Positron Affinity, Deformation Potential and Diffusion Constant in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ Ternary Semiconductor Alloys

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Abstract The present investigation deals with the positron behaviour in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys in the zinc-blende phase. The calculations are mainly based on a pseudopotential approach coupled with the independent particle model. Features such as elastic constants, electron and positron chemical potentials, positron deformation potential and positron diffusion constant are determined. Moreover, the positron affinity to InSb, AlSb and their related ternary alloys and heterostructures is calculated. The present results are compared to experiment and found to be in reasonably good agreement. The information gathered from the present study can help in understanding the positron trapping at interfaces and precipitates and might be useful in slow-positron-beam experiments.

KEY WORDS: Semiconductor alloys; Positrons; Diffusion; Surface and interface states; Heterostructures

1 Introduction

The III–V semiconductors are important materials for the high-tech photonic and optoelectronic devices, due to their large bulk moduli, high melting temperature and high thermal conductivity. Several techniques such as molecular beam epitaxy, metal organic vapour phase epitaxy and liquid phase epitaxy can be used to obtain the film materials of devices [1].

The III–V compounds that have different fundamental properties can be mixed to ternary alloys so as to obtain a

new material with intermediate properties which allow light emission and absorption at desired wavelength.

Among these materials, $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys have an immense potential for many applications in semiconductor technology. Besides, InSb/ $\text{Al}_x\text{In}_{1-x}\text{Sb}$ -based quantum wells have received a growing interest. This is because of their importance to the lasers [2], the devices exhibiting quantum effects such as quantized conductance [3, 4] and for quantum information applications [5].

The study of solid surfaces and defect profiles using slow beams of mono-energetic positrons is currently a well-established tool for non-destructive evaluation of layered structures as well as for other surface and near-surface investigations [6–8]. However, experimental techniques require a comprehensive theory for deep, quantitative understanding of the results. Computational methods for examining positron experiments have matured and are reported in the literature [9–11]. In fact, Monte Carlo simulations can be used to investigate the positron slowing-down process in solid targets [12–15]. The positron affinity and positron deformation potential are useful parameters for positron penetration in semiconducting materials.

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Moreover, the positron deformation potential is related to positron diffusion in metals and semiconductors [16, 17]. These parameters can be measured experimentally and may serve as a test of the quality of the theoretical models employed for the determination of the electron and positron chemical potentials.

In the current contribution, the electron and positron energy levels in zinc-blende $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys have been calculated. This has allowed the determination of the positron affinity, positron deformation potential and positron diffusion constant in the material system of interest. The calculations are mainly based on the empirical pseudopotential method (EPM) under the virtual-crystal approximation (VCA), whereas the point-core approximation for the ionic potential has been used to evaluate the positron wave function.

2 Computational Details

The electronic band structure has been computed by using the EPM [18]. It is an approach in which the potential in the Schrödinger equation is approximated by a truncated Fourier series, where the expansion coefficients are obtained by fitting to experiment. In the present work, a set of symmetrical and anti-symmetrical pseudopotential form factors are adjusted in order to yield band-gap energies that agree with the experimental measurements. The empirical pseudopotential parameters are optimized using the non-linear least-squares method as described in references [19, 20]. The used empirical energy band-gaps at Γ , X and L k-points in the fitting procedure at zero pressure for InSb and AlSb semiconductor compounds are shown in Table 1.

The potential of ternary semiconductor alloys $\text{Al}_x\text{In}_{1-x}\text{Sb}$ is calculated using the VCA and including the compositional disorder effect on the effective potential as described in [23–25], whereas the Vegard's law is assumed for the calculation of the alloy system lattice constant.

The positron wave function is represented by plane wave and evaluated using the point-core approximation for the ionic potential as described elsewhere [10, 11, 26]. It is assumed that there is only one positron for many electrons.

Table 1 Experimental band-gap energies for InSb and AlSb fixed in the fits at zero pressure

Compound	$E_{\Gamma-\Gamma}$ (eV)	$E_{\Gamma-X}$ (eV)	$E_{\Gamma-L}$ (eV)
InSb	0.18 ^a	1.63 ^a	0.93 ^a
AlSb	2.30 ^b	1.615 ^b	2.211 ^b

^a Ref. [21]

^b Ref. [22]

Hence, the exchange term can be neglected since there is no positron–positron interaction.

3 Results and Discussion

Elastic properties of materials are relating to various fundamental solid-state properties such as inter-atomic potential and associated with longitudinal wave of the acoustic phonons. Thus, it is important to determine elastic constants of the material system of interest. In this respect, the elastic constants, namely C_{11} , C_{12} and C_{44} , of $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys have been calculated using the same approach used by Bouarissa [27] for calculating C_{11} and C_{12} and the valence force field model as reported in Refs. [28, 29] for C_{44} . Our results are given in Table 2. For comparison the available experimental data are also reported in the literature. Note that our results agree well with the experimental ones reported in Ref. [30] for InSb and AlSb. We also predicted the results for $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$. The variation of the elastic constants of $\text{Al}_x\text{In}_{1-x}\text{Sb}$ as a function of the Al concentration is displayed in Fig. 1. The solid, dashed and dotted lines are fitted curves drawn using the least-squares method. The corresponding expressions to the fit are

$$C_{11}(x) = 6.24 + 3.78x - 0.25x^2, \quad (1a)$$

$$C_{12}(x) = 2.70 + 1.58x - 0.092x^2, \quad (1b)$$

$$C_{44}(x) = 2.52 + 1.55x - 0.11x^2, \quad (1c)$$

where C 's are expressed in 10^{11} dyn/cm². One can observe that by increasing the Al concentration x , C_{11} and C_{44} increase nonlinearly whereas C_{44} increases almost linearly. All constants vary monotonically exhibiting the same qualitative behaviour. Nevertheless, the rate of variation seems to be more important for C_{11} .

Table 2 Elastic constants and the average in $\langle C_{ii} \rangle$ for zinc-blende InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb

Material	Elastic constants (10^{11} dyn/cm ²)			
	C_{11}	C_{12}	C_{44}	$\langle C_{ii} \rangle$
InSb	6.26 ^a 6.608 ^b	2.71 ^a 3.531 ^b	2.526 ^a 3.027 ^b	7.011 ^a
$\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$	8.073 ^a	3.471 ^a	3.267 ^a	9.039 ^a
AlSb	9.766 ^a 8.769 ^b	4.188 ^a 4.341 ^b	3.956 ^a 4.076 ^b	10.933 ^a

^a This work

^b Experimental data reported in Ref. [30]

Fig. 1 Elastic constants in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

The knowledge of elastic constants makes it possible to proceed with the average in $\langle C_{ii} \rangle$ following the approximation of Boev et al. [16]. In fact, $\langle C_{ii} \rangle$ is the elastic constant associated with longitudinal wave and averaged over the directions of propagation. The latter has been calculated using the approximate expression [16].

$$\langle C_{ii} \rangle \approx 1/2(C_{11} + C_{12} + 2C_{44}), \quad (2)$$

Our results are depicted in Table 2 and may serve as a reference for future studies. The compositional dependence of $\langle C_{ii} \rangle$ for $\text{Al}_x\text{In}_{1-x}\text{Sb}$ in the zinc-blende phase is displayed in Fig. 2. The solid line is a fitted curve plotted using the least-squares method and corresponds to the relation,

$$\langle C_{ii} \rangle(x) = 6.99 + 4.23x - 0.28x^2, \quad (3)$$

$\langle C_{ii} \rangle$ here is expressed in 10^{11} dyn/cm^2 . Note that on going from InSb ($x = 0$) to AlSb ($x = 1$), $\langle C_{ii} \rangle$ increases

Fig. 2 Elastic constant associated with longitudinal waves and averaged over the directions of propagation in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

monotonically from 7.011×10^{11} to $10.933 \times 10^{11} \text{ dyn/cm}^2$.

Another important parameters obtained from the electron and positron band structures are the internal electron and positron chemical potentials. These features are denoted by μ_- and μ_+ for the electron and positron, respectively, and are purely bulk properties. μ_- is equal to the Fermi energy in the electron band structure, whereas μ_+ is the lowest energy in the positron band structure. The calculated electron and positron chemical potentials for InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb semiconducting materials are shown in Table 3. Due to the absence of both theoretical and experimental data regarding μ_- and μ_+ for the materials of interest, to the best of our knowledge, our results are only for reference and may serve for future investigations.

The variation of μ_- and μ_+ as a function of the Al content in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys is plotted in Figs. 3 and 4, respectively. The solid lines in both figures are the curves that fit best the obtained data in the present work, which correspond to the following expressions:

$$\mu_-(x) = -0.044 - 1.32x + 0.51x^2, \quad (4)$$

$$\mu_+(x) = -7.44 + 0.19x - 0.08x^2, \quad (5)$$

where μ_- and μ_+ are expressed in eV.

Note that as ones proceed from InSb to AlSb, μ_- decreases, whereas μ_+ increases.

Both variations are monotonic. However, μ_+ exhibits a weaker bowing parameter as compared to that of μ_- (see the quadratic terms in Eqs. (4) and (5)). The increase of the positron chemical potential when going from InSb to AlSb is consistent with the positron bulk lifetime in these compounds reported very recently by Fares et al. [31], bearing in mind that the thermalized positrons are near the bottom of the lowest energy band at $k_+ = 0$.

The positron affinity denoted by A_+ is a basic bulk characteristic of materials. It has an important role in the understanding of positron trapping at interfaces and precipitates [32]. It can be obtained simply by using the relation [33]

Table 3 Electron and positron chemical potentials and positron affinity for zinc-blende InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb

Material	μ_- (eV)	μ_+ (eV)	A_+ (eV)
InSb	-0.09 ^a	-7.43 ^a	-7.52 ^a
$\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$	-0.57 ^a	-7.36 ^a	-7.92 ^a
AlSb	-0.81 ^a	-7.31 ^a	-8.12 ^a

^a This work

Fig. 3 Electron chemical potential in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

Fig. 4 Positron chemical potential in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

$$A_+ = \mu_- + \mu_+. \quad (6)$$

Our results concerning A_+ for InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb are listed in Table 3. In Fig. 5 we display the positron affinity against the alloy composition x for $\text{Al}_x\text{In}_{1-x}\text{Sb}$. Note that by increasing the alloy concentration x , A_+ decreases monotonically. The solid line is the best fit of our results using a least-squares procedure which corresponds to the following expression,

$$A_+(x) = -7.48 - 1.13x + 0.43x^2, \quad (7)$$

A_+ is expressed in eV.

The quadratic term in Eq. (7) is the bowing parameter of the positron affinity.

It indicates that the behaviour of A_+ versus the alloy composition x is nonlinear.

It should be noted that A_+ is a bulk material property. However, its practical usage concerns material surfaces and interfaces [32]. Thus, for heterostructures formed by distinct materials M_1 and M_2 in contact, the electron chemical

Fig. 5 Positron affinity in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

potentials align mutually, and hence, the difference between the positron levels can give the difference between the positron affinities in M_1 and M_2 as [16, 33],

$$\Delta A_+^{M_1, M_2} = A_+^{M_1} - A_+^{M_2}. \quad (8)$$

Using the values of A_+ given in Table 3, the positron affinity to different heterostructures formed by InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb semiconducting materials has been calculated. For example, InSb and $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ in contact (InSb/ $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ heterostructure), the positron favours $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ with an affinity difference of 0.40 eV. On the other hand, for InSb and AlSb in contact (InSb/AlSb heterostructure), the positron favours AlSb with an affinity difference of 0.60 eV, whereas it favours AlSb with an affinity difference of -0.20 eV for AlSb/ $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ heterostructure. It is worth noting that if M_2 is a precipitate, the relation $\Delta A_+^{M_1, M_2} > 0$ is a necessary condition for the trapping of positrons in this precipitate.

Another interesting quantity regarding the positron characteristics is the positron deformation potential denoted by E_d^+ which has been calculated using Eq. [16],

$$E_d^+ = -V_0 \frac{dA_+}{dV}, \quad (9)$$

where V_0 is the crystal volume at zero pressure. The volume derivatives of the positron affinity are obtained by performing electron and positron band structure calculations based on the EPM coupled with the independent particle model for various lattice constants which are obtained by using different pressures. The change in the lattice constant as a function of pressure is calculated using the Murnaghan equation of state. The values of the equilibrium bulk modulus (B_0) and its first pressure derivative (B'_0) used in the present contribution are $B_0 = 4.56 \times 10^{11} \text{ dyn/cm}^2$, $B'_0 = 4.899$ and $B_0 = 5.82 \times 10^{11} \text{ dyn/cm}^2$,

$B'_0 = 4.55$ for InSb and AlSb, respectively [30]. The pressure derivatives of the pseudopotential form factors required in the present calculation are obtained empirically by fitting the first-order coefficients of the band gaps at Γ , X and L high-symmetry points in the Brillouin zone to those of $\frac{dE_{\Gamma\Gamma}}{dp} = 17.6$, $\frac{dE_{\Gamma X}}{dp} = 2.7$, $\frac{dE_{\Gamma L}}{dp} = 8.3(\times 10^{-3} \text{ eV/kbar})$ and $\frac{dE_{\Gamma\Gamma}}{dp} = 10$, $\frac{dE_{\Gamma X}}{dp} = -1.5$, $\frac{dE_{\Gamma L}}{dp} = 6.4(\times 10^{-3} \text{ eV/kbar})$ reported in Ref. [34] for InSb and AlSb, respectively. Table 4 shows pseudopotential parameters used in this work for InSb and AlSb at pressures ranging from 0 to 20 kbar. In Table 5, we list the calculated positron deformation potential for InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb. Once again our results are only for reference.

The variation of E_d^+ as a function of the Al concentration for $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys is plotted in Fig. 6. The solid line in Fig. 6 represents the curve that fit best the obtained data, which gives the analytical relation,

$$E_d^+(x) = 3.88 - 0.64x + 0.04x^2, \quad (10)$$

where E_d^+ is expressed in eV. We observe that as the Al content increases from $x = 0$ to $x = 1$, the positron deformation potential decreases monotonically exhibiting an almost linear behaviour. This can be confirmed from Eq. (10) where one can see a very weak bowing parameter. From the deformation potential theory, one can get the positron diffusion constant due to acoustic phonon scattering as follows [16],

Table 5 Positron deformation potential and positron diffusion constant for zinc-blende InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb

Material	E_d^+ (eV)	D_+ (cm^2/s)
InSb	3.88 ^a	6.86 ^a
$\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$	3.57 ^a	7.29 ^a
AlSb	3.28 ^a	8.53 ^a

^a This work

Fig. 6 Positron deformation potential in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

Table 4 Pseudopotential parameters for zinc-blende (a) InSb and (b) AlSb at various pressures up to 20 kbar

Pseudopotential parameters	$P = 0$ kbar	$p = 5$ kbar	$p = 10$ kbar	$p = 15$ kbar	$p = 20$ kbar
(a) InSb					
$V_s(3)$ (Ry)	-0.201294	-0.201109	-0.200967	-0.200878	-0.200727
$V_s(8)$ (Ry)	0.01	0.01	0.01	0.01	0.01
$V_s(11)$ (Ry)	0.028338	0.030451	0.031422	0.034612	0.036643
$V_A(3)$ (Ry)	0.064495	0.063882	0.063319	0.062763	0.062233
$V_A(4)$ (Ry)	0.03	0.03	0.03	0.03	0.03
$V_A(11)$ (Ry)	0.015	0.015	0.015	0.015	0.015
Lattice constant (at. units)	12.2684	12.2248	12.1835	12.1443	12.1070
(b) AlSb					
$V_s(3)$ (Ry)	-0.225597	-0.223732	-0.221471	-0.219438	-0.217605
$V_s(8)$ (Ry)	0.028086	0.025325	0.021853	0.018512	0.015273
$V_s(11)$ (Ry)	0.062230	0.065721	0.069888	0.073990	0.078050
$V_A(3)$ (Ry)	0.007109	0.007109	0.007109	0.007109	0.007109
$V_A(4)$ (Ry)	0.058960	0.058960	0.058960	0.058960	0.058960
$V_A(11)$ (Ry)	0.004544	0.004544	0.004544	0.004544	0.004544
Lattice constant (at. Units)	11.5983	11.5658	11.5345	11.5045	11.4755

Fig. 7 Positron diffusion constant in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary alloys versus Al content

$$D_+ = \left[\frac{8\pi}{9} \right]^{1/2} \frac{\hbar^4 \langle C_{ii} \rangle}{m_+^{*5/2} (k_B T)^{1/2} E_d^{+2}}, \quad (11)$$

where m_+^* is the positron effective mass, T the absolute temperature and $\langle C_{ii} \rangle$ the elastic constant mentioned above. m_+^* has been calculated following the approach used by Bouarissa [35]. Our predicted results as regards D_+ for InSb, $\text{Al}_{0.5}\text{In}_{0.5}\text{Sb}$ and AlSb semiconducting materials are listed in Table 5. The variation in D_+ as a function of the Al concentration x for $\text{Al}_x\text{In}_{1-x}\text{Sb}$ is displayed in Fig. 7. The solid line is a fitted curve drawn using the least-squares method, which corresponds to the following analytical expression,

$$D_+(x) = 6.86 + 0.05x + 1.62x^2, \quad (12)$$

where D_+ is expressed in cm^2/s . Note that as one goes from InSb to AlSb parent compounds, the positron diffusion constant increases monotonically showing a nonlinear behaviour with a large bowing parameter. This can be seen from Eq. (12). On the basis of the energy band-gap trend [25], and the positron diffusion constant in $\text{Al}_x\text{In}_{1-x}\text{Sb}$ semiconductor ternary alloys, one may conclude that the positron diffusion constant follows the same trend as that of the energy band-gap.

4 Conclusion

In summary, the theoretical investigation of electron and positron energy levels in zinc-blende $\text{Al}_x\text{In}_{1-x}\text{Sb}$ ternary semiconductor alloys has been performed using a pseudopotential approach coupled with the independent particle model. The alloy potential has been calculated within the VCA that takes account of the disorder effect. Quantities

such as a positron deformation potential, positron affinity and positron diffusion constant have been obtained for materials of interest, and heterostructures formed by these materials. Besides, elastic constants and the elastic constant associated with longitudinal waves averaged over the directions of propagation have been determined. The present results were compared to those of experiments and found to be in reasonably good agreement. Other case, our results are predictions and may serve for a reference for future studies. The compositional dependence of all features being studied here has been examined and expressed by quadratic polynomial forms. The present study was capable of predicting quantities which can be measured directly using the slow-positron-beam techniques. This is very useful for the investigation of both bulk and surface solids.

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