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Abstract

Two new minimum-energy surface structures have been identified for p(1x1) overlayers of Sb on the (110) surface of III-V compound semiconductors using a tight-binding total-energy formalism previously developed for these systems. The first is the "commensurate chain" structure in which Sb zig-zag chains are commensurate with, and on top of, the Ga-As unreconstructed surface zig-zag chains. This structure differs from the previously found epitaxical-chain structure by virtue of the registry of the Sb chains "on top of" rather than "in between" the substrate Ga-As chains. Like the epitaxical chain structure, it is compatible with both scanning tunneling microscopy (STM) and photoemission data. The second is an "overlapping chain" structure in which the Sb chains are 180° out-of-phase with, and on top of, the Ga-As substrate chains. This structure is, however, incompatible with both low-energy-electron-diffraction and STM data for GaAs(110)-p(1x1)-Sb although it may be a possible structure for other systems. Computations for GaP(110)-p(1x1)-Sb and InSb(110)-p(1x1)-Sb reveal that the energy difference between the commensurate chain and traditional epitaxical structure is approximately constant over this range of overlayer/substrate lattice mismatch.

I. Introduction

The GaAs(110)-p(1x1)-Sb overlayer system has been studied extensively[1,2,3], and its atomic geometry determined quantitatively by a low-energy electron diffraction (LEED) intensity analysis[4]. The resulting "epitaxical" structure, shown in Fig.1a, has been confirmed via theoretical total-energy model predictions[5,6], and by comparison of the predictions of this model with angle-resolved photoemission[7,8] (ARPES) data, inverse photoemission[9] (IP) data, and scanning tunneling microscopy (STM) images[10]. Nevertheless, two recent developments suggest that a reexamination of the structure of Group V overlayers on zincblende structure cleavage faces might reveal a more extensive array of surface geometries. First, the latest STM study[10], concluded that in addition to the accepted epitaxical structure (Fig.1a), the "p^3" model of Skeath *et al.*[2] (Fig. 1b) also was compatible with the data. Second, recent studies of Bi overlayers on the (110) surface of the III-V's show differences from the Sb systems[11,12,13] suggesting the possibility of different surface structures.

In this paper we utilize a tight-binding total energy model, previously applied to these systems[5,6], to derive two new minimum-energy surface atomic structures for Column V adsorbates on the (110) surface on III-V compound semiconductors, and show that one of these structures, the "commensurate chain" model, is compatible with the current STM, ARPES, and IP data for the GaAs(110)-p(1x1)-Sb system. The other structure, the "overlapping chain" model, has been eliminated by a LEED intensity analysis[4], but the commensurate chain model has not yet been tested against LEED intensity data. Finally, we explore the hypothesis that the relative stability of these surface structures is a function of the mismatch between the overlayer and substrate lattices.

II. The Model

Tight-binding total energy minimization computations were performed for the III-V(110)-p(1x1)-Sb(1ML) using a 17-layer slab consisting of fifteen(15) III-V substrate layers with layers of Sb at both the top and bottom surfaces making each surface equivalent. All thirty-four(34) atoms in each unit cell of the slab were allowed to relax. The tight-binding model used was a slightly modified version of the of the nearest-neighbor sp^3s^* empirical tight-binding models of Vogl *et al.*[14] and Chadi[15] as applied to the Sb/III-V(110) epitaxical structures by Mailhiot *et al.*[5-6].(See Table I for the model parameters.) The modification involves the parameters describing the interactions of the Sb adatoms with themselves, which were derived in Ref. 6 using the d^{-2} scaling law and a value of 2.87 Å for the Sb-Sb equilibrium bond length (the value in bulk Sb). Likewise, the parameters given in Ref. 6 describing the interaction of the Sb adatoms with the P substrate atoms in GaP were derived using the d^{-2} scaling law and a value of 2.11 Å for the Sb-P equilibrium bond length. These two values for the bond lengths are different from the sum of the covalent radii (the criterion used to obtain all other equilibrium bond lengths in cases where they are unknown) of 2.72 Å for d(Sb-Sb) and 2.46 Å for d(Sb-P). Since we are interested in the scaling between the relative stabilities of the surface structures and the overlayer/substrate lattice mismatch in a systematic way, the Sb-Sb and Sb-P parameters were rederived using the d^{-2} scaling law and the sum of the covalent radii as the equilibrium bond length. (See Table I.) The remaining parameters are those given in Ref. 6. Since we are using a different tight-binding model parameter set, the structural parameters listed in Table II for the epitaxical structures are different from those reported in Ref. 6, although for Sb/GaAs(110) they are still quantitatively comparable (*i.e.,* within the combined LEED and model uncertainties) with the results of the LEED study.[6]

The new aspect of our analysis relative to those given earlier[5,6] is the recognition that a number of structurally inequivalent local minima in the total energy surface exist and that these can be located by using different starting geometries in the energy minimization process. By utilizing a variety of starting structures corresponding to conceptually distinct types of Sb-substrate bonding we have been able to locate three separate local minima in the total energy surface. One of these, the epitaxical structure, corresponds to the results of earlier calculations.[5,6] The other two correspond to different types of Sb-substrate bonding which lead to locally optimized surface structures which we refer to as the "commensurate chain" and "overlapping chain" structures, respectively. The tight-binding total energy model is probably inadequate to give absolute magnitudes of the energy differences between these minima, but by indicating their existence it can guide the experimental search for the various structures, *e.g.*, by LEED intensity analysis.

III. GaAs(110)-p(1x1)-Sb(1ML)

Using the model described above, total-energy minimization computations[15] were performed for GaAs(110)-p(1x1)-Sb(1ML) using three chemically distinct starting geometries; each of which differed in the registry of the Sb overlayer zig-zag chains with the (110) surface Ga-As zig-zag chains. Three minimum-energy surface structures were found. The first consists of the the epitaxical chain structure (Fig. 1a) reported previously[5,6] and shown to be compatible with LEED[4], ARPES[7,8], IP[9], and STM[10] data. The second consists of the analogous Sb zig-zag chains commensurate with, but on top of, the the underlying GaAs zig-zag chains on the unrelaxed (110) surface (Fig. 1c - "commensurate chain" (CC) structure). This structure, obtained by starting with the proposed "*p3*" model of Skeath[2] (Fig. 1b) and allowing it to relax, also is compatible with the recent STM data.[10] The third structure is the "overlapping chain" (OC) model described by Duke *et al.*[4]. (See Fig. 1d.) It consists of Sb zig-zag chains in which the Sb-Sb bonds overlap the Ga-As bonds in the unreconstructed surface zig-zag chains, and exhibits metallic bonding. This structure is not compatible with the STM data for GaAs(110)-p(1x1)-Sb, yet may be a possible structure for other systems. The specification and listing of the relevant geometrical parameters for these three minimum-energy structures are given in Fig. 1 and Table II.

Using the tight-binding total energy model the OC structure is computed to be substantially lower in energy than either the epitaxical or CC structures. An examination of the bonding in the OC structure quickly reveals why. As shown in Fig. 1d, each Sb surface atom is fivefold-coordinated, as opposed to threefold-coordinated plus a lone pair in the epitaxical and CC structures, bonding to two other Sb ad-atoms in the chain and to three surface atoms. This fact results in each surface atom being sixfold-coordinated. Because of the simplified treatment of the Coulomb repulsion in the tight-binding total energy model[15], the more bonds that are formed, the lower the energy without regard to the Coulomb interactions between the electrons in the various bonds. Hence, no argument can be made, on the basis of the tight-binding total-energy model, for the preference of this structure over a structure with a different bonding pattern. All that can be concluded is that the OC structure represents a stable minimum-energy conformation. The question of whether it is a local or global minimum can only be inferred via comparison of the predicted structures with experimental data. Since the OC structure is incompatible with the experimental data for Sb/GaAs(110) we limit further consideration in this paper to the CC structure, even though the OC model may be an alternative structure for other systems.

For GaAs(110)-p(1x1)-Sb(1ML), the tight-binding total energy of the epitaxical structure is lower than that of the CC structure by ~0.21 eV/surface atom/unit cell. This energy is the total energy difference between the two structures for the 34 atom slab divided by 2 surface atoms per unit cell. We regard it as sufficiently small so as to make the two structures comparable within the intrinsic accuracy of the model. Therefore in the following subsections we turn to a survey of the experimental evidence permitting a discrimination to be made between the epitaxical and CC structures.

A. Scanning Tunneling Microscopy

As noted previously, the CC structure is compatible with the most recent STM results[10]. Mårtensson and Feenstra found, as shown in Fig. 2b, that the proposed "p^3" model (Fig. 1b) is only marginally incompatible with the experimental data[10]. The CC model however (Figs. 1c and 2c) gives a better fit to the data than the epitaxical structure (Figs. 1a and 2a). It is important to remember that in the originally proposed p^3 model the substrate was assumed to remain fully reconstructed after adsorption, while in the CC structure the adsorption of Sb largely un-relaxes the substrate (see Fig. 1 and Table II). The OC model, shown in Fig. 2d is clearly incompatible with the data.

B. Surface State Eigenvalue Spectrum

Figures 3 and 4, respectively, show the computed surface state eigenvalue spectrum for the CC structure and the surface state eigenvalue spectrum for the epitaxical structure as calculated by Mailhiot *et al.*[6]. While the two are similar there are notable differences which arise from the different character of the bonding in the two structures. The epitaxical structure is characterized by a p^2 bonding within the Sb chain, while the overlayer-substrate bond arises from the interaction of the Sb $p\pi$ orbital with the sp^3 hybridized dangling bond of the substrate atom.[5,6,16] Consequently, the surface states associated with the intrachain bonding p orbitals do not, effectively, interact with the substrate, and only the $p\pi$ states of the chain (S_5-S_8) are split into overlayer-substrate bonding and anti-bonding pairs.[6] (See Fig. 5.)

In the CC structure however, the intrachain and overlayer-substrate bonding is not separable. The bonding is best characterized as a p^3 hybridization - hence the original name - which is responsible for both the intrachain and overlayer-substrate interactions. The s orbital bands remain separated from the p AO hybrids and are therefore labelled in Fig. 3 with the same surface state notation as that of Ref. 6 (and Fig. 4). Because of the different hybridization, and the fact that the p AO mixing in the p^3 states is a function of the wavevector $\mathbf{k}_{||}$, however, the orbital nature of the surface states changes as the p AO mixing changes throughout the surface Brillouin zone (SBZ). Therefore the p^3 states are simply labelled S^{I}-S^{VII} (Fig. 3). For comparison with the orbital character of the eigenvectors in the epitaxical structure shown in Fig. 5, in Fig. 6 we schematically illustrate the orbital nature of the surface states near X.

As Fig. 3 reveals, the effect of the p^3 hybridization on the surface states is large. Interestingly, because the un-relaxation of the substrate in the CC structure is not as complete as in the epitaxical structure (see Table II), the persistance of the in-plane (reconstructed) substrate p orbital bands A_3 (at the top of the stomach gap) and A_4 (at the bottom of the fundamental gap) is seen near point X'. (See Fig. 3.)

To date there have been two ARPES[7-8] studies of GaAs(110)-p(1x1)-Sb(1ML). The tight-binding total energy computations of Mailhiot *et al.*[6], based on the epitaxical model, have been in qualitative agreement with both of them, although it encountered some difficulties with the interpretation of the data of Ref. 8. Figures 5 and 6 compare the ARPES data of references 7 and 8 respectively, with the surface state eigenvalue spectrum based on the CC model. These figures reveal that, within the ability of the data to distinguish between different surface states, the predictions of the CC model are qualitatively consistent with the ARPES data from Ref. 7. As in the case of the epitaxical model, however, there are some fundamental disagreements between the data of Ref. 8 and the tight-binding computations for the CC structure. These discrepancies may be explainable via the changes in surface state orbital character but at the present time we cannot account for them in detail.

The single IP study[9], on the basis of three data points, determined that the lowest unoccupied surface state band had a slight upward dispersion away from Γ towards X, and was ~2 eV above the valence band maximum at Γ. Examination of Fig. 3 reveals that the CC model is consistent with these data as well.

III. Scaling

As the adatom-adatom bond length is increased, preservation of the p(1x1) symmetry of the surface requires the lateral expansion of the adatom chain along the [100] direction[6]. Although the increased adatom-adatom bond length can also be accommodated via a shearing of the surface layer in the direction perpendicular to the surface, the data in

Table II indicate that this is a small contribution. Thus, we might expect that different overlayer structures would occur as a function of the mismatch between the adatom-adatom bond length in the overlayer, and the anion-cation bond length in the substrate. This section is devoted to an examination of this topic.

It can be seen from Fig. 1a that for the epitaxical structure, expansion of the overlayer chain in the [100] direction diminishes the overlap between the *sp*^{3} dangling bonds of the substrate and the *p*π orbital of the adatom. As a consequence, the surface atoms are forced to rehybridize in an energetically unfavorable way, thereby destabilizing this structure. However, in the CC structure (Fig. 1c) lateral expansion of the overlayer chain *increases* the overlap between the overlayer chain orbital and the substrate *sp*^{3} dangling bond, stabilizing the structure. Therefore, there exists the interesting possibility that the realization of either one of these surface structures is primarily a function of the mismatch between the overlayer bond length and that of the substrate. According to this line of reasoning, well lattice-matched adsorbate-substrate systems, such as Sb/InSb(110) where d(Sb-Sb) = 2.72 Å and d(In-Sb) = 2.81 Å, the epitaxical structure should be favored while for less well lattice-matched systems, such as Sb/GaP(110) where d(Sb-Sb) = 2.72 Å and d(Ga-

P) = 2.36 Å, the CC structure may be favored. The Sb/GaAs(110) system (d(Ga-As) = 2.45 Å) may be a borderline epitaxical system.

Since the InSb(110)-p(1x1)-Sb system is well lattice-matched (d(Sb-Sb) = 2.72 Å; d(In-Sb) = 2.81 Å), if the relative stabilities of these structures is controlled by the lattice mismatch, the epitaxical structure should be favored over the CC structure to a greater extent than in the GaAs system. Our computations indicate, however, that although the epitaxical structure is lower in energy, the energy difference between the two structures is on the same order as that for Sb/GaAs(110) at ~0.14 eV/surface atom/unit cell. Likewise, in the even less-well lattice-matched system of GaP(110)-p(1x1)-Sb the epitaxical structure is favored over the CC structure by ~0.19 eV/surface atom/unit cell. Therefore the energy difference between these two surface structures is approximately constant, implying that the concept of overlayer/substrate lattice mismatch being the primary factor determining the surface structure is not supported by our calculations *within this limited range of lattice mismatch.*

Indeed, it is uncertain where, if anywhere, a "crossover" point between the epitaxical and CC structures occurs. One possible figure of merit is the intrachain bond angle, θ. (See Fig. 1) Since larger adatom-

adatom bond lengths are accommodated primarily via lateral expansion of the chain in the [100] direction, for a series of adatoms on a single substrate θ scales inversely with the intrachain bond length. Conversely, for a single adatom species θ scales directly with the bulk substrate lattice constant. For isolated Sb chains, the equilibrium value of θ is ~91°, hence any significant deviation from this value will be energetically unfavorable. The CC structure is expected to be favored over the epitaxical structure for those cases in which $\theta << 90°$.

Table III lists values of θ computed by assuming that the Sb adatoms occupy the epitaxical positions and that neither the substrate nor the overlayer relax. Moreover, these values are compared to those obtained via the tight-binding total energy minimization computations in which the entire system is allowed to relax. As expected, θ scales directly with the bulk substrate lattice constant, but none of these systems satisfy the condition that $\theta << 90°$. It is interesting to note that, based on θ, the largest overlayer/substrate "mismatch" actually occurs for the Sb/InSb(110) system, and is evidenced by the larger substrate relaxation, and value of $\Delta_{2,\perp}$ for this system.

Finally in Table III we present the values of θ computed simply by placing Bi atoms in the epitaxical positions and assuming only lateral expansion with no substrate relaxation. Evidently both the Bi/GaP(110) and Bi/GaAs(110) are expected to show values of $\theta < 90°$. Whether they are sufficiently less than 90° to display the CC structure remains to be determined.

V. Synopsis

By searching over chemically distinct starting structures in total-energy minimization calculations, two new possible minimum-energy surface atomic structures for p(1x1) overlayers of Column V elements on the (110) face of III-V compound semiconductors have been identified. The electronic structure and bonding on one of these (the CC structure) has been explored in detail. This structure is compatible with current STM, ARPES, and IP data, thereby rendering it a viable potential alternative to the previously determined epitaxical structure to be checked by analysis of LEED intensity data. The systematics of the energy difference between these two structures as a function of the mismatch between overlayer and substrate have been examined for a limited set of overlayer/substrate systems, *i.e.*, p(1x1)-Sb on the (110) surface of GaP, GaAs, and InSb. The tight-binding total energy difference between the epitaxical and CC structures for these systems were found to be approximately constant, and within the intrinsic accuracy of the tight-binding model. The adatom intrachain bond angle, θ, is predicted to vary inversely with the adatom-adatom bond length for a given substrate, and directly with the bulk substrate lattice constant for a given overlayer. The condition that $\theta << 90°$ was established as the criterion for the CC structure to be clearly more stable than the epitaxical structure. None of the systems listed above met this condition, although simple geometric considerations suggest that the Bi/GaP(110) and Bi/GaAs(110) may do so.

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Table I: Empirical tight-binding interactions for the sp^3s^* model. The notation is of Refs. 6 and 13. Units are eV for the interactions and Å for d_o.

Tight Binding Interactions	Sb/GaP	Sb/GaAs	Sb/InSb
$E_s[1]$	-8.112	-8.343	-8.016
$E_s[2]$	-2.198	-2.657	-3.464
$E_s[3]$	-7.321	-7.321	-8.016
$E_{s^*}[1]$	8.515	8.591	6.454
$E_s^*[2]$	7.185	6.739	5.936
$E_s^*[3]$	6.635	6.635	6.454
$E_p[1]$	1.125	1.041	0.674
$E_p[2]$	4.115	3.669	2.916
$E_p[3]$	0.855	0.855	0.674
$V_{ss}\sigma[1,2]$	-1.868	-1.613	-1.380
$V_{ss}\sigma[1,3]$	-1.746	-1.638	-1.462
$V_{sp}\sigma[1,2]$	1.852	1.940	1.640
$V_{sp}\sigma[2,1]$	2.736	2.504	1.987
$V_{sp}\sigma[1,3]$	2.292	2.150	1.922
$V_{sp}\sigma[3,1]$	2.436	2.285	1.544
$V_{s^*p}\sigma[2,1]$	2.206	2.082	1.474
$V_{s^*p}\sigma[1,3]$	2.072	1.943	1.599
$V_{s^*p}\sigma[3,1]$	2.451	2.299	1.599
$V_{pp}\sigma[1,2]$	3.106	3.028	2.289
$V_{pp}\sigma[1,3]$	2.789	2.616	2.425
$V_{pp}\pi[1,2]$	-0.746	-0.781	-0.619
$V_{pp}\pi[1,3]$	-0.723	-0.678	-0.655
$U_1[1,2]$	-18.55	-17.79	-13.18
$U_1[1,3]$	-19.36	-17.70	-14.21
$U_1[2,3]$	-15.62	-15.62	-13.18
$U_1[3,3]$	-14.92	-14.92	-14.21
$U_2[1,2]=U_2[1,3]=U_2[3,3]$	59.08	56.50	47.52
$U_2[2,3]$	52.64	52.64	47.52
$d_o[1,2]$	2.36	2.45	2.81
$d_o[1,3]$	2.63	2.63	2.81
$d_o[2,3]$	2.46	2.54	2.72
$d_o[3,3]$	2.72	2.72	2.72

Table II: Parameters predicted for the commensurate chain (CC) and epitaxical (Epi) structures of $M_{III}A_{V}(110)$-p(1x1)-Sb as shown in Fig. 1. The values in parentheses were determined via ELEED for GaAs(110)-p(1x1)-Sb (epitaxical model- Ref. 4). Uncertainty in predicted structural parameters is ±0.2 Å (Ref. 6) and the units are Å. Also listed is the tight-binding total-energy per unit cell (E_{Total}) for each structure as well as the total-energy per unit cell of the CC and OC structures relative to that of the epitaxical structure ($E_{Rel.}$). Energy units are eV.

		GaP			GaAs			InSb	
	CC	Epi	OC	CC	Epi	OC	CC	Epi	OC
$\Delta_{1,\perp}$	0.16	0.07	0.10	0.33	0.04 (0.1±0.05)	0.13	0.34	0.01	0.04
$\Delta_{1,y}$	1.90	1.90	2.14	1.83	1.86 (1.96±0.3)	2.11	1.64	1.66	1.95
$d_{12,\perp}$	2.81	2.30	2.13	2.93	2.35 (2.39±0.1)	2.11	3.13	2.46	2.05
$d_{12,y}$	1.46	4.42	1.73	1.25	4.47 (4.62±0.3)	1.74	1.24	4.84	1.87
$\Delta_{2,\perp}$	−0.26	0.00	−0.27	−0.27	0.03 (0.1±0.05)	−0.16	−0.17	0.12	0.05
$\Delta_{2,y}$	1.26	1.34	1.59	1.32	1.41 (1.41±0.3)	1.69	1.52	1.67	2.01
E_{Total}	−355.48	−355.89	−367.17	−358.93	−359.36	−370.09	−327.85	−328.13	−337.57
$E_{Rel.}$	0.41	0.0	−11.28	0.43	0.0	−10.73	0.28	0.0	−9.44

Table III: Value of intrachain bond angle, Θ, for epitaxical model of V/III-V(110) systems.

Substrate	a_0(Å)	Adatom		
		Sb		Bi[*]
		No Relaxation	Full Relaxation	No Relaxation
GaP	5.45	90°	91°	82°
GaAs	5.65	94°	94°	86°
InSb	6.48	114°	108°	103°

[*] d_o(Bi-Bi) = 2.92 Å

Figure Captions

Figure 1. Schematic diagram of the surface geometry for the $M_{III}A_{V}$(110)-p(1x1)-Sb systems and definition of the structural parameters. (a) epitaxical structure, (b) "*p*^{3}" structure, (c) commensurate chain structure, and (d) overlapping chain structure.

Figure 2. Schematic diagram of the surface geometry for the $M_{III}A_{V}$(110)-p(1x1)-Sb systems; (a) epitaxical structure, (b) overlapping chain structure, (c) "*p*^{3}" structure, and (d) commensurate chain structure. Shaded areas indicate uncertainty in the position of Sb adatoms as determined by STM (Ref. 10). Adapted from Mårtensson and Feenstra (Ref. 10).

Figure 3. (a) Energy dispersion of surface bound states for GaAs(110)-p(1x1)-Sb commensurate chain structure. Sb- derived surface states are denoted by S_n and indicated by a dashed line. Substrate derived states are denoted by A_n (anion derived) and C_n (cation derived) and are indicated by a bold dot-dashed line.

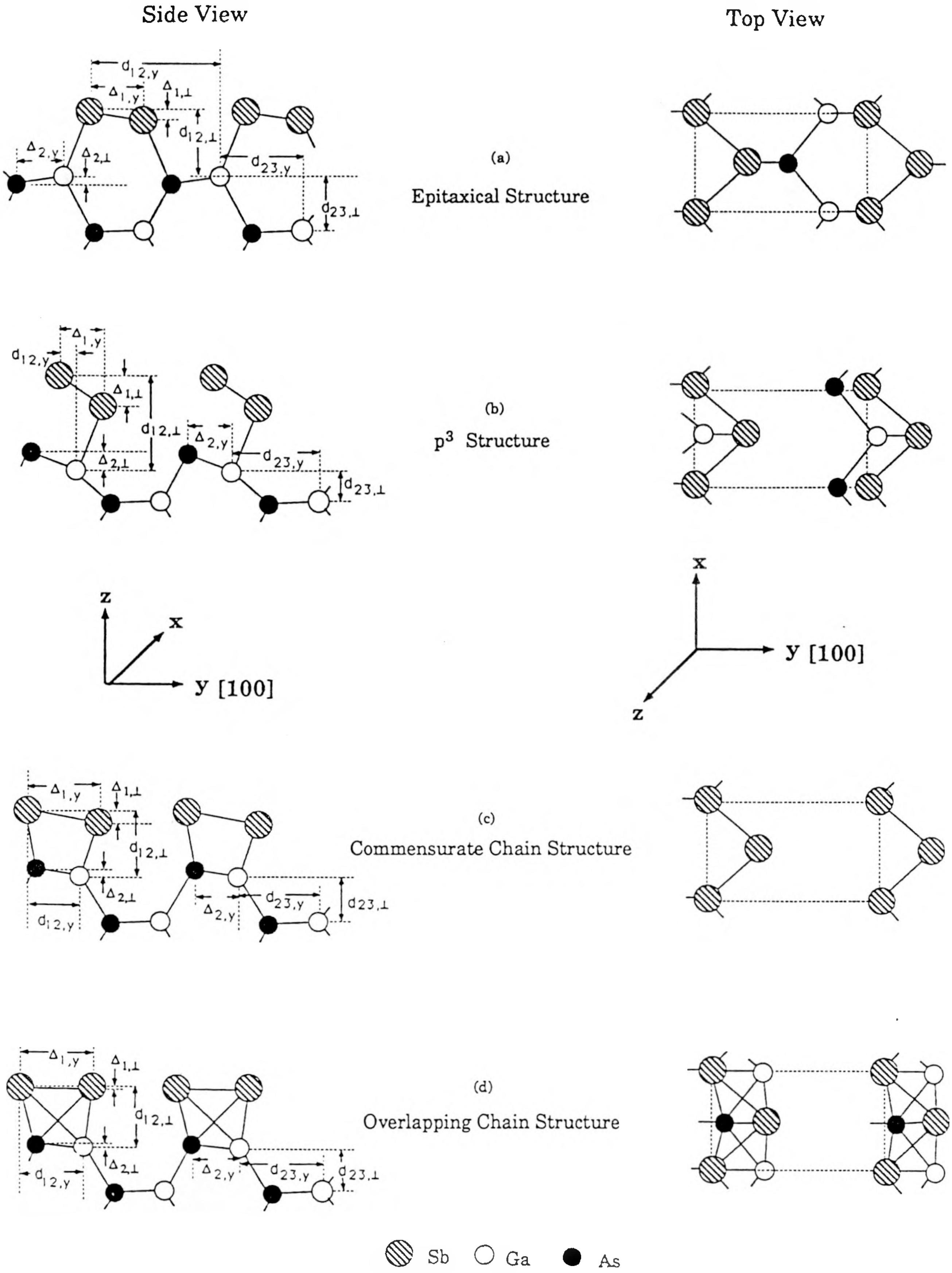
Figure 4. Energy dispersion of surface bound states for GaAs(110)-p(1x1)-Sb epitaxical structure (adapted from Mailhiot *et al.*, Ref. 6). Sb- derived surface states are denoted by S_n and indicated by a dashed line. Substrate derived states are denoted by A_n (anion derived) and C_n (cation derived) and are indicated by a bold dot-dashed line.

Figure 5. Schematic indication of the orbitals associated with the surface states S_5-S_8 at X for the epitaxical structure. (Adapted from Mailhiot *et al.*, Ref. 6.)

Figure 6. Schematic indication of the orbitals associated with the surface states S^{III} - S^{VI} near X for the CC structure.

Figure 7. Comparison of surface state dispersions for GaAs(110)-p(1x1)-Sb computed for the commensurate chain structure (solid lines) and the experimental ARPES values of Ref. 7. The experimental values were shifted by 1eV to put the highest occupied surface state at 0 eV at Γ. Shaded area indicates the projection of the bulk bands.

Figure 8. Comparison of surface state dispersions for GaAs(110)-p(1x1)-Sb computed for the commensurate chain structure (solid lines) and the fit to experimental ARPES values of Ref. 8. Shaded area indicates the projection of the bulk bands.



(a) Epitaxical Structure

(b) p^3 Structure

(c) Commensurate Chain Structure

(d) Overlapping Chain Structure

FIG. 1

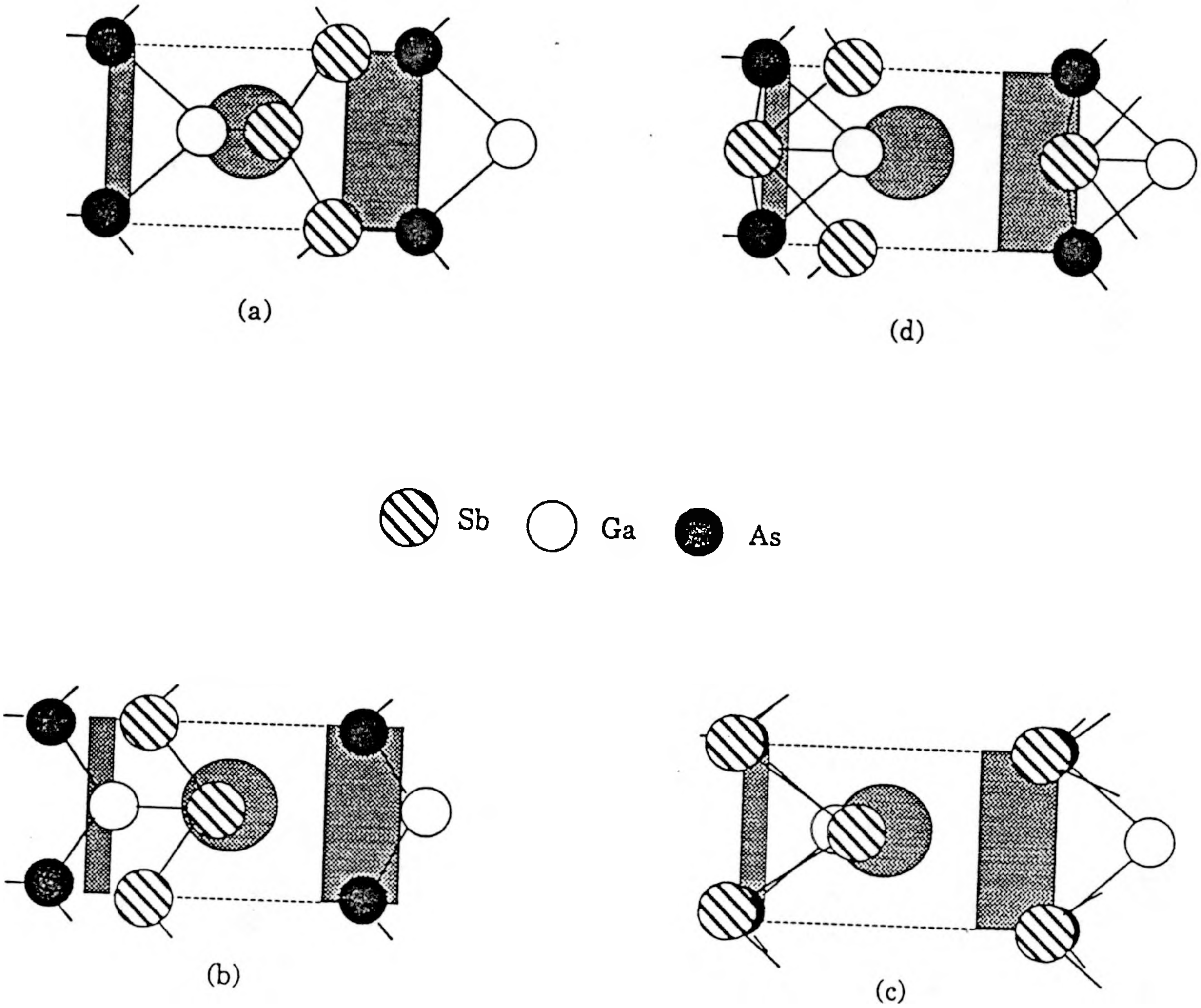
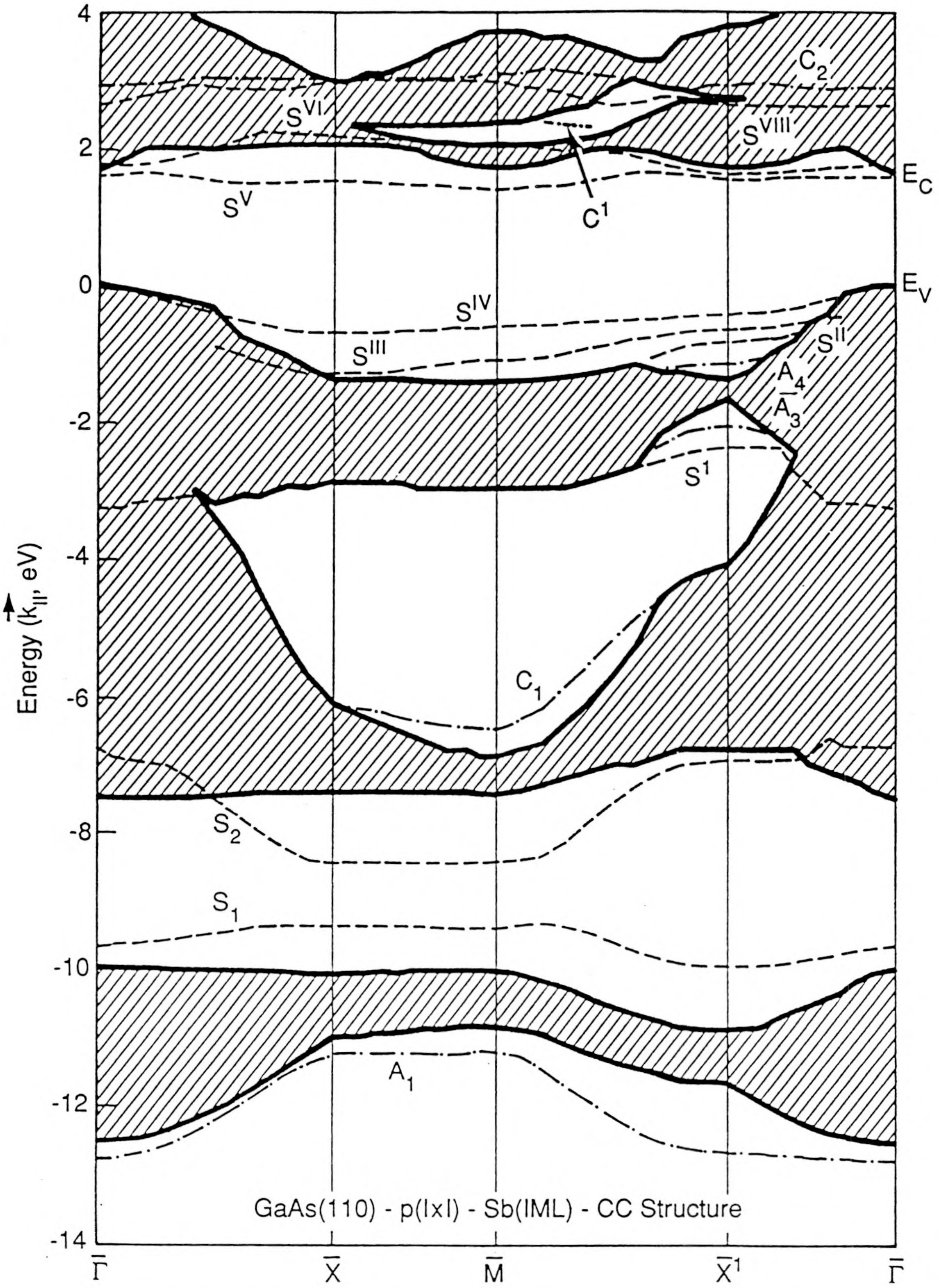
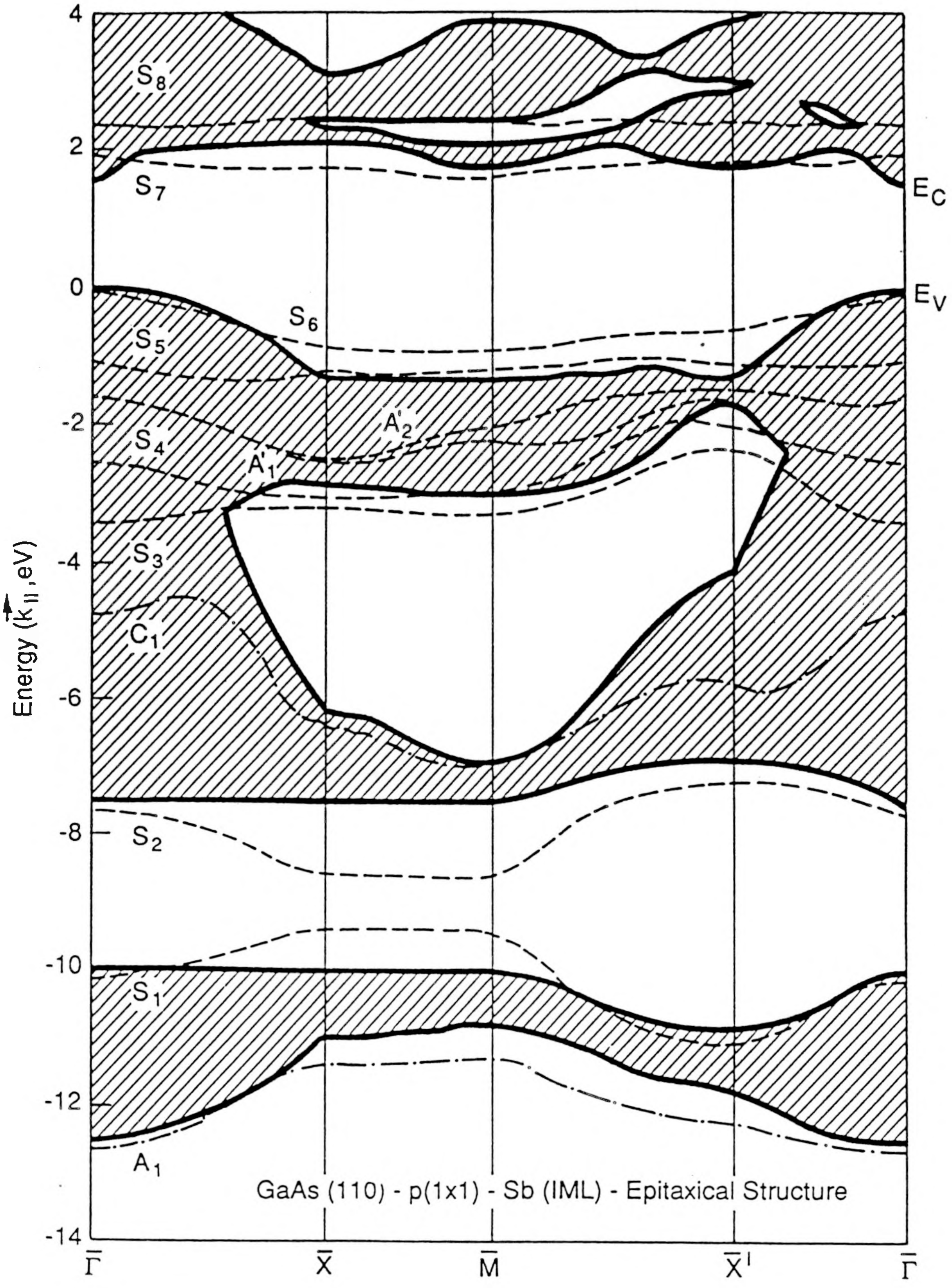


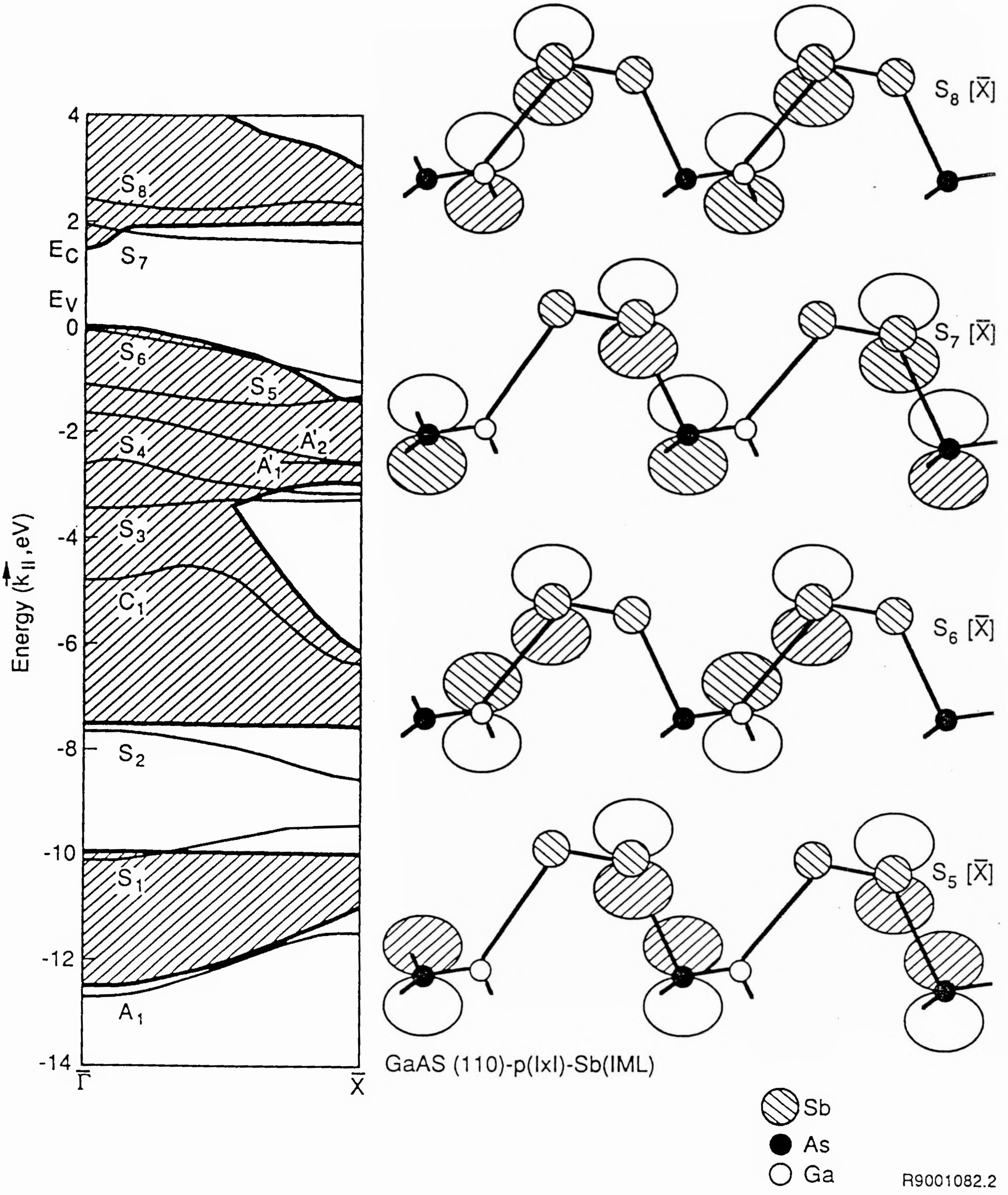
FIG 2



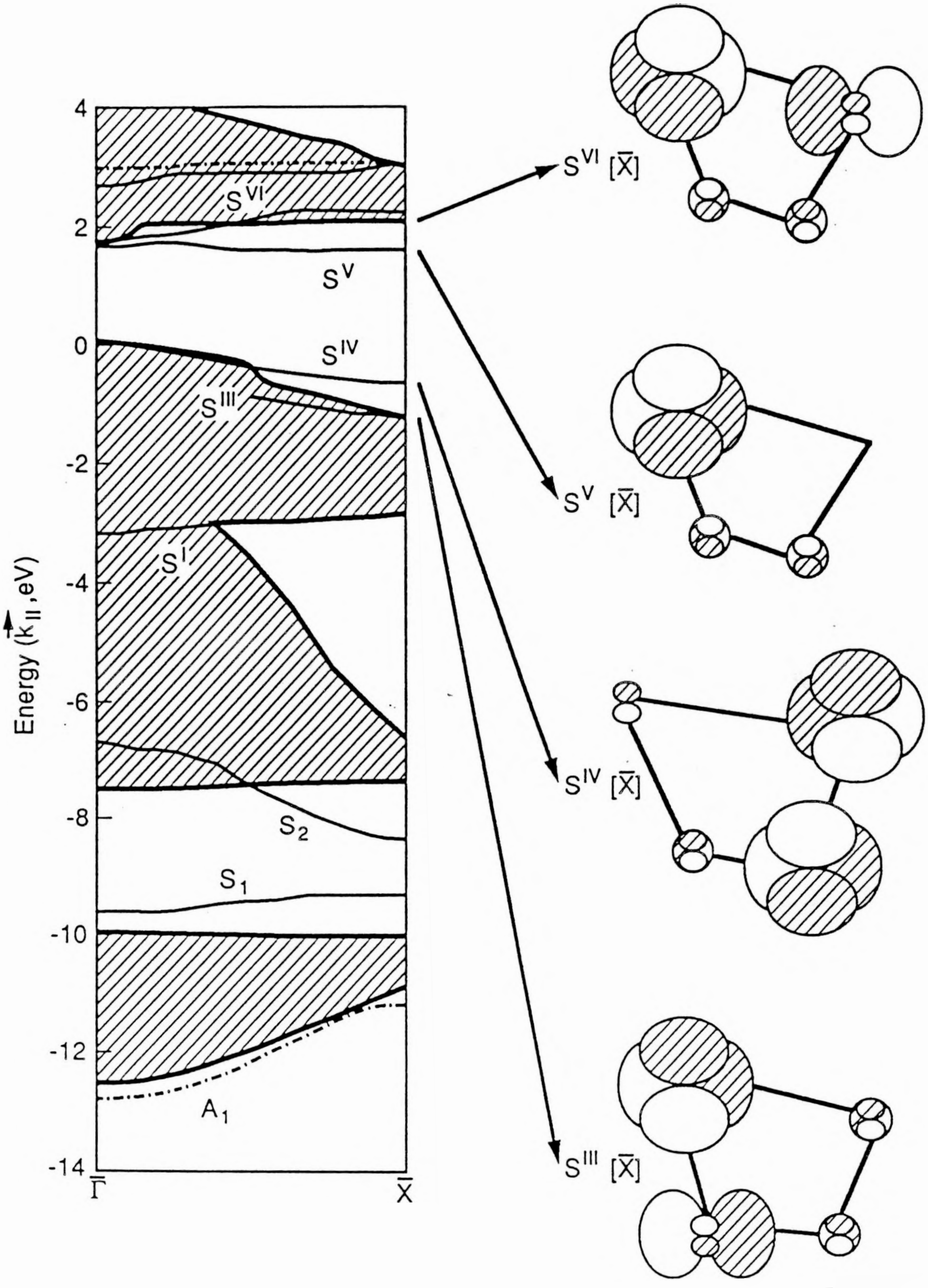
4
2
0
-2
-4
-6
-8
-10
-12
-14
Energy (k_II, eV)
C2
S^VI
S^VIII
E_C
S^V
C^1
E_V
S^IV
S^III
S^II
A4
A3
S^1
C1
S2
S1
A1
GaAs(110) - p(IxI) - Sb(IML) - CC Structure
Γ̄
X̄
M̄
X̄^1
Γ̄



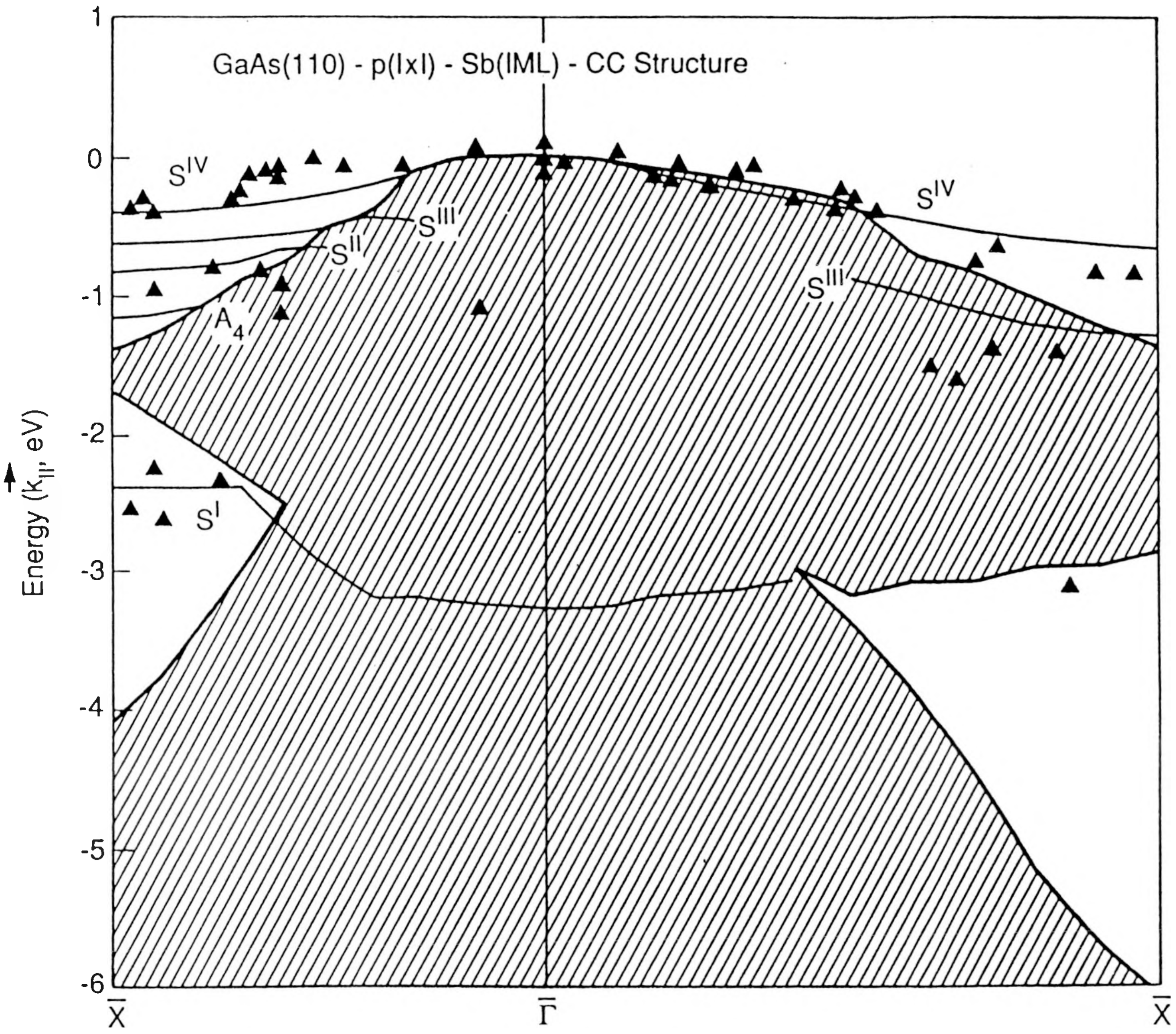
4
2
0
-2
-4
-6
-8
-10
-12
-14
Energy ($\vec{k}_{\parallel}$, eV)
S_8
S_7
S_6
S_5
S_4
S_3
C_1
S_2
S_1
A_1
A'_1
A'_2
E_C
E_V
$\bar{\Gamma}$
$\bar{X}$
$\bar{M}$
$\bar{X}'$
$\bar{\Gamma}$
GaAs (110) - p(1x1) - Sb (IML) - Epitaxical Structure

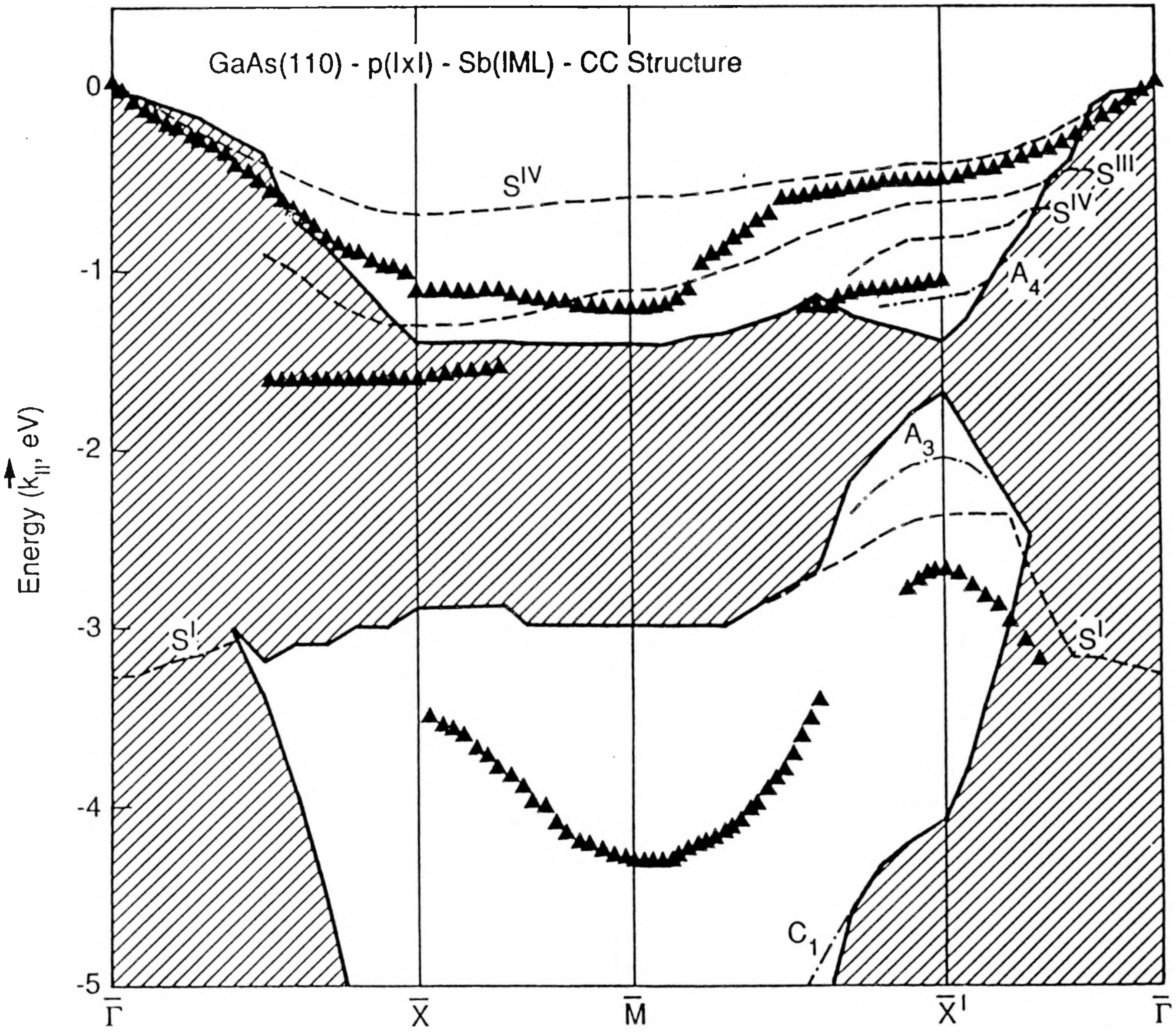

Energy ($k_{\parallel}$,eV)
4
2
0
-2
-4
-6
-8
-10
-12
-14
E_C
E_V
S_8
S_7
S_6
S_5
S_4
S_3
C_1
S_2
S_1
A_1
A'_1
A'_2
$\bar{\Gamma}$
$\bar{X}$
S_8 [$\bar{X}$]
S_7 [$\bar{X}$]
S_6 [$\bar{X}$]
S_5 [$\bar{X}$]
GaAS (110)-p(lxl)-Sb(lML)
Sb
As
Ga

R9001082.2


Energy (k_{II}, eV)
4
2
0
-2
-4
-6
-8
-10
-12
-14
$\bar{\Gamma}$
$\bar{X}$
S^{VI}
S^{V}
S^{IV}
S^{III}
S^{I}
S_2
S_1
A_1
S^{VI} [$\bar{X}$]
S^{V} [$\bar{X}$]
S^{IV} [$\bar{X}$]
S^{III} [$\bar{X}$]

R9001082.1


GaAs(110) - p(1x1) - Sb(1ML) - CC Structure
Energy (k$_{||}$, eV)
1
0
-1
-2
-3
-4
-5
-6
S^{IV}
S^{III}
S^{II}
A_4
S^{I}
S^{IV}
S^{III}
$\bar{X}$
$\bar{\Gamma}$
$\bar{X}$


GaAs(110) - p(1x1) - Sb(1ML) - CC Structure
Energy ($\vec{k}_{||}$, eV)
0
-1
-2
-3
-4
-5
$\bar{\Gamma}$
$\bar{X}$
$\bar{M}$
$\bar{X}'$
$\bar{\Gamma}$
S^{IV}
S^{III}
S^{IV}
A_4
A_3
S^{I}
S^{I}
C_1