energy $\hbar\omega_p$ and the microhardness H of $B_xAl_{1-x}Sb$ semiconducting alloys as a function of boron concentration x in the range 0 – 1. So the accuracy of the data obtained here for both the plasmon energy and the microhardness of $B_xAl_{1-x}Sb$ alloys are limited by the correctness of the reflective index data reported by Benchehima et al. [9].

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2. Theory, results and discussion

The evaluation of refractive index n of a semiconducting material is of considerable importance for many optoelectronic applications, it is the key parameter for the optoelectronic devices [17]. For $B_xAl_{1-x}Sb$alloys, we observe that the results of the reflective index n reported by Benchehima et al. [9] are fitted with the following quadratic function: $n(x) = 1.562 - 3.054\ x + 2.472\ x^2$ [9]. It is very important to note that the previous quadratic fit is incorrect. Taken for example x = 0, which gives n(0) = 1.562, this value is very lower than the value 3.069 reported by Benchehima et al. [9] (see the Table 5 of the Ref. [9]). So an incorrect bowing parameter of the reflective index n reported in Ref. [9] for $B_xAl_{1-x}Sb$ alloys which is + 2.472. In Figure 1, we remade the fitting of the of the reflective index data reported by Benchehima et al. [9]. So the correct quadratic dependence of n reported by Benchehima et al. [9] versus the boron concentration x obeys the following variation: $n(x) = 3.060 + 1.161\ x - 1.041\ x^2$. Our data for the bowing parameter of the reflective index n for $B_xAl_{1-x}Sb$ alloys is − 1.041.

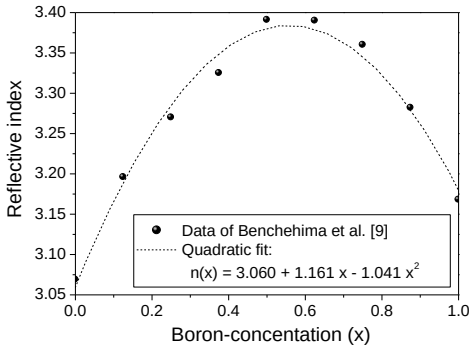

Fig. 1: Correct Quadratic Fit of the Reflective Index n Reported by Benchehima et al. [9] for $B_xAl_{1-x}Sb$ Alloys as a Function of x.

It shows that the energy band gap of semiconductor is inversely proportional to static value of dielectric constant which is explained by Penny model [19], given by the following relation: $\varepsilon(0) = 1 + (\hbar\omega_p / Eg)^2$ [20], where Eg is the energy gap which is related to the real part of the dielectric function, while $\hbar\omega_p$ is the valence electron plasmon energy. The value of the valence electron plasmon energy $\hbar\omega_p$ can be determined using the following empirical relationship [20]:

$$\hbar\omega_p = k_1 e^{-k_2 n} \tag{1}$$

where k_1, k_2 are two constants. The numerical values of the constants (k_1, k_2) are (22.079, 0.1779) and (47.924, 0.3546), respectively for II-VI and III-V group semiconductors [20].

Replacing the reflective index values reported by Benchehima et al. [9], into Eq. (1), the predicted values of the plasmon energy $\hbar\omega_p$ for $B_xAl_{1-x}Sb$ alloys are plotted in Figure 2, along the theoretical data of the Ref. [11]. We can observe clearly that the plasmon energy $\hbar\omega_p$ of $B_xAl_{1-x}Sb$ change gradually but not monotonically with increasing of boron concentration x in the range 0 –1. The best fit of our data on the plasmon energy $\hbar\omega_p$ (in eV) versus boron concentration x obeys the following expression: $\hbar\omega_p = 16.17 - 6.26\ x + 5.61\ x^2$.

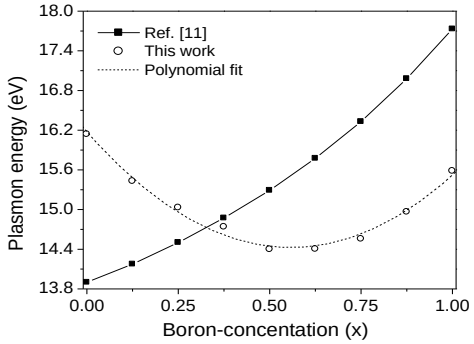

Fig. 2: Variation of $\hbar\omega_p$ for $B_xAl_{1-x}Sb$ Semiconducting Alloys as a Function of x, Along the Theoretical Data of the Ref. [11].

The plasmon energy $\hbar\omega_p$ of AlSb was found to be 16.14 eV, while that of BSb was found to be 15.58 eV, respectively. Our value (16.14 eV) of $\hbar\omega_p$ for AlSb compound is higher than the results 13.8 eV and 13.72 eV reported by Böer and Pohl [2] and Kumar et al. [21], respectively. Our value (15.58 eV) of $\hbar\omega_p$ for BSb compound is lower than the theoretical value 17.26 eV reported by Bioud et al.[22].

Bulk modulus B is still used as a preliminary measure of the hardness of material but in order to confirm it, other properties must also be taken into account [23].There are several approaches usually used to determine the microhardness H of materials [24-33]. Chen et al. [34] found that the hardness of polycrystalline materials correlated with the product of the squared Pugh's modulus ratio and the shear modulus, while Attard [35] found a linear function between the covalent charge and the reduced microhardness for several III-V semiconducting materials. For many semiconducting materials with tetrahedral structure, the microhardness H and the plasmon energy $\hbar\omega_p$ are related by $H = K_1 (\hbar\omega_p)^{7/3} - K_2$ [11], [21], where H and $\hbar\omega_p$ are expressed in GPa and in eV, respectively. K_1 and K_2 are two constants, the numerical values of the constants K_1 and K_2 are 0.0202 and 5.743, respectively for III–V semiconducting materials [21].

The variation of the microhardness H as a function of x in $B_xAl_{1-x}Sb$ alloys is displayed in Figure 3, along the data of the Ref. [11]. The best fit of our data on H (in GPa) versus boron concentration x obeys the following expression: $H = 7.58 - 11.12\ x + 9.94\ x^2$.

The microhardness H of AlSb was found 7.56 GPa, while that of BSb was found to be 6.51 GPa. The minimum value of H was found to be 4.45 GPa for both $B_{0.5}Al_{0.5}Sb$ and $B_{0.625}Al_{0.375}Sb$ semiconducting alloys. Experimentally, the microhardness H of solid is infected with

the density defects existing in the material [36]. Several techniques were usually used to characterize the defects in the solids, such as transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM), and time-of-flight secondary ion mass spectrometry (TOF-SIMS) [13].

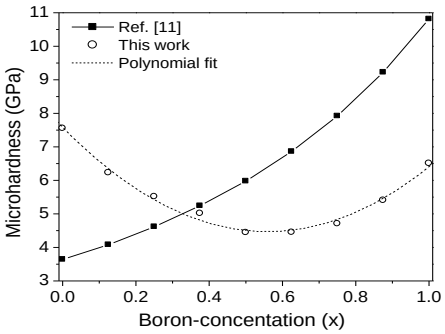

Fig. 3: Variation of the Microhardness H for $B_xAl_{1-x}Sb$ Alloys as a Function of x, Along the Theoretical Data of the Ref. [11].

Similarly to the plasmon energy, our obtained value (7.56 GPa) of the microhardness H for AlSb binary compound is higher than the experimental result (4 GPa) reported by Adachi [37], while our obtained value (6.51 GPa) of the microhardness for BSb compound is slightly lower than the theoretical value 9.80 GPa reported by Bioud et al.[22]. Our value (6.51 GPa) of H for BSb compound is very lower than the theoretical value 34.05 GPa reported by Kr. Pathak et al.[7]. To the best of our knowledge, there are no experimental data available in the literature on the microhardness H for BSb compound.

In the case of covalently bonded semiconducting materials, the homopolar or covalent contribution to the bonding is expressed as: $E_h = 39.74/(d^{2.5})$ [38], where d is the nearest-neighbor distance, which is expressed in Å, while E_h is expressed in eV. Using the nearest neighbor distance d deduced from the lattice parameters reported by Benchehima et al. [9], the variation of the homopolar band gap energy E_h as a function of x in $B_xAl_{1-x}Sb$ alloys is displayed in Figure 4. The polynomial fit of our obtained data on E_h (in eV) versus boron concentration x for $B_xAl_{1-x}Sb$ alloys obeys the following expression: $E_h = 0.433 + 0.077\ x + 0.134\ x^2$.

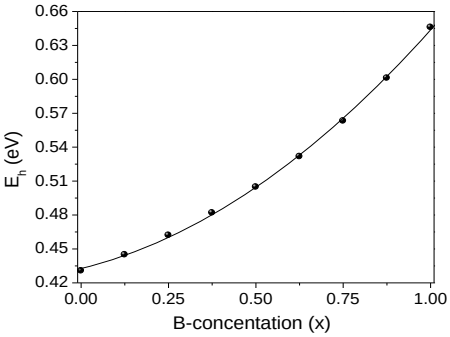

Fig. 4: Variation of The Homopolar Band Gap Energy E_h for $B_xAl_{1-x}SbAlloys$ as a Function of x.

To the best of our knowledge no experimental data or theoretical calculation for the boron concentration x dependence of the homopolar band gap energy E_h for $B_xAl_{1-x}Sb$ has been reported yet. We believe that, our results can serve as a prediction for future investigations.

3. Conclusion

Firstly, we give the correct quadratic fit of the reflective index data reported by Benchehima et al. [9] for $B_xAl_{1-x}Sb$ ternary alloys as a function of boron concentration x, which is incorrectly established. Second one, we predicted the plasmon energy $\hbar\omega_p$ and the microhardness H of $B_xAl_{1-x}Sb$ semiconducting alloys based on the theoretical data of the reflective index n reported in the literature. Some discrepancies were noted, where we found that both the plasmon energy and the microhardness of $B_xAl_{1-x}Sb$ alloys change gradually but not monotonically with increasing of boron concentration x in the range 0 – 1, while normally, both plasmon energy $\hbar\omega_p$ and the microhardness H monotonically increase with increasing x as it was mentioned in the literature. The maximum of the plasmon energy $\hbar\omega_p$ was found to be 16.14 eV for AlSb binary compound, while the minimum of the plasmon energy $\hbar\omega_p$ was found to be 14.4 eV for both $B_{0.5}Al_{0.5}Sb$ and $B_{0.625}Al_{0.375}Sb$ alloys. The shame behavior was observed also for the microhardness H. The accuracy of the data reported in this work for both the plasmon energy and the microhardness of $B_xAl_{1-x}Sb$ alloys are limited by the correctness of the reflective index data reported by Benchehima et al. [9].

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