OPEN ACCESS

International
Journal
Of Modern Engineering Research (IJMER)

Structural, Electronic and Gamma Shielding Properties of $B_xAl_{1-x}As$

Sinem Erden Gulebaglan[*], Emrah Kaya[**], Gulsah Saydan Kanberoglu[***] and Berna Oto[****]

[*]*Department of Electric Program, Vacational School of Van, Yuzuncu Yıl University, 65080 Van, Turkey*
[**]*Department of Physics, Faculty of Science, Yuzuncu Yıl University, 65080, Van, Turkey.*
[***]*Department of Chemistry, Faculty of Science, Yuzuncu Yıl University, 65080, Van, Turkey.*
[****]*Department of Marine Engineering, Faculty of Maritime, Yuzuncu Yıl University, 65080, Van, Turkey.*

ABSTRACT: *The structural and electronic properties of $B_xAl_{1-x}As$ ternary alloys in the zincblende structure were systematically investigated by using the first principles calculations. The local density approximation was used for exchanged and correlation interaction. The calculated band gap bowing parameter was discovered to be mightily composition dependent of the Boron concentration. Additionally, we have calculated some gamma shielding parameters of $B_xAl_{1-x}As$ ternary alloys. Primarily, the values of mass attenuation coefficients (μ_ρ) were calculated using WinXCom computer program and then these parameters were utilized to calculate the values of electron density (N_{el}) and effective atomic number (Z_{eff}) in the wide energy range (1 keV - 100 GeV).*

Keywords: *Electronic Properties, Gamma Shielding Properties, Ternary Alloy.*

I. INTRODUCTION

Ternary and quaternary alloys have important microelectronic industrial applications [1-3]. Therefore, structural and electronic properties of alloy are studied. In particular, the energy band gap is of great importance. The energy band gap can be controlled by doping. For this reason, this issue has been studied by many researchers. The ternary alloys have performed an very important role in different scientific fields, and confirm of their physical constants such as mass attenuation coefficients, electron numbers and mass effective atomic are very important for realization their physical properties. The (μ_ρ) is a measure of the probability of interaction of gamma-ray with the shielding medium [4] and its value interconnects on incident photon energy and chemical composition of the medium. The atomic number of a composite material which interacts with a photon cannot be represented with a single value. It is possible to describe this number as effective atomic number, Z_{eff}, for multi element materials such as compound, mixture. This number varies with incident photon energy as well as the atomic number of the constituent elements [5]. The another physcial parameter for photon interactions is the effective electron density (N_{el}) which is defined as an electron per unit mass of the shielding matter. In the literature, there are some reports on the study of gamma shielding parameters of different types of alloys [6-9]. In the present work, we have demonstrated some gamma shielding parameters such as mass attenuation coefficient (μ_ρ), effective atomic number (Z_{eff}) and electron density (N_{el}) for $B_xAl_{1-x}As$ alloy.

II. COMPUTATIONAL DETAILS AND THEORY

The structural and electronic properties of BAs and AlAs compounds and $B_xAl_{1-x}As$ alloys are investigated by using the plane wave pseudopotentials methods within the Quantum Espresso [10] software package and this package is based on density functional theory (DFT) and pseudopotentials. Exchange and correlation potentials are described within the Local Density Aproximation (LDA). [11] A 16 atom supercell in this structure which comply to 2 × 2 × 2 conventional cubic cell is used for all alloys. As a result Self consistency was observed with an 12 x 12 x 12 Monkhorst-Pack [12] grid of k-points and the electronic wave functions were seen as broadened in the plane wave basis set with the kinetic energy cut-off of 80 Ryd.

In this study, the values of mass attenuation coefficient (μ_ρ) are investigated using WinXCom code attributed on the mixture rule

$$\mu_\rho = \sum_i w_i (\mu_\rho)_i \tag{1}$$

where w_i and $(\mu_\rho)_i$ are the proportion by weight and mass attenuation coefficient of the ith element, respectively. w_i is given as

$$w_i = \frac{a_i A_i}{\sum_j a_j A_j} \tag{2}$$

where A_i is the atomic weight of the ith element and a_i is the number of formula units [13].

The total molecular cross-section (σ_m) values are computated from the following equation

$$\sigma_m = \frac{(\mu_\rho)_{comp.}}{N_A} M \tag{3}$$

and

$$\mathrm{M} = \sum n_i A_i \tag{4}$$

where M is the molecular weight, N_A is the Avagadro number and n_i is the number of atoms of the ith element [14]. The values of electronic cross-sections (σ_{el}) and total atomic cross-sections (σ_a) are calculated as follows

$$\sigma_a = \frac{\sigma_m}{\sum n_i} \tag{5}$$

and

$$\sigma_e = \frac{1}{N_A} \sum \frac{A_i}{Z_i} f_i \mu_i \tag{6}$$

where Z_i and f_i are the atomic number and fractional abundance of constituent element, respectively. The effective atomic number (Z_{eff}) for total photon interaction is given by [14]

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} . \tag{7}$$

As a result, electron density [14], N_{el} can be defined

$$N_{el} = \frac{(\mu_\rho)_{comp.}}{\sigma_e} . \tag{8}$$

III. RESULT AND DISCUSSION

3.1 Structural and electronic properties of $B_xAl_{1-x}As$

At the beginning of this investigation the structural properties of the BAs and AlAs compounds in zincblende structure were calculated by using LDA scheme. With these calculations it was seen that the total energies for many different volumes, around stability, comply the Murnaghan's equation [15] of state, in order to acquire the stability lattice constant for the BAs and AlAs. The structural parameters for BAs and AlAs including the lattice parameters and band gaps are calculated a_{BAs} = 4.724 Å, $E_{g,BAs}$ = 1.15 eV and

a_{AlAs} =5.62 Å, $E_{g,AlAs}$= 1.363 eV. The calculated lattice constant is in good agreement with other theoretical and experimental values [16-21].

Our reviews contain an 16 atom for $B_xAl_{1-x}As$ ternary alloys in a supercell. We commence at AlAs supercell and complete at BAs supercell. The lattice constant and energy band gap of alloys are important. The lattice constant of ternary alloys depends on the lattice constant of binary compounds. We deal with $B_xAl_{1-x}As$ ternary alloy. In this study, Vegard rule is used for the lattice constant.

$$a(x) = xa_{BAs} + (1-x)a_{AlAs} \quad (9)$$

where a_{BAs} is the lattice parmeter of Bas, a_{AlAs} is lattice constant of AlAs and x is concentration.

Bowing parameter is very important for exploring the energy gap of the alloy.

$$E_g(x) = xE_{g,BAs} + (1-x)E_{x,AlAs} - bx(1-x) \quad (10)$$

$E_{g,BAs}$ is band gap of BAs, $E_{g,AlAs}$ is band gap of AlAs and $E_g(x)$ is band gap of $B_xAl_{1-x}As$. Situated lattice constant and band gap are represented in Tab. 1.

Tab 1. Calculated lattice constant and band gap of $B_xAl_{1-x}As$.

a (Å)/x	**0.25**	**0.50**	**0.75**
Vegard's Law	20.39	19.55	18.71
Present Work	20.42	19.67	18.80
Band Gap(eV)	0.64	0.62	0.53

Bowing parameters of these three components is expressed as follows. [22]

$$b = b_{VD} + b_{CE} + b_{SR} \quad (11)$$

$$b_{VD} = \frac{E_{BAs}(a_{BAs}) - E_{BAs}(a)}{1-x} + \frac{E_{AlAs}(a_{AlAs}) - E_{AlAs}(a)}{x}, \quad b_{CE} = \frac{E_{BAs}(a)}{1-x} + \frac{E_{AlAs}(a)}{x} - \frac{E_{BAlAs}(a)}{x(1-x)} \quad (12)$$

$$b_{SR} = \frac{E_{BAlAs}(a) - E_{BAlAs}(a_{eq})}{x(1-x)} \quad (13)$$

$\mathbf{b_{VD}}$ is concerned with the effect of volume deformation, $\mathbf{b_{CE}}$ is related to charge transfer and $\mathbf{b_{SR}}$ relates to structural relaxation [21]. Calculated bowing parameter and bowing parameter of three components are represented in Tab. 2.

Tab 2. Calculated bowing parameter of $B_xAl_{1-x}As$.

x	**0.25**	**0.50**	**0.75**
b	3.593	2.509	3.575
b_{VD}	1.263	0.654	0.786
b_{CE}	2.33	1.855	2.830
b_{SR}	0.0	0.0	-0.001

Numerical simulation using on first-principle calculations is performed the structural characteristics the bowing parameters of the zincblende $B_xAl_{1-x}As$ alloys. The electronic structure calculation the band gap energy are acquired for different compositions of the $B_xAl_{1-x}As$ alloys. We executed that bowing parameter and bowing parameter of three components display very strong composition dependence for the $B_xAl_{1-x}As$ alloys.

3.2 Mass attenuation coefficients (μ_ρ)

The mass attenuation coefficient (μ_ρ) of $B_xAl_{1-x}As$ alloy have been computed by WinXCom computer program in energy range from1 keV to 100 GeV. And results are presented in Fig. 1 and it is seen from this figure that the mass attenuation coefficients depend largely upon gamma energies. And also it is seen from Fig.1. that there are three energy regions. In the low energy region (E<0.1 MeV); values of μ_ρ decrease sharply while the incident photons energy increase. In this energy region, photoelectric effect is overpowering process and μ_ρ values of the alloy are the highest because the cross-section of the photoelectric effect is proportional to the incident photon energy and atomic number as ($\sim Z^{4-5}/E^{7/2}$). In the intermediate energy region

(1 MeV<E<10 MeV); the values of μ_ρ decrase slightly with the increasing incident energy. The trend of μ_ρ may explained by means of the dominance of the Compton scattering process and that Compton scattering cross-section is proportional to Z/E. In the high energy region (10 MeV<E), μ_ρ values increase and then become constant at around 100 MeV energy. Because in this region, the pair production interaction happens overpowering process and cross-section of its interconnects on atomic number as (Z^2) and it is proportional to the incident photon energy. This material could potentially be explicated by absorption K-edges of the Al (1.56 KeV) and As (11.86KeV) elements and absorption L-edges of As (L1:1.52 KeV; L2:1.39 KeV; L3: 1.32 KeV) element the in the alloy.

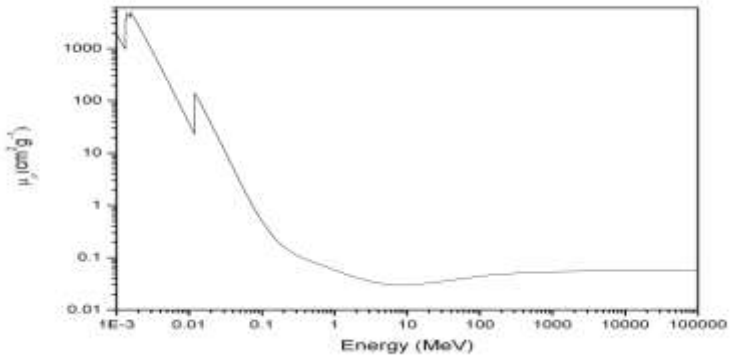

Fig. 1. The calculated mass attenuation coefficients of $B_xAl_{1-x}As$ as a function of photon energies.

3.3 The effective atomic number and effective electron density

The moleculer (σ_m), atomic (σ_a), electronic cross-sections (σ_e), effective atomic numbers *(Z_{eff})* and electron densities *(N_{el})* of the compound were calculated at photon energies from 1 keV to 100 GeV and the variation of *(Z_{eff})* and *(N_{el})* values versus photon energy is presented in Figs. 2a-2b, respectively. It is seen from these figures that the values of *(Z_{eff})* and *(N_{el})* depend on the entire photon energy and the energy dependence of Z_{eff} and N_{el} are dominated by different photon interaction processes; Compton scattering, photoelectric absorption and pair production.

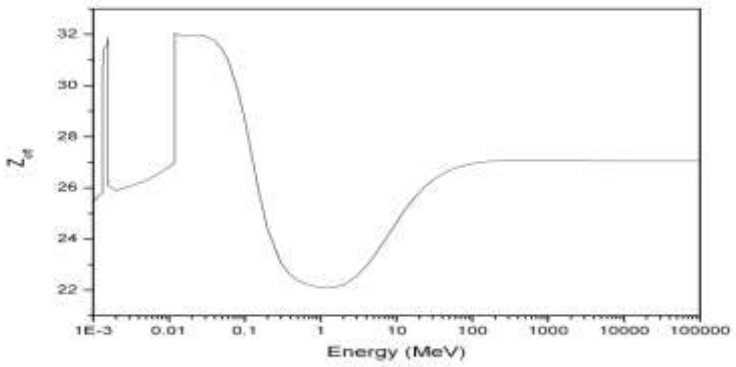

Fig. 2a. The variations of effective atomic number Z_{eff} with photon energy

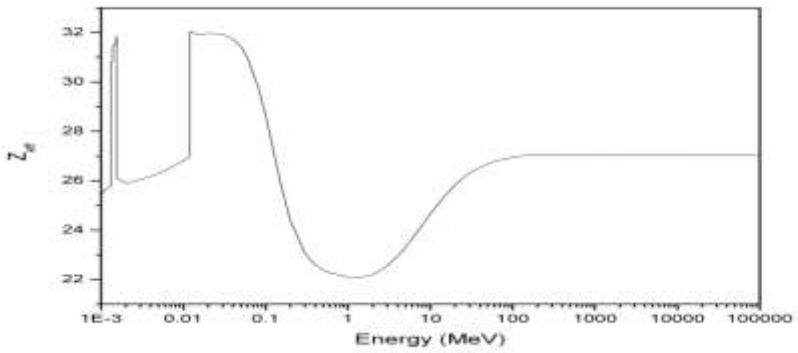

Fig. 2b. The variations of electron density N_{el} with photon energy.

IV. CONCLUSION

In summary, the structural, electronic and Gamma shielding properties of $B_xAl_{1-x}As$ ternary alloys have been studied as a function of the composition x within density functional theory. Considering the lattice constant and energy band gap calculations, it has been proved that these alloys can be used as good materials for optoelectronic device applications. Additionally, we reported new data on (μ_ρ), (Z_{eff}) and (N_{el}) in the energy region of 1keV to 100 GeV for $B_xAl_{1-x}As$ alloy. These data are expected to be useful in the field of radiation application.

REFERENCES

[1]. Schnohr C S, Kluth P, Giulian R and. Llewellyn D J, Byrne A P, Cookson D J, Ridgway M C. Swift heavy ion irradiation of III-V semiconductors. Physical Review B 2010 81, 075201-1/9.
[2]. Negache M, Taibi K, Souami N and Lounis Z. Microstructural, Investigations On Ni-Ta-Al Ternary Alloys, 2010 1202.
[3]. Zhao G, Xu X, Li H, Wei H, Han D, Ji, Z, Meng, Y, Wang L, Yang S. The immiscibility of InAlN ternary alloy, DOI: 10.1038/srep26600
[4]. Hubbell J H, Review of photon interaction cross section data in the **medical** and biological context. Phys. Med. Biol. 1999 44, R1-R22.
[5]. Hine G J, The Effective Atomic Number of Materials for Various Gamma Ray Interactions. In Physical Review 1952 **85**, 725-725.
[6]. Han, I., and Demir L. Mass attenuation coefficients, effective atomic and electron numbers of Ti and Ni alloys. Radiation Measurements 2009 44.3 289-294.
[7]. Limkitjaroenporn, P, Kaewkhao J, Chewpraditkul W, Limsuwan P, Physical,Optical, Structural and gamma-ray shielding properties of lead sodium borate glasses Procedia Engin., 2002 32,847-854.
[8]. Kaewkhao J, Laopaiboon J, and Chewpraditkul W, Determination of effective atomic numbers and effective electron densities for Cu/Zn alloy. J. of Quant. Spect. and Radiative Transfer 2008 109.7, 1260-1265.
[9]. Prasad, S. Guru, K. Parthasaradhi, and W. D. Bloomer. Effective atomic numbers for photo absorption in alloys in the energy region of absorption edges. Radiation Phys. and Chem. 1998 53.5, 449- 453.
[10]. S. Baroni, A. Dal Corso, S. de Gironcoli and P. Giannozzi, (http://www.pwscf.org)
[11]. Hou Q Y, Li J J, Ying C, Zhao C W, Zhao E J and Zhang Y, First-principles study on the effect of high In doping on the conductivity of ZnO. 2013 Chin. Phys. B, **22,** 077103.
[12]. Monkhorst H J and Pack J D , Special points for Brillonin-zone integrations. Physical Review B 1976 5188-5192.
[13]. Gerward L, Guilbert N, Jensen K B, Levring H, WinXCom—a program for calculating X-ray attenuation coefficients, Radiation Physics and Chemistry 2004 71 653–654.
[14]. Gowda S, Krishnaveni S , Yashoda T, Umesh T K and Gowda R, Photon mass attenuation coefficients, effective atomic numbers and electron densities of some thermoluminescent dosimetric compounds. Pramana 2004 63(3), 529-541.
[15]. F. D. Murnaghan, "The compressibility of media under extreme pressures", Proc. Nat. Acad. Sci. USA vol. 30, pp. 244-247, Sept. 1944.
[16]. Gowda S, Krishnaveni S, and Gowda R, Studies on effective atomic numbers and electron densities in amino acids and sugars in the energy range 30–1333 keV. Nuclear Instruments and Methods in Physics Research Section B 2005 239(4), 361-369.
[17]. Briki M, Abdelouhaba M, Zaoui A, Ferhat M, Superlatt. Microstruct. 45 (2009)80.
[18]. Annane F, Meradji H, Ghemid S, El Haj Hassan F, First principle investigation of AlAs and AlP compounds and ordered AlAs1xPx alloys .Computational Materials Science 2010 50 274–278
[19]. Hellwege K H, Madelung O (Eds.), Semi-Conductor, Intrinsic Properties of Group IV Elements and III_V, II_VI and I_VII Compounds, Landolt-Bornstein New Series, Group III, vol. 22, Pt Springer, Berlin, 1982.

[20]. Adachi S, Properties of Group-IV, III–V and II–VI Semiconductors, John Wiley & Sons, England, 2005.
[21]. Ahmed R, Hashemifar S J , Akbarzadeh H , Ahmed M, Aleem F. Ab initio study of structural and electronic properties of III-arsenide binary compounds,.Computational Materials Science. 2007 39 580–586
[22]. Ferhat M and Bechstedt F, First-principles calculations of gap bowing in $In_xGa_{1-x}N$and $In_xA_{l1-\ x}N$ alloys: Relation to structural and thermodynamic properties. PRB, 2002 **65**, 075213.