IL NUOVO CIMENTO VOL. 20 D, N. 12 Dicembre 1998

Electronic structure of $Ga_xIn_{1-x}As_ySb_{1-y}$ quaternary alloy by recursion method

M. EL-HASAN and H. ALAYAN
Physics Department, An-Najah N. University - Nablus, West Bank, Palestine

(ricevuto il 28 Aprile 1997; revisionato il 25 Luglio 1998; approvato il 31 Luglio 1998)

Summary. — This work reports the electronic structure of GaInAsSb quaternary alloy by recursion method. A five-orbital sp^3s^* per atom model was used in the tight-binding representation of the Hamiltonian. The local density of states (LDOS), integrated density of states (IDOS) and structural energy (ST.E) were calculated for Ga, In, As and Sb sites in $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$ and GaInAsSb lattice matched to GaAs and the same alloy lattice matched to GaSb. There are 216 atoms in our cluster arranged in a zincblend structure. The results are in good agreement with available information about the alloy.

PACS 71.20 – Electronic density of states and band structure of crystalline solids.

Introduction

The quaternary alloy $Ga_xIn_{1-x}As_ySb_{1-y}$ is a promising material in the technology of photodevices. The importance of this material comes from the fact that one of its constituents, $InAs_xSb_{1-x}$ ternary, has the smallest band gap energy among all III-V semiconductors [1]. It was observed that the energy gap for this ternary is 99 meV when $x = 0.68$ [2]. So this quaternary has important applications as light emitter or photodetector in infrared and near-infrared ranges. The fact is that in quaternaries concentrations of anions and cations could be varied independently, so the average lattice constant and the band gap energy could be varied independently too [3]. For this reason epitaxial layers of quaternary alloys of desired compositions can be fabricated to match a certain substrate.

Some experimental groups were successful in preparing this material with compositions which match with GaAs [4, 5] substrates, while other groups prepared the alloy with compositions which match GaSb substrates [6, 7]. Various methods have been used in fabricating this material as Molecular Beam Epitaxy [4, 5] and Liquid Phase Epitaxy [6, 7]. Also actual devices as light-emitting heterostructure laser diodes [8], multiple quantum wells [9, 10] and photodetectors [11, 12] have been fabricated.

Experimental work on this material has been carried in the form of photoluminescence at low temperature [6, 7]. Band gap energy and its temperature

© Società Italiana di Fisica

dependence have been studied by performing Fourier Tranform Infrared Spectroscopy (FTIRS) measurements at different temperatures [4].

On the other hand, the theoretical work on quaternary alloys is not extensive. It was started by Chen and Sher [13] by performing Coherent Potential Approximation (CPA) to study the valance bands for GaInAsP. After then Gera *et al.* [14] used Coherent Potential Approximation (CPA) and Virtual Crystal Approximation (VCA) to study both valence and condition bands for GaInAsP too. Ekpenuma *et al.* used CPA and VCA to study both valence and condition bands for four quaternaries where GaInAsSb was one of them. Recently, the recursion method was used to study electronic structure of GaInAsP [15].

In this work, the recursion method was used to study the electronic structure of GaInAsSb. In the next section the method is summarized. Details of calculations and results are given in sect. 3.

2. – The recursion method

The recursion method has been extensively discussed in the literature [16]. Therefore only a brief discussion of the essentials is given here. The main quantity of interest in the recursion method is the local density of states (LDOS) which is defined by

$$N_\alpha(E, R) = \sum_n |\langle n|\alpha R\rangle|^2 \delta(E - E_n), \tag{1}$$

where $|n\rangle$ and E_n are the eigenfunction and eigenvalues of the system and $|\alpha R\rangle$ is a localized orbital α located at R. Using the Green function $G(E) = (E - H)^{-1}$, eq. (1) can be written as

$$N_\alpha(E, R) = -\frac{1}{\pi} \lim_{s \to 0} \mathrm{Im}\langle \alpha R|G(E + i\delta)|\alpha R\rangle. \tag{2}$$

The method generates by means of the following recursion algorithm: an orthogonal basis $|n\}$, which contains the orbital $|\alpha R\rangle$ as starting element $|0\rangle$ and in which the Hamiltonian H is tridiagonal

$$b_{n+1}|n+1\rangle = (H - a_n)|n\rangle + b_n|n-1\rangle, \tag{3}$$

$$\langle n|H|m\rangle = \begin{cases} a_n, & \text{if } m = n\,, \\ b_n, & \text{if } m = n+1\,, \\ b_n^*, & \text{if } m = n-1\,, \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{4}$$

The 0-0 element of G

$$\langle 0|G|0\rangle = \frac{1}{E - a_0 - b_1^2/(E - a_1 \ldots)}$$

is equal to the local density of states $N_\alpha(E, R)$. Thus, the essential information needed for LDOS is contained in the set of coefficients a_n, b_n. Once the coefficients a_n, b_n are determined, the continued fraction can immediately be calculated for any E.

3. – Results and conclusions

The recursion method is not providing detailed k-space information about the structure, but it yields valuable information on LDOS at chosen atomic sites. Encouraged by the smallness of the alloy scattering effects, we use an interpolation procedure and try to make a reliable use of the known properties of the constituent binaries GaAs, GaSb, InAs and InSb.

A cluster of 216 atoms with zincblende structure, lattice constants and Slater-Koster (SK) parameters used in describing the Hamiltonian H is given in table I. The five orbitals sp^3s^* per atom are used so that there are 1080 orbitals in the system. Here s^* is the extra s-orbital originally introduced by Vogl *et al.* [17] to correct the conduction bands instead of extending the interaction to second nearest neighbors.

The number of coefficients a_n, b_n^2 calculated in all calculations reported is 17*.

The alloy lattice constant, and Slater-Koster (SK) parameters were calculated from the values of the constituent binaries according to Vegard's law including cation and anion concentrations. For the alloy $A_xB_{1-x}C_yD_{1-y}$, Vegard's law for the lattice constant and the SK parameter will be

$$a_{\text{alloy}} = yxa_{\text{AC}} + y(1-x)\,a_{\text{BC}} + x(1-y)\,a_{\text{AD}} + (1-y-x+xy)\,a_{\text{BD}},$$

$$V_{\text{alloy}} = yxV_{\text{AC}} + y(1-x)\,V_{\text{BC}} + x(1-y)\,V_{\text{AD}} + (1-y-x+xy)\,V_{\text{BD}}.$$

The self-energy of the starting state was also averaged according to the concentration of the two environments of each species as

$$SE(\text{A}) = SE_{\text{A}}(\text{AC}) * y + (1-y) * SE_{\text{A}}(\text{AD}),$$

$$SE(\text{B}) = SE_{\text{B}}(\text{BC}) * y + (1-y) * SE_{\text{B}}(\text{BD}),$$

$$SE(\text{C}) = SE_{\text{C}}(\text{AC}) * x + (1-x) * SE_{\text{C}}(\text{BC}),$$

$$SE(\text{D}) = SE_{\text{D}}(\text{AD}) * x + (1-x) * SE_{\text{D}}(\text{BD}),$$

TABLE I.

	GaAs	GaSb	InAs	InSb
a(Å)	5.6337	5.8732	6.036	6.4782
$-ss\sigma$	1.6133	1.5392	1.4006	1.3798
$S_aP_c\sigma$	1.9399	2.1478	1.3144	1.6403
$-S_aP_c\sigma$	2.5045	2.0211	2.3551	1.9875
$pp\sigma$	3.0276	2.4590	2.6946	2.2885
$-pp\pi$	0.7808	0.6633	0.6574	0.6186
$S_c^*P_a\sigma$	2.0967	2.1605	1.4612	1.5444
$-S_c^*P_c\sigma$	2.1651	1.8265	1.6930	1.4743
$-E(s, c)$	2.6569	3.8993	2.7219	3.4643
$-E(s, a)$	8.3431	7.3207	9.5381	8.0157
$E(p, c)$	3.6686	2.9146	3.7201	2.9162
$E(p, a)$	1.0414	0.8554	0.9099	0.6738
$E(S^*, c)$	6.7386	5.9846	6.7401	5.9362
$E(S^*, a)$	8.5914	6.6354	7.4099	6.4530

where $SE(\mathrm{A})$ is the self-energy of atom A, $SE_{\mathrm{A}}(\mathrm{AC})$ the self-energy of atom A in compound AC, $SE_{\mathrm{A}}(\mathrm{AD})$ the self-energy of atom A in compound AD, and similar definitions hold for the other quantities.

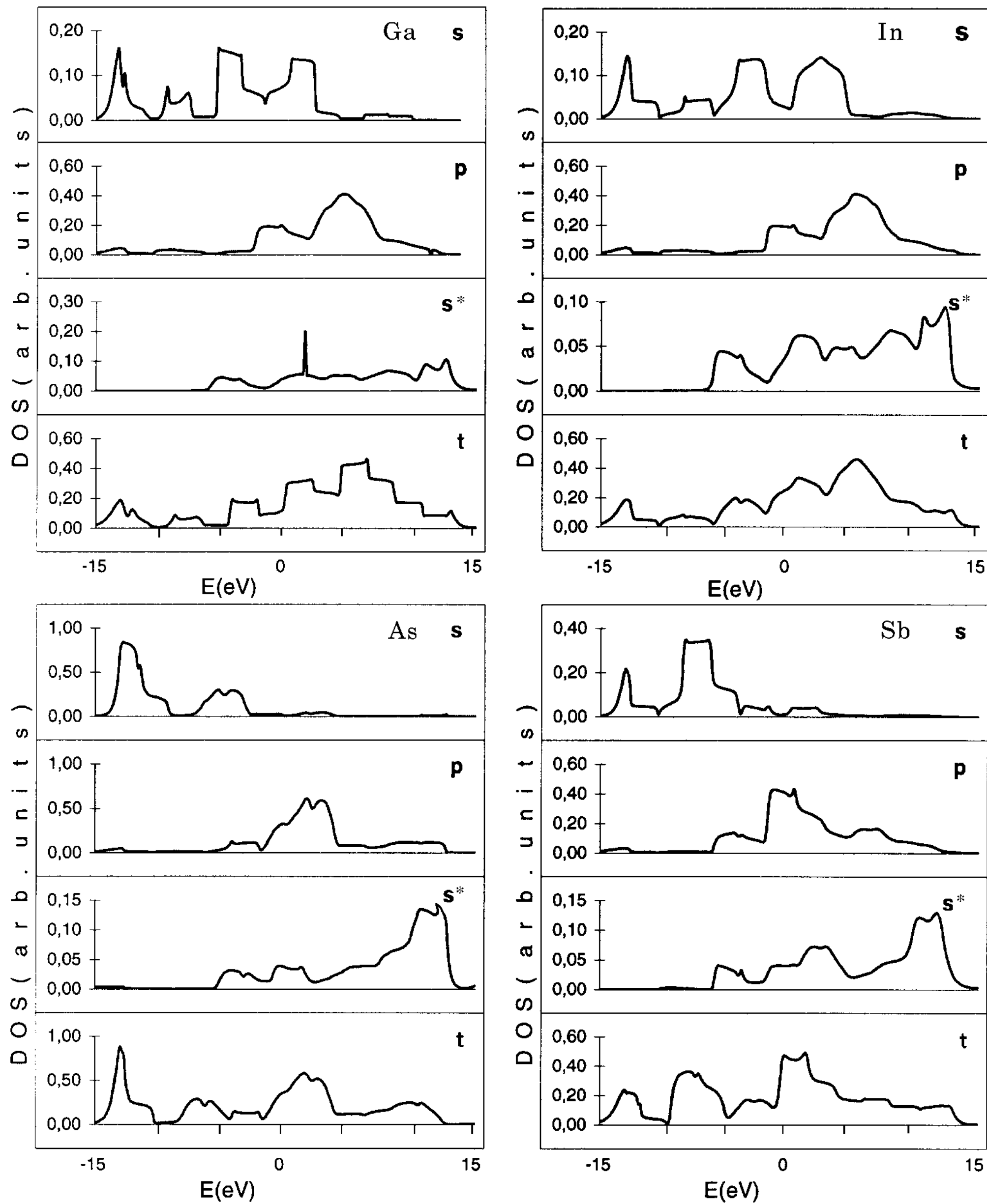

Fig. 1. – Partial LDOS and its orbital decomposition at Ga, In, As and Sb sites in $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$.

The integrated density of state (IDOS) was calculated by integrating LDOS over all the entire band as

$$\text{IDOS} = \sum_{\alpha} \int_{E_{\min}}^{E_{\max}} N_{\alpha}(E, R)\, \mathrm{d}E$$

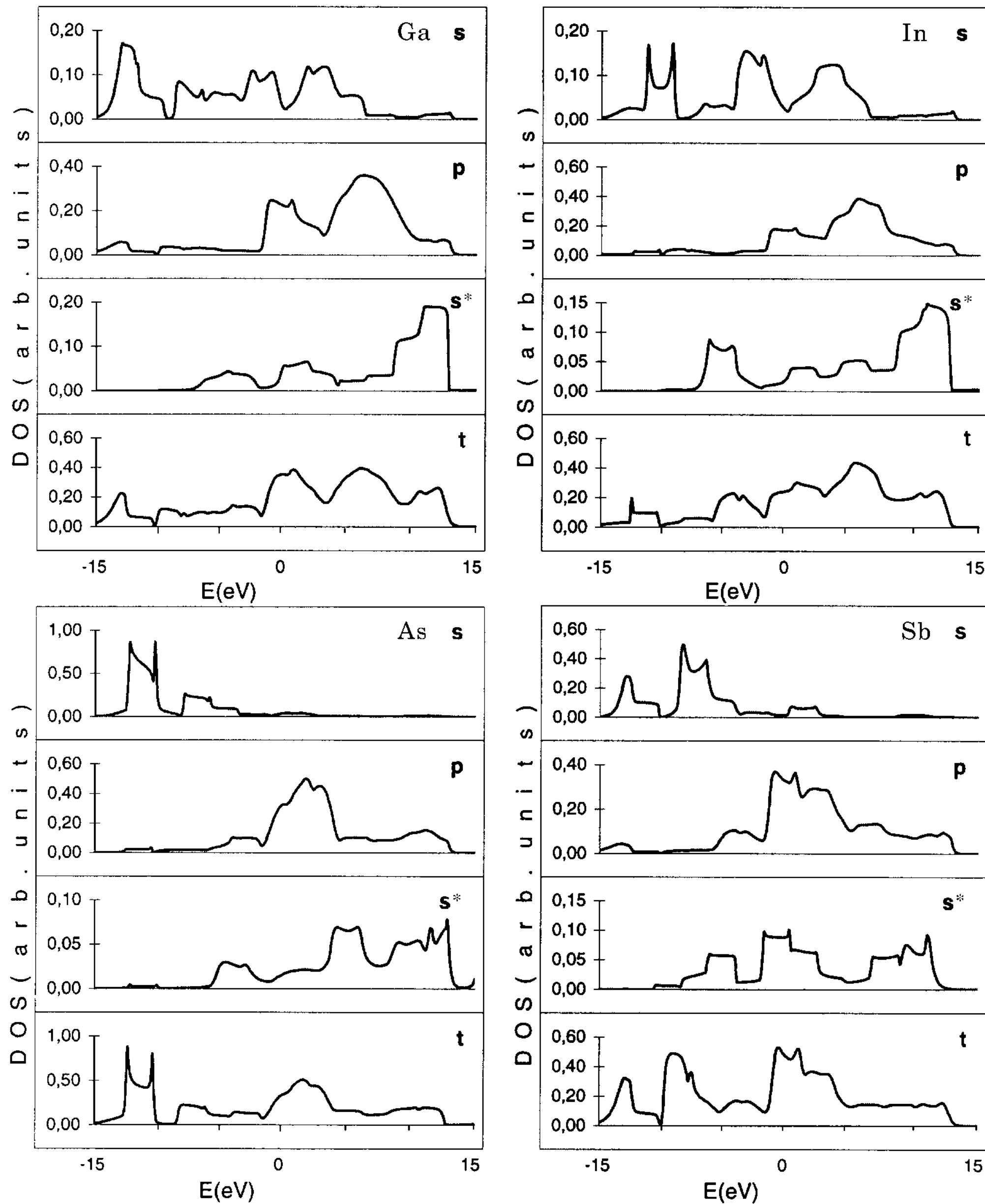

Fig. 2. – Partial LDOS and its orbital decomposition at Ga, In, As and Sb sites in $Ga_{0.222}In_{0.778}As_{0.812}Sb_{0.188}$.

and the structural energy (ST.E) contains almost all the interesting structure-dependent parts of the energy and was calculated as

$$\mathrm{ST.E} = \sum_{\alpha} \int_{E_{\min}}^{E_{\max}} E N_{\alpha}(E, R)\, \mathrm{d}E .$$

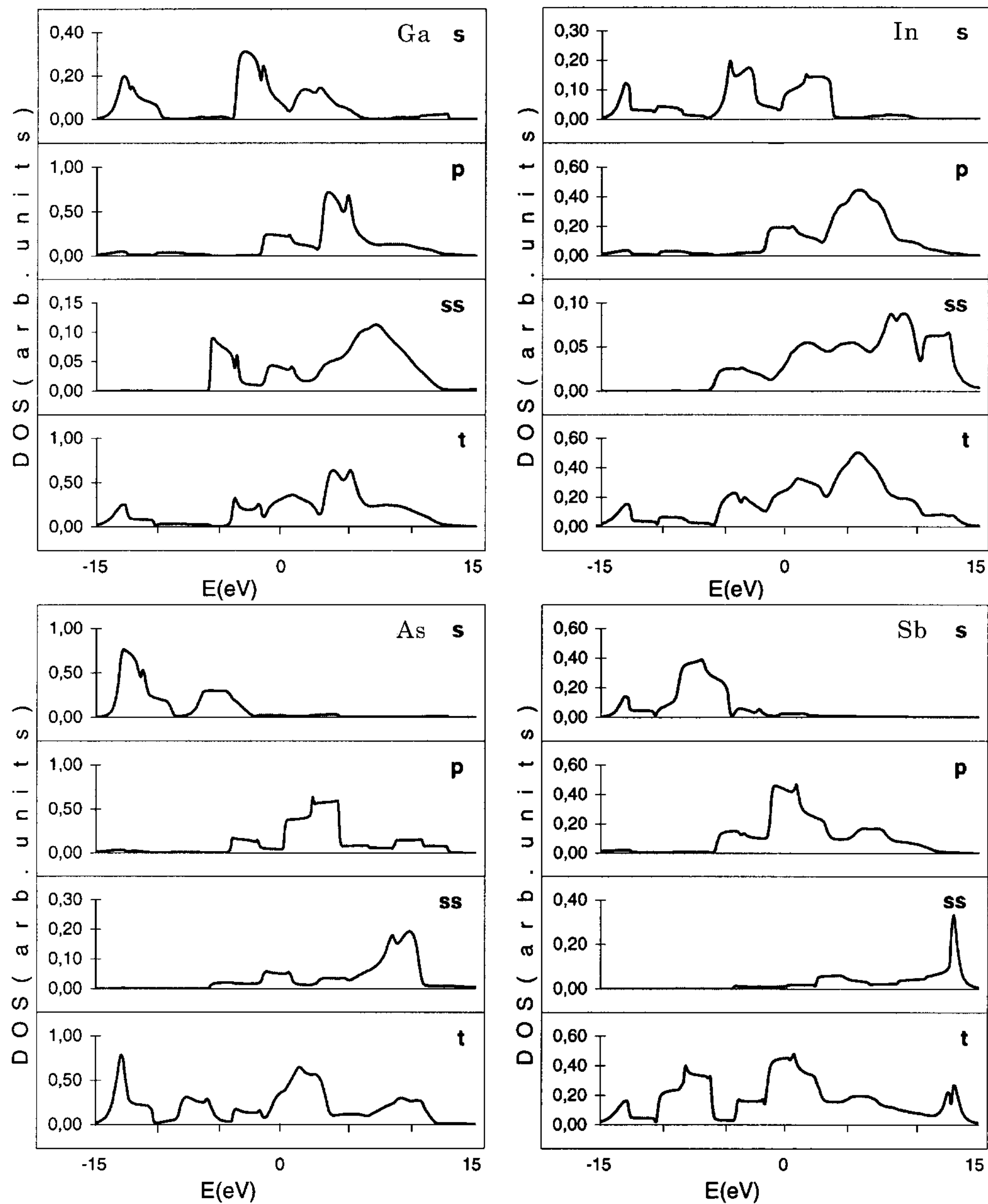

Fig. 3. – Partial LDOS and its orbital decomposition at Ga, In, As and Sb sites in $Ga_{0.77}In_{0.23}As_{0.19}Sb_{0.81}$.

The LDOS curves and its orbital decomposition have the general shape of such systems. It is difficult to compare with other calculations because the only (as far as we know) reported DOS for such alloys are those of ref. [3]. They used VCA and CPA in their calculations, but they are not reporting the local density of states nor its orbital decomposition. In our results, fig. 1 represents the LDOS and its orbital decomposition

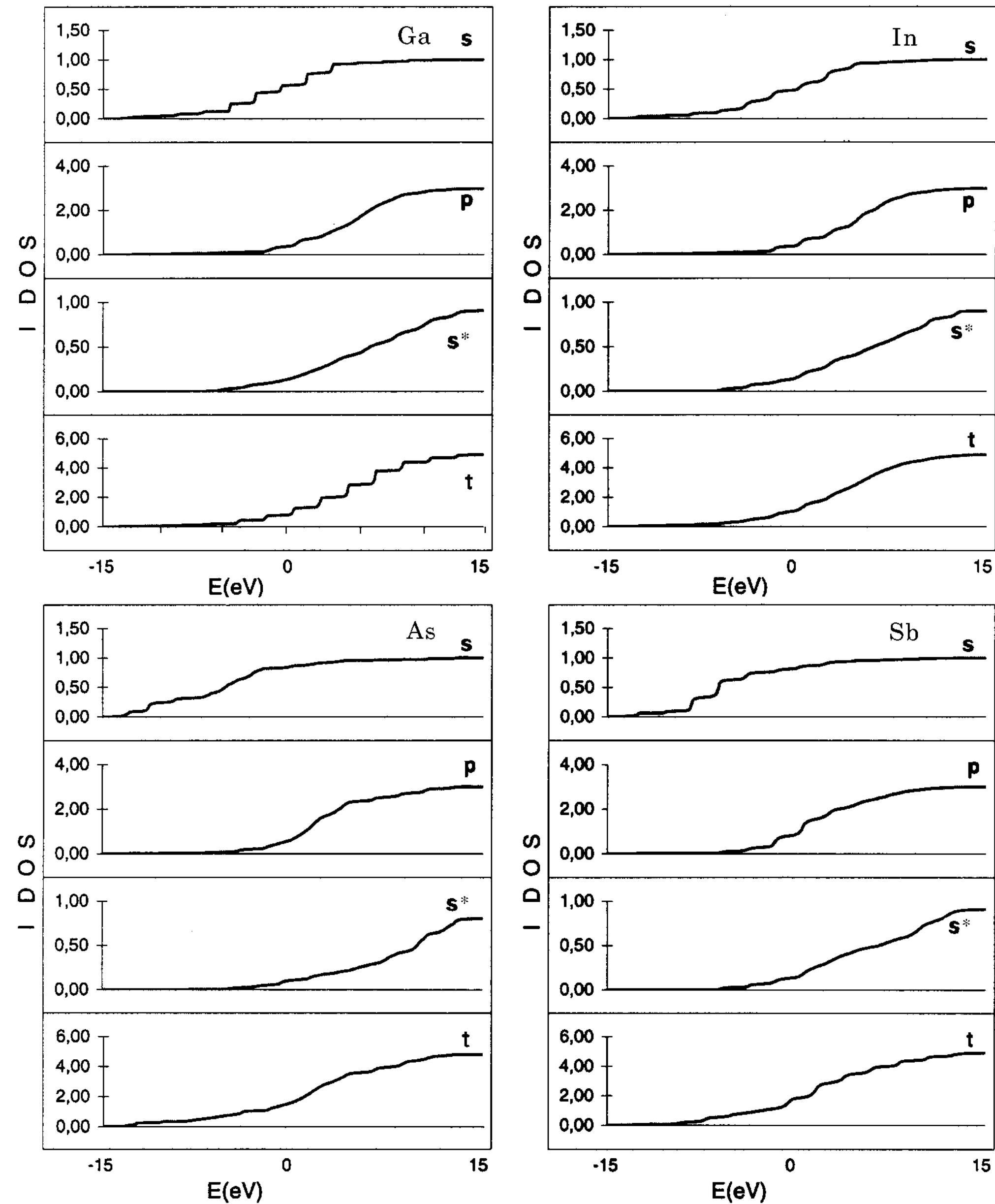

Fig. 4. – IDOS and its orbital decomposition at Ga, In, As and Sb sites in $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$.

for Ga, In, As and Sb sites of $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$ which is the same alloy and concentration as fig. 1(d) of ref. [3]. So we can roughly compare with their results. We have the same number of peaks as they have, three in valence band and three in conduction band, but our beaks are generally wider than theirs. Studying carefully our results for this alloy, we find that the contribution from the *s*-orbital of As is more than

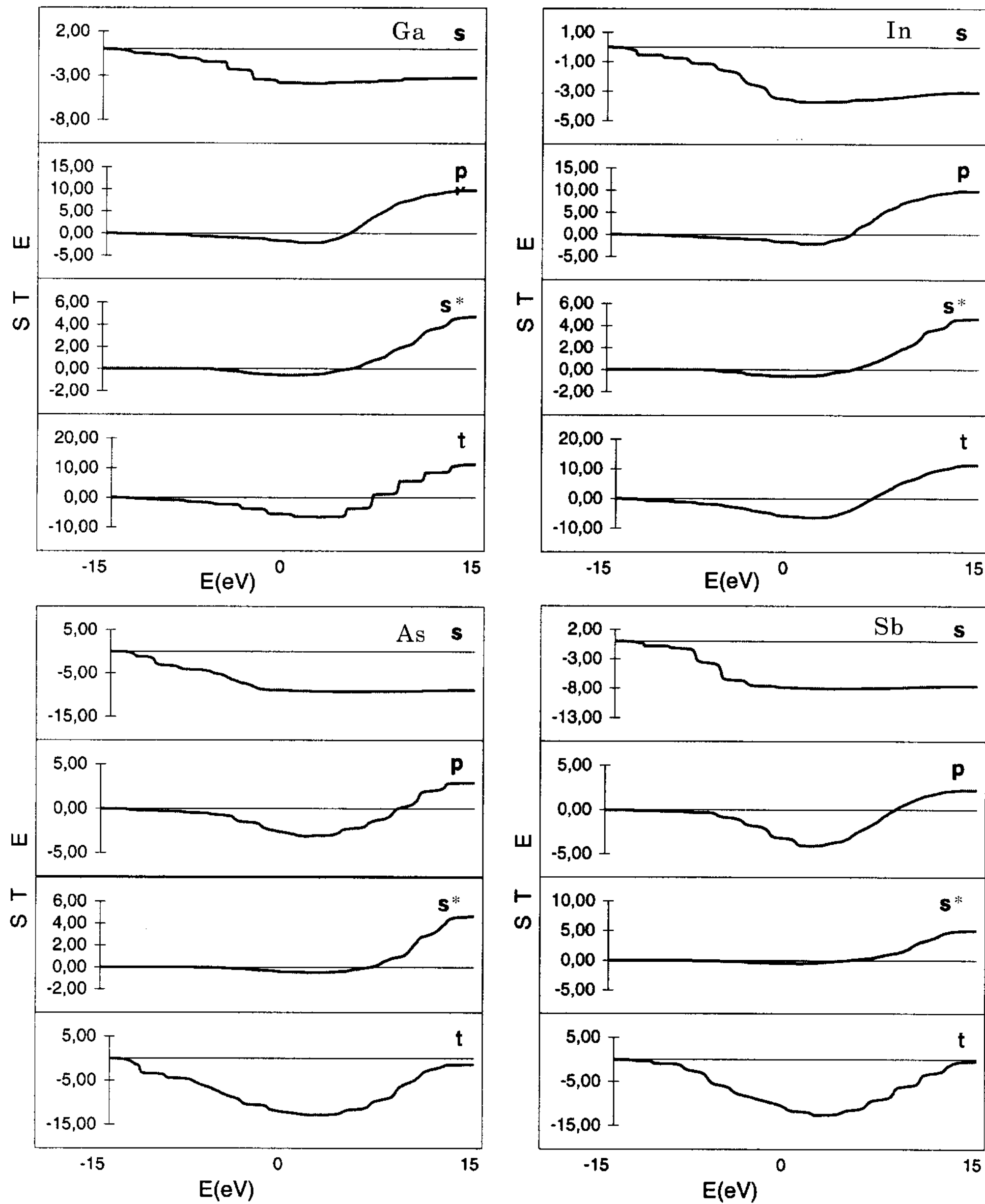

Fig. 5. – Structural energy and its orbital decomposition at Ga, In, As and Sb sites in $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$.

that of the Sb orbital and this is due to the difference in energy of the *s*-orbital for both of them, while the contribution to the *p*-bands is almost the same for both As and Sb. The same holds for contributions from Ga and In: they are almost the same for both *s*- and *p*-orbitals.

Figures 2 and 3 show the LDOS and its orbital decomposition in Ga, In, As and Sb sites in $Ga_{0.222}In_{0.778}As_{0.812}Sb_{0.188}$ (lattice matched to GaAs), and $Ga_{0.77}In_{0.23}As_{0.19}Sb_{0.81}$ (lattice matched to GaSb).

Although the integrated density of states (IDOS) and the structural energy (ST.E) were calculated at different atomic sites in the all three alloys, we present here in fig. 4 and 5 the results for the first alloy only for simplicity.

To study the compositional dependence of band gap variation is not easy with this method because of the well-known difficulties with band gaps in this technique. They do not become sharp enough for an easy determination.

REFERENCES

[1] OSBOURN G. C., *J. Vac. Sci. Technol. B*, **4** (1986) 1423.
[2] BETHEA C. G., YEN M. Y., LEVINE B. F., CHOI K. K. and CHO A. Y., *Appl. Phys. Lett.*, **51** (1987) 1431.
[3] EKUPENUMA S. N., MYLES C. W. and GREGG J. R., *Phys. Rev. B*, **41** (1990) 3582.
[4] BI WENGANG and LI AIZHEN, *Chinese Phys. Lett.*, **9** (1992) 53.
[5] LI A. Z. *et al.*, *Proceedings of the XVI International Symposium on GaAs and Related Compounds*, Vol. **106** (1989) p. 159.
[6] TRONC P., REID B., MACIEJKO R., LECLERCQ J. L. and LAZZARI J. L., *Solid State Commun.*, **85** (1993) 2177.
[7] TRONC P., REID B., MANI H., MACIEJKO R., TITKOV A. N., LAZZARI J. and ALIBERT C., *Phys. Status Solidi*, **180** (1993) 1087.
[8] MESSANH MOHOU A., internal report LAMP/95/2. ICTP, Trieste (1995).
[9] EGLASH S. J. and CHOI H. K., *Appl. Phys. Lett.*, **57** (1992) 1292.
[10] CHOI H. K., TURNER G. W. and EGLASH S. J., *IEEE 4990 Photon Technol. Lett.*, Vol. **6**, **7** (1994).
[11] ANDREEV I. A., AFRAILOVA M. A., BARANOV A. N., KONNIKOV S. G., MIRSAGATOV M. A., MIKHAILOVA M. P., SALATA O. V., UMANSKII V. B., FILARETOVA G. M. and YAKOVLEV YU. P., *Sov. Tech. Phys. Lett.*, **14** (1989) 935.
[12] TITKOV A. N., CHEBAN V. N., BARANOV A. N., GUSEINOV A. A. and YAKOVLEV YU. P., *Sov. Phys Semicond.*, **24** (1990) 666.
[13] CHEN A.-B. and SHER A., *Phys. Rev. B*, **19** (1979) 3057.
[14] GERA V. A., GUPTA R. and JAIN K. P., *Phys. Rev. B*, **36** (1987) 9657.
[15] EL-HASAN M., *to be published in Int. J. Mod. Phys. B*.
[16] HEINE V., HAYDOCK R. and KELLY M., in *Solid State Physics*, edited by H. EHRENREICH, F. SEITZ and TURNBULL, Vol. **35** (Academic Press, New York) 1980.
[17] VOGL HJALMARSON H. P. and DOW J. D., *J. Phys. Chem. Solids*, **44** (1983) 365.