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Electron and positron characteristics in $Al_xIn_{1-x}Sb$: A comparative study performed by using a pseudopotential approach

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ABSTRACT

Based on a pseudopotential approach under the virtual-crystal approximation, the electron and positron band structures and their derived properties have been investigated for zinc-blende $Al_xIn_{1-x}Sb$ ternary semiconductor alloys. The effect of compositional disorder on electron and positron band structures has been examined and discussed. Moreover, the differences and the similarities between electron and positron characteristics in the material system of interest have been analyzed. The present study reveals possibilities for the investigation of the positron annihilation in $Al_xIn_{1-x}Sb$.

1. Introduction

Positron annihilation spectroscopy is a characterization method for probing the local electron density and atomic structure at the site chosen by the electrostatic interaction of the positron with its environment [1–4]. In positron beam studies [3,5–8], positrons are implanted at a high initial kinetic energy but they rapidly lose their energy through interactions with electrons and phonons and become thermalized in a time short compared to their average lifetime in the material of interest. The thermal stage ends when the positron annihilates with an electron. The concomitant radiation conveys information which can be used to reconstruct host electronic properties near the site of annihilation [3,9]. Thus, the state of electrons in semiconducting materials might be studied by investigating the characteristics of the positron annihilation process [9–11]. The differences and similarities between electron and positron band structures and their related fundamental properties are also of considerable interest, and an understanding of positron annihilation characteristics in solids underpins and strengthens the description of the structure and properties of condensed matter.

The present contribution deals with electron and positron states in $Al_xIn_{1-x}Sb$ ternary alloys in the zinc-blende phase. The calculations are based on the pseudopotential approach within the virtual-crystal approximation (VCA). The positron wave function is evaluated using the point-core approximation for the ionic potential. Special attention has been given to the effect of compositional disorder on the electron and positron band structures of $Al_xIn_{1-x}Sb$ ternary semiconductor alloys. The aim of this work is to compare the electron and positron band structures and their related fundamental properties in $Al_xIn_{1-x}Sb$ so as to investigate the differences and the similarities. The choice of $Al_xIn_{1-x}Sb$ ternary alloys is based on their importance for many applications in semiconductor technology. These materials have an immense potential for technological applications in the fields of fabrication of microwave, optoelectronic, and electric devices. As a matter of fact, $Al_xIn_{1-x}Sb$ ($x = 1–0.5$) with a composition closely lattice matched to the channel layers, $Ga_xIn_{1-x}Sb$ and $InAs_xSb_{1-x}$, was used for barrier layers [12]. Besides, the InSb-like channel in the $Al_xIn_{1-x}Sb/InAs_xSb_{1-x}$ heterostructures offers very high room-temperature as well as 77 K electron mobility [12]. Furthermore, transistors were fabricated on a semi-insulating GaAs substrate using a relaxed metamorphic buffer layer of $Al_xIn_{1-x}Sb$ to accommodate lattice mismatch, a compressively strained InSb quantum well confined between layers of $Al_xIn_{1-x}Sb$ and Schottky barrier metal gate [13].

2. Computational method

The electronic wave functions are determined from the band-structure using the pseudopotential approach, more specifically the empirical pseudopotential method (EPM) [14]. It is, of course, just such Fourier components with respect to reciprocal lattice vectors that enter directly into the secular equation that determines the

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Table 1
Experimental band-gap energies for InSb and AlSb fixed in the fits.

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

[a] Ref. [17].
[b] Ref. [18].

energies and wave functions. The EPM involves adjusting the pseudopotential form factors which are modified in order to reproduce the experimental band-gap energies at selected points in the Brillouin zone as accurately as possible. In the present contribution, the non-linear least-squares method as described by Kobayasi and Nara [15,16] has been used so as to optimize the empirical pseudopotential parameters. Table 1 shows the experimental band-gap energies at Γ, X and L high-symmetry points in the Brillouin zone used in the fitting procedure for semiconductor compounds InSb and AlSb of interest.

The alloy potential has been obtained using the VCA. However, when the compositional disorder is taken into consideration, a correction to the VCA is made by introducing the disorder effect as an effective disorder potential as described in [19,20].

The lattice constant of the alloy system of interest has been determined assuming the Vegard's law.

The positron wave function is evaluated using the point-core approximation for the ionic potential. More details about the approach can be found in [9–11]. As a matter of fact, after implantation and thermalization the positron in a semiconductor is in a Bloch-like state in a perfect periodic crystal lattice. It can be then described to a ground approximation by a single-particle Schrödinger equation [3]. The positron potential results from two parts, the first part is due to the nuclei and the second one results from the electron. Both parts are purely Coulombic in nature. The nuclear part is expressed in terms of point charges situated at the lattice sites where its Fourier coefficients are easily found. Note that the electron-positron correlation potential has been neglected here. This has been justified by the fact that this potential is a slow function of the electron density. Thus, it is generally flat in the interstitial region and is swamped by the ionic and Coulombic potentials in the ion core region.

The positron wave function has been represented by plane waves as described in [9]. The positron can be assumed to thermalize in a time short compared to its lifetime [3]. This makes the solution of the secular equation simple.

3. Results and discussion

The pseudopotential parameters used in the present calculations for InSb and AlSb are given in Table 2, whereas the Fourier coefficients of the valence charge densities for InSb, $Al_{0.5}In_{0.5}Sb$ and AlSb are shown in Table 3.

The computed electron and positron energy band structures of $Al_{0.5}In_{0.5}Sb$ in the zinc-blende phase at the high-symmetry points and along the principal symmetry directions in the Brillouin zone are displayed in Figs. 1 and 2, respectively. In both cases, the effect of compositional disorder on the band structure has been examined. The electron valence band maximum is taken to be the zero energy reference (Fig. 1). Note that the electron conduction band minimum occurs at the Γ point. This is consistent with the fact that $Al_{0.5}In_{0.5}Sb$ is a direct band gap semiconductor as reported in Ref. [20]. The largest degree of localization is exhibited by the wave functions for the minimum conduction band at Γ. Taking an overall look at the electron band structure featured in Fig. 1, one can see that it is similar to other electronic band structure of III–V ternary semiconductor alloys [21] with different dispersive bands and band crossings. This difference accounts for the difference in the ionicity of the semiconducting materials. The positron band structure (Fig. 2) exhibits similarities to that of the electron counterpart (Fig. 1). Nevertheless, the positron energy spectrum does not show a band gap between the fourth and the fifth bands at the Γ point in the Brillouin zone. This is consistent with the fact that all the positron bands are conduction ones. Going back to the electron band structure (Fig. 1), one can observe a presence of a band gap between the first and second valence bands at the X point in the Brillouin zone. This gap is termed as the antisymmetric gap and found to be useful for getting information about the trend of the ionicity in semiconducting materials [22,23]. Interestingly, this gap is also present in the positron band structure and may serve as a source of information on the crystal ionicity. It is to be noted that the effect of compositional disorder is more important on the electron band structure than on the positron band structure counterpart. The alloy disorder effect affects both the valence and conduction bands in the electronic band structure (Fig. 1) and hence it should be taken into account in the electron band structure calculations. The same conclusion can be drawn for the positron band structure even seen that the compositional disorder effect is not as important as that on the electron band structure. This particularly is more important for the positron thermalization energy that is the lowest energy level in the positron band structure.

The knowledge of the electronic and positronic band structures allowed us to determine the electron and positron effective masses that are important parameters in transport properties of semiconductors. Following the approach used by Bouarissa [24] for both electrons and positrons, the electron and positron effective masses have been calculated. The electron effective mass has been determined in the electronic conduction band minimum at the Γ valley, whereas, the positron effective mass counterpart was obtained in the bottom of the positronic lowest energy band and termed as the positron band mass (m_b^*). Our findings showed that the electron effective mass for InSb is $0.03m_0$ and that for AlSb is $0.13m_0$, where m_0 is the electron free-particle mass. These values agree reasonably with the experimental ones of $0.013m_0$ [25] and $0.14m_0$ [25] reported by Adachi for InSb and AlSb, respectively. Taking into account the disorder effect, the variation of the electron effective mass as a function of the alloy composition x for $Al_xIn_{1-x}Sb$ with zinc-blende structure is displayed in Fig. 3. The solid line is a fitted curve drawn using the least-squares method. Note that by increasing the Al content on going from 0 up to 1, the electron effective mass increases almost linearly. The behavior suggests that the electron mobility may decrease with increasing the composition x. As regards the positron case, our calculations found that the positron effective band mass is $1.03m_0$ for InSb and $1.29m_0$ for AlSb, where m_0 is the positron free-particle mass. The positron effective mass of $1.5m_0$ has been reported to be a compromise over the various theoretical and experimental determinations [26]. As compared to our obtained values, it seems that our results are smaller than this value. As a matter of fact, the positron effective mass contains the contributions due to the periodic lattice (m_b^*) and due to the screening electron cloud (correlation effective mass) [26]. Recently, Panda et al. [27] have determined the positron effective mass in Si using first-principles calculations. Their results showed that the obtained positron effective mass is smaller than $1.5m_0$. The discrepancy has been attributed to the neglect of the positron–phonon and positron–plasmon interactions. By including the positron–plasmon interaction in their calculation, Panda et al. [27] found that the positron effective mass becomes in good agreement with that of $1.5m_0$, suggesting thus that the positron self-interaction with the phonon field is negligible. Accordingly, one can believe that the discrepancy in our case is due to the neglect of the positron-plasmon interaction. Nevertheless, one can note that the largest contribution to the positron effective mass comes from m_b^*. This is