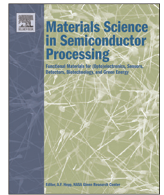
Materials Science in Semiconductor Processing 40 (2015) 539–542

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp



Valence band anticrossing model for $GaSb_{1-x}Bi_x$ and $GaP_{1-x}Bi_x$ using k.p method

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ARTICLE INFO

Article history:
Received 6 May 2015
Received in revised form
9 June 2015
Accepted 25 June 2015
Available online 17 July 2015

Keywords:
VBAC
Spin–orbit split-off energy
III–V-Bismides
Band offset
Auger recombination
Light hole/heavy hole

ABSTRACT

The reduction in band gap as well as the increase in spin–orbit splitting energy in $GaSb_{1-x}Bi_x$ and $GaP_{1-x}Bi_x$ are explained by the Valence Band Anticrossing (VBAC) model. This restructuring of the valence band is due to the interaction of the Bi related impurity levels with the extended states of the valence band of the host semiconductor. The band gap reduction in $GaSb_{1-x}Bi_x$ and $GaP_{1-x}Bi_x$ calculated using VBAC model are respectively 40.2 meV and 206 meV/at% Bi. A comparison of the theoretical and experimentally obtained values of band gap in GaSbBi shows good agreement. Valence band structure for GaPBi is obtained by the extrapolation of the parameters used for modeling of the GaSbBi system. The upward movement of the spin–orbit split-off E_+ energy level in GaSbBi by 19.2 meV/at% Bi is also responsible for the suppression of Auger recombination processes making it a potential candidate for near and mid-infrared optoelectronic applications.

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1. Introduction

III–V-Bi alloy systems have received a great deal of interest in the last few years for potential applications in near- and mid-infrared optoelectronic devices. A review of this new class of materials is presented in a recent Springer Series volume [1]. The most prominent property of III–V-bismides is a substantial reduction in band gap caused by the addition of a little amount of Bi. For example, addition of only 1 at% Bi in GaAs has been found to reduce the band gap by about 88 meV [2]. Similar effects have been studied in InPBi [3], InSbBi [4], InAsBi [5] and GaSbBi [6]. This property makes the bismides similar to comparatively older and more studied dilute III–V-nitrides [7]. However, contrary to the dilute nitrides, where the interaction of the N related resonant state with the conduction band of the host semiconductor causes the reduction in band gap, the band gap reduction in bismides is primarily due to a restructuring of the valence band as a result of an anticrossing interaction with the Bi related impurity levels [8]. The incorporation of a small amount of Bi into the host lattice forms Bi related impurity states close to the valence band edge of the host semiconductor. These impurity states interact with the valence band states, i.e. the light hole (LH) and heavy hole (HH) bands, resulting in an reduction of the material band-gap and the phenomenon is well-explained by the Valence Band Anticrossing (VBAC) model [9]. The increase in the spin–orbit splitting in III–V bismides is due to the interaction of the Bi related spin–orbit split-off energy level with the spin–orbit split-off band of the host lattice [5]. The effect enhances the spin orbit splitting energy of the alloy and offers a potential way to reduce or even suppress the loss processes such as Auger recombination and inter valence band absorption (IVBA) [1]. Moreover, bismides offer the possibility of realizing lasers with temperature insensitive emission wavelengths [10] due to the reduced temperature dependence of the band gap [11] in the material. Degradation of electron mobility in bismides is also reported to be less than nitrides since there is little perturbation in the conduction band in the former [12,13].

GaSbBi appears to be a potential member of the III–V-Bi family, where the band gap tuning property may be effectively utilized for fabricating devices in the mid-infrared regions [1,6,14]. GaPBi, on the other hand, could be useful for tuning the emission from optical sources in the visible range. However, till date, we could not find any published result on the growth of this material. In this paper, we present a mathematical model, based on VBAC, to explain the reduction in band gap and enhancement in the spin orbit splitting energy in GaSbBi and GaPBi. VBAC model for GaPBi is obtained by extrapolating the parameters used for modeling GaSbBi as the growth of GaPBi has not yet been reported.

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http://dx.doi.org/10.1016/j.mssp.2015.06.065
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2. Mathematical modeling

When a small amount of bismuth is incorporated into GaSb or GaP, localized defect states are produced near the extended states of the valence band of the host semiconductor. The interaction of these impurity states with the light hole (LH), heavy hole (HH) and spin–orbit split-off band (SO) causes the splitting of these bands into E_+ and E_- subbands. While the E_+ subbands maintain the extended nature of the host semiconductor, E_- subbands retain the properties of the defect states [8]. This anticrossing interaction can be well explained by the VBAC Model. The resultant valence band structure of III–V-Bi can be described by a 12×12 Hamiltonian H to include the 6p-like states of the host and 6p-like states of the defect Bi [15]. The solution of the Hamiltonian yields six distinct eigen values corresponding to the six subbands. Hence the reduced form of the Hamiltonian H for the $<100>$ $[k_x=1, k_y=k_z=0]$ plane can be written as

$$H_0=\begin{pmatrix} H & Ck_x^2 & 0 & V(x) & 0 & 0 \\ Ck_x^2 & L & 0 & 0 & V(x) & 0 \\ 0 & 0 & S & 0 & 0 & V(x) \\ V(x) & 0 & 0 & E_{Bi} & 0 & 0 \\ 0 & V(x) & 0 & 0 & E_{Bi} & 0 \\ 0 & 0 & V(x) & 0 & 0 & E_{Bi-so} \end{pmatrix} \quad (1)$$

where,

$$H=Ak_x^2+\Delta E_{VBM}x$$
$$L=Bk_x^2+\Delta E_{VBM}x$$
$$S=Ek_x^2+(\Delta E_{VBM}-\Delta E_{SO})x-\Delta_0$$
$$V(x)=C_{Bi}\sqrt{x}$$
$$A=\frac{-\hbar^2}{2m_0}[\gamma_1+\gamma_2]$$
$$B=\frac{-\hbar^2}{2m_0}[\gamma_1-\gamma_2]$$
$$C=\frac{\sqrt{3}\hbar^2}{2m_0}\gamma_2$$
$$E=\frac{-\hbar^2}{2m_0}\gamma_1$$

ΔE_{VBM} and ΔE_{SO} in the above expressions denote the difference in the valence band maximum and the spin–orbit split-off energies between the end point compounds. A, B, C and E are constants which are dependent on the Luttinger parameters γ_1, γ_2 and γ_3 and Δ_0 is the spin orbit splitting energy for GaSb or GaP. $V(x)$ is the matrix element which takes into account the coupling between the host valence band and the Bi-related impurity levels is taken into account by the matrix element $V(x)$ with C_{Bi} used as a fitting parameter [16]. E_{Bi} and E_{Bi-so} are the Bi related impurity levels corresponding to the LH/HH and SO bands of GaSb/GaP. At the Γ point, where $k=0$, all the off-diagonal elements of the Hamiltonian matrix H_0 becomes zero. The solution of the Hamiltonian then yields four distinct eigen values corresponding to the E_+ and E_- sub-bands of the LH/HH and SO energy levels which are given by the equations [17]

$$E_{LH/HH\pm}=\frac{1}{2}\left(H+E_{Bi}\pm\sqrt{H^2-2HE_{Bi}+E_{Bi}^2+4V^2}\right) \quad (2)$$

$$E_{SO\pm}=\frac{1}{2}\left(S+E_{Bi-so}\pm\sqrt{\left(S^2-2SE_{Bi-so}+E_{Bi-so}^2+4V^2\right)}\right) \quad (3)$$

The above equations are obtained by using the reduced form H_R of the Hamiltonian in Eq. (1) as [17]

$$H_R=\begin{bmatrix} H/L & 0 & V & 0 \\ 0 & S & 0 & V \\ V & 0 & E_{Bi} & 0 \\ 0 & V & 0 & E_{Bi-so} \end{bmatrix} \quad (4)$$

The value of the spin orbit splitting energy for GaSb and GaBi is reported as 0.76 eV [18] and 2.2 eV [19] respectively. The direct E_0 energy gap for GaBi is calculated as -2.35 eV by using Quantum Dielectric Theory [20]. We have calculated the values of the valence band offset (VBO), conduction band offset (CBO) and spin–orbit split-off band offset between GaSb and GaBi as 0.38 eV, -2.78 eV and -1.06 eV respectively. Valence band offset (VBO) for GaBi is obtained by extrapolating the graph between VBO and lattice constant for Ga containing binary compounds using Ref. [18]. The VBO for GaBi is found out to be 0.35 eV corresponding to its lattice constant 6.324 Å [19]. Using the value of the atomic spin–orbit splitting energy for Bi of 1.5 eV [9] and value of the heavy/light hole levels for Bi E_{Bi} of 1.17 eV [21] below the valence band maximum (VBM) of GaSb, the location of corresponding spin–orbit split-off level E_{Bi-so} is found out to be 2.67. The value of coupling parameter is calculated to be 1.01 eV and is obtained by using the band gap reduction value of 40 meV/at% Bi reported by Dhar et al. [14]. The coupling parameter C_{Bi} determines the magnitude of shift of the E_+ and E_- levels of the HH, LH and SO subbands as is evident from Eqs. (2) and (3).

For $GaP_{1-x}Bi_x$, the value of spin orbit splitting energy is taken as 0.08 eV using [18]. The values of VBO, CBO and spin–orbit split-off band offset are calculated as 1.62 eV, -3.00 eV and -0.50 eV respectively. The value of the heavy/light hole levels for Bi E_{Bi} is taken as 0.1 eV [9] above the valence band maximum (VBM) of GaP and the location of corresponding spin–orbit split-off level E_{Bi-so} is found out to be 1.4 eV below the VBM of GaP. These values are obtained using Fig. 5 of [9]. The location of E_{Bi} above the VBM makes GaPBi a multiband semiconductor similar to that of AlAsBi as the anticrossing interactions of the impurity level with the host matrix are predicted to push the Bi-related HH/LH E_+ bands into the band gap of these semiconductors resulting in the formation of narrow impurity-related band [9]. The coupling parameter C_{Bi} is taken as 2.1 eV which is obtained following the general trend in ionization energy vs coupling parameter used for modeling the $GaAs_{1-x}Bi_x$ and $GaAs_{1-x}Sb_x$ alloy systems [9].

3. Results and discussions

Fig.1 shows the E–k diagram for $GaSb_{1-x}Bi_x$ in the ⟨100⟩ direction with $x=0.05$. The broadening of the LH/HH E_+ band, as can be seen from the band diagram, causes an increase in the hole effective mass and affects the hole transport properties of GaSbBi [8]. The changes in the spin orbit split-off band is insignificant due to the weak interaction of the localized Bi related spin–orbit split-off states with the SO band GaSb. The E_+ subband maintain the nature of the host semiconductor lattice whereas the E_- subband retain the localized character of the defect states [8].

Fig. 2 shows the band structure of $GaSb_{1-x}Bi_x$ as a function of Bi mole fraction, calculated at $\Gamma=0$. The positions of the energy levels are calculated using Eqs. (2) and (3). It can be observed from the figure that the E_+ and E_- levels corresponding to the heavy/light hole and the spin–orbit split-off energy bands repel each other. The heavy hole/light hole (HH/LH) E_+ band moves upward by about 12.4 meV/at% Bi. The upward movement of the heavy hole/light hole E_+ level is responsible for the most part of energy gap reduction in III–V bismides. The band structure is drawn by taking a total band gap reduction of 40 meV/at% Bi [14]. The lowering of the conduction band minimum for $GaSb_{1-x}Bi_x$

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