

Electronic properties in heterostructures

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Using the interface response, the effect of internal surface of Single Quantum Well (SQW) and of Superlattice (SL) (i.e. Substrate / Single Quantum Well and of Substrate / Superlattice interfaces) are studied in term of changing the heterostructures parameters and keeping constant the parameters of substrate. Surface and interface considered as well as planar defects are associated with the states which are localised in minigaps (MG). Electronic properties are touched in this way and their investigation is made by band structures and variational density of states (DOS).

I. INTRODUCTION

The electronic properties of heterostructures investigated in recent year¹⁻⁷ are related as generally known to the bulk properties. In particular their electronic structures are characterised by energy bands separated by minigaps which result from the interaction between the states of constituted wells. The electronic structures of these materials have been studied by using the envelope function approach^{2,4}, the transfer matrix formalism^{5,8}, the tight banding and the pseudo-potential approximation^{6,9,10}. Through their surface and interfaces, the heterostructures can interact with the media surrounding them, this leads to take account of them experimentally and theoretically.

The aim of this paper, is to provide the different aspects related the SQW and SL studies as corresponding to electronic surface and interface properties. After this great deal of work concentrated on bulk properties of semiconductors SL, also the surface and interface effects became a subject of interest of theoretical and experimental study worked in this field.

Starting from all these facts, among the other objectives of this paper is to investigate in a way similar to that used for the phonons problem, the properties of surface (or interface) states in an unprecedented line. In fact, it does matter that the first systematic study of the surface states behaviour when varying the location of the terminating place with the period of SL. The Kronig-Penney type model is adopted, since it has already been recognised that such potential taken (well-barrier) can serve as a justified approach for treating the electronic properties of the SL. The analogy between the transverse mode in elastic phonons and the Kronig-Penney potential with the modulated effective mass allow us to make a transposition from one case to another easily.

The same process is followed in order to investigate the existence and the behaviour of localised and resonant modes of the optical waves, associated with the substrate.

The most common system which have been experimentally investigated is GaAs- $\text{Ga}_{1-x}\text{Al}_x\text{As}$ because of its importance in many application in realisation of devices. Its characteristics constitute a field which attracts researchers in way to form a subject of interest to both theorists and experimentalists. In particular the observation of surface Tamm-like¹¹ as a single localised states lying inside the energy gap, which has been reported by Ohno et al^{12,13}. The features of this heterostructure geometry is that the location of the surface plane relative to the bulk can vary, as indicated below, within the width of the layer. This in turn, causes the surface states to move across the entire

MG going from one energy of Mini-Band (MB) to the other and thus allowing the investigation of the surface states properties in a new way.

This paper will be organised as follows: we present at first the study of SQW which is constituted of two parts ; the formalism and some results with their discussion, and at second we give the statement of problem for SL (because the formalism is very similar to the phonon problem), which will be followed also by some results and their discussion. For the SQW case, we find ourselves obliged to give some elements of its formalism because this system has not been studied before for the phonons.

II. SINGLE- QUANTUM WELL

In such systems, the medium surrounding the well must form a « barrier » which prevents well wave function from extending much outside it. In particular, it has been shown recently⁷⁻¹¹ that the ideal quantum well (QW) potential in which one considers a QW system to be terminated on either side by barriers of finite height, but infinite in extent, needs to be modified to take into account the finite size effect of the barriers surrounding the QW.

Recently, many authors have presented works on this subject⁷⁻¹¹, and over all their studies the effect of the substrate (i.e., the buffer layer of large extent), which serve as support for the devices, on electron states in these structures is usually ignored. However, a minor contribution devoted to the substrate effect but only under the form of continuum states above the barrier of the well has been presented¹². Let us mention that Moison et al¹⁴ have performed an extended study by in situ photoluminescence to the effect of a cap layer (barrier of finite extent) on bound states in $\text{GaAs/Ga}_{0.7}\text{Al}_{0.3}\text{As}$ QW's and their interaction with surface states. Also Fafard et al^{15,16} have studied the effect of the high potential at the device surface on the above barrier (continuum) states in a simple GaAs/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ structure; intense above barrier oscillations related to the oscillations in the probabilities of finding carriers in the various region induced by finite cap layers were observed in photoluminescence spectra. Above-barrier optical transitions in $\text{Ga}_{1-x_1}\text{Al}_{x_1}\text{As/GaAs/Ga}_{1-x_2}\text{Al}_{x_2}\text{As}$ compositionally asymmetric SQW have been investigated with piezomodulation spectroscopy by Parks et al¹⁷.

A. Basic calculation

In our case²¹, the heterostructure is composed of slabs of materials i ($i = 1, 2$) with thickness d_i sandwiched between two semi-infinite materials $i = 0$ and $i = 3$. The calculation of $\mathbf{g}(\mathbf{DD})$ is obtained by the knowledge of $\mathbf{g}(\mathbf{MM})$ which is given by inverting the matrix $\mathbf{g}^{-1}(\mathbf{MM})$. If $\mathbf{g}_{si}(\mathbf{MM})$ is the interface Green's function of the slab i ($i = 1, 2$) and of the substrate j ($j = 0, 3$).

The first step before addressing the problem is to know the surface element of the Green function \mathbf{g}_{si} of a slab of medium i and substrate j . These surface elements can be written as follows:

$$\mathbf{g}_{si}^{-1}(\mathbf{M}_i \mathbf{M}_j) = \begin{bmatrix} \mathbf{A}_i & \mathbf{B}_i \\ \mathbf{B}_i & \mathbf{A}_i \end{bmatrix} \quad (1)$$

where

$$\mathbf{A}_i = -\mathbf{F}_i \frac{\mathbf{C}_i}{\mathbf{S}_i}, \quad \mathbf{B}_i = \frac{\mathbf{C}_i}{\mathbf{S}_i}, \quad \mathbf{C}_i = \text{ch} \alpha_i d_i, \quad \mathbf{S}_i = \text{sh} \alpha_i d_i,$$

$$\mathbf{F}_i = \frac{\hbar^2}{2m_i} \alpha_i \quad \text{and} \quad \alpha_i^2 = -\frac{2m_i}{\hbar^2} (E - E_i) \quad \text{with } i = 1, 2 \quad (2)$$

The inverse of the Green function within the total interface space \mathbf{M} is obtained²² and gives the formula of $\mathbf{g}(\mathbf{MM})$.

From the knowledge of these interface matrix elements one can obtain the Green's function between any two points of the whole system (see eq. (1)). Therefore, we only give their expressions for two points belonging both either to the two substrates ($j = 0, 3$) or to the two layers ($i = 1, 2$).

Let us recall first that the bulk Green function of the medium i is given by²²

$$G_i(x_3, x'_3) = -\frac{e^{-\alpha_i |x_3 - x'_3|}}{2F_i} \quad (3)$$

where α_i and F_i are given by eq. (2)

Between any two points of each medium i , the Green's function is written as follows :

i- when the two points are inside the medium $i=0$
($x_3, x'_3 \leq 0$)

$$g(x_3, x'_3) = -\frac{e^{-\alpha_0 |x_3 - x'_3|}}{2F_0} + \left\{ \frac{1}{2F_0} - \frac{1}{W} \left[C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 + \frac{F_3}{F_2} C_1 S_2 + \frac{F_3}{F_1} C_2 S_1 \right] \right\} e^{\alpha_0 (x'_3 + x_3)}, \quad (4)$$

ii- when the two points are inside the medium $i = 1$
($0 \leq x_3, x'_3 \leq d_1$)

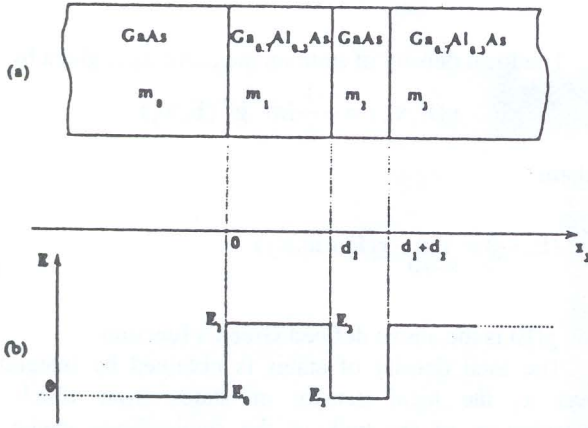


Figure 1. Schematic representation (a) and potential profile (b) of a single quantum well with a well layer GaAs surrounded by two barriers $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ of finite and infinite extent, the whole system is deposited on a GaAs substrate. d_1 and d_2 are respectively, the thickness of the barrier and well layers.

We have examined the below-and above-barrier resonant states in a single GaAs QW of a given thickness d_1 (see figure 1) confined in one side $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ barrier of infinite extension, and on the other side by a $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ barrier of finite extension. The whole system is deposited on GaAs substrate, which represents the buffer layer of infinite extension. Among different mathematical approaches, the Green's function method is quite suitable for studying the spectral properties of these heterostructures. The Green function approach allowed us to determine the transmission and reflection rates as well as the phase times. There are several other times¹⁸⁻²⁰, however the only well-defined and well-established one¹⁹ is the 'dwell time' which is the average time spent in a given region by all incoming particles.

It is well established that DOS is a much better characteristic of resonant states than transmission rate. However, to our knowledge there has been no comparison between the DOS and the reflection and transmission phase times until this date. Furthermore we add that the same resonances appear in the DOS and in the phase times which mean the same behaviour.

The structure of fig. 1 has no similarity in the vibrational properties, this reason have led the development some details of calculation in this text.

$$g(x_3, x'_3) = -\frac{e^{-\alpha_1 |x_3 - x'_3|}}{2F_1} + \frac{1}{S_1^2} \left\{ A \operatorname{sh}(\alpha_1(d_1 - x_3)) \operatorname{sh}(\alpha_1(d_1 - x'_3)) + B \left[\operatorname{sh}(\alpha_1 x_3) \operatorname{sh}(\alpha_1(d_1 - x'_3)) + \operatorname{sh}(\alpha_1(d_1 - x_3)) \operatorname{sh}(\alpha_1 x'_3) \right] + C \left(\operatorname{sh}(\alpha_1 x_3) \operatorname{sh}(\alpha_1 x'_3) \right) \right\}, \quad (5)$$

where

$$A = -(C_1 C_2 + S_1 S_2 F_2 / F_1 + C_1 S_2 F_3 / F_2 + C_2 S_1 F_3 / F_1) / W + 1 / (2F_1), \quad (6)$$

$$B = -\frac{1}{W} \left(C_2 + \frac{F_3}{F_2} S_3 \right) + \frac{e^{-\alpha_1 d_1}}{2F_1}, \quad (7)$$

and

$$C = -\frac{1}{W} \left(C_1 C_2 + \frac{F_0}{F_1} C_2 C_1 + \frac{F_3}{F_2} C_1 S_2 + \frac{F_0 F_3}{F_1 F_2} S_1 S_2 \right) + \frac{1}{2F_1}, \quad (8)$$

iii- when the two points are inside the medium $i = 2$
($d_1 \leq x_3, x'_3 \leq d_1 + d_2$)

$$g(x_3, x'_3) = -\frac{e^{-\alpha_2 |x_3 - x'_3|}}{2F_2} + \frac{1}{S_2^2} \left\{ D \operatorname{sh}(\alpha_2(d - x_3)) \operatorname{sh}(\alpha_2(d - x'_3)) + E \left[\operatorname{sh}(\alpha_2(d - x_3)) \operatorname{sh}(\alpha_1(x'_3 - d_1)) + \operatorname{sh}(\alpha_2(x_3 - d_1)) \operatorname{sh}(\alpha_2(d - x'_3)) \right] + F \operatorname{sh}(\alpha_2(x_3 - d_1)) \operatorname{sh}(\alpha_1(x'_3 - d_1)) \right\},$$

where

$$D = -\frac{1}{W} \left(C_1 C_2 + \frac{F_0}{F_1} C_2 S_1 + \frac{F_3}{F_2} C_1 S_2 + \frac{F_0 F_3}{F_1 F_2} S_1 S_2 \right) + \frac{1}{2F_2}, \quad (10)$$

$$E = -\frac{1}{W} \left(C_1 + \frac{F_0}{F_1} S_1 \right) + \frac{e^{-\alpha_2 d_2}}{2F_2},$$

$$F = \frac{-1}{W} \left(C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 + \frac{F_0}{F_1} C_2 S_1 + \frac{F_0}{F_2} C_1 S_2 \right) + \frac{1}{2F_2}, \quad (11)$$

iv- when the two points are inside the medium $i=3$
($x_3, x'_3 \geq d_1 + d_2$)

$$g(x_3, x'_3) = -\frac{e^{-\alpha_3 |x_3 - x'_3|}}{2F_3} + \left\{ \frac{1}{2F_3} - \frac{1}{W} \left[C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 + \frac{F_0}{F_2} C_1 S_2 + \frac{F_0}{F_1} C_2 S_1 \right] \right\} e^{-\alpha_3 (x'_3 + x_3 - 2d)}, \quad (12)$$

The local density of state on the plane x_3 is given by

$$n(E, x_3) = -\frac{1}{\pi} \operatorname{Im} g^+(E, x_3) \quad (13)$$

where

$$g^+(E, x_3) = \lim_{\epsilon \rightarrow 0} g(E + i\epsilon, x_3) \quad (14)$$

and $g(E)$ is the above defined Green's function

The total density of states is obtained by integrating over x_3 the local density of states from which the contribution of the bulk of the semi-infinite media are subtracted. This variation $\Delta n(E)$ can be written as

$$\Delta n(E) = \Delta n_0(E) + n_1(E) + n_2(E) + \Delta n_3(E) \quad (15)$$

where $\Delta n_0(E)$ and $\Delta n_3(E)$ are the variation of the DOS in mediums $i = 0$ and $i = 3$ respectively, $n_1(E)$ and $n_2(E)$ the DOS in the layers 1 and 2 respectively. The explicit expression of these four quantities were found to be

$$\Delta n_0(E) = -\frac{1}{\pi} \operatorname{Im} \left\{ \frac{1}{2\alpha_0} \left[\frac{1}{2F_0} - \frac{1}{W} \left(C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 + \frac{F_3}{F_2} C_1 S_2 + \frac{F_3}{F_1} C_2 S_1 \right) \right] \right\} \quad (16)$$

$$n_1(E) = -\frac{1}{\pi} \operatorname{Im} \left\{ -\frac{d_1}{2F_1} + \frac{1}{2\alpha_1 S_1^2} \left[(A + C)(C_1 S_1 - \alpha_1 d_1) + 2B(\alpha_1 d_1 C_1 - S_1) \right] \right\} \quad (9)$$

$$n_2(E) = -\frac{1}{\pi} \operatorname{Im} \left\{ -\frac{d_2}{2F_2} + \frac{1}{2\alpha_2 S_2^2} \left[(D + F)(C_2 S_2 - \alpha_2 d_2) + 2E(\alpha_2 d_2 C_2 - S_2) \right] \right\} \quad (16)$$

$$\Delta n_3(E) = -\frac{1}{\pi} \operatorname{Im} \left\{ \frac{1}{2\alpha_3} \left[\frac{1}{2F_3} - \frac{1}{W} \left(C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 + \frac{F_0}{F_2} C_1 S_2 + \frac{F_0}{F_1} C_2 S_1 \right) \right] \right\} \quad (18)$$

For the reflection and transmission effect in the substrates $i = 0$ and $i = 3$, their coefficients are expressed, respectively, as

$$C_R e^{\alpha_0 x_3} \text{ and } C_T e^{-\alpha_3(x_3-d)} \quad (19)$$

where

$$C_R = \frac{2F_0}{W} (C_1 C_2 + \frac{F_2}{F_1} S_1 S_2 + \frac{F_3}{F_2} C_1 S_2 + \frac{F_3}{F_1} C_2 S_1) - 1 \quad (20)$$

and

$$C_T = -\frac{2F_0}{W} \quad (21)$$

C_R and C_T are the reflection and transmission amplitudes respectively. The reflection rate R and transmission rate T are defined by

$$R = |C_R|^2 \text{ and } T = |C_T|^2 \quad (22)$$

The reflection and transmission phase times are given respectively, in the stationary phase approximation, by^{13,14}

$$\tau_R = \hbar d\theta_R / dE \text{ and } \tau_T = \hbar d\theta_T / dE \quad (23)$$

where $\hbar = 2\pi \hbar$ is the Plank's constant and θ_R and θ_T are the phases of the reflected and transmitted amplitudes of electrons scattered off the two embedded layers.

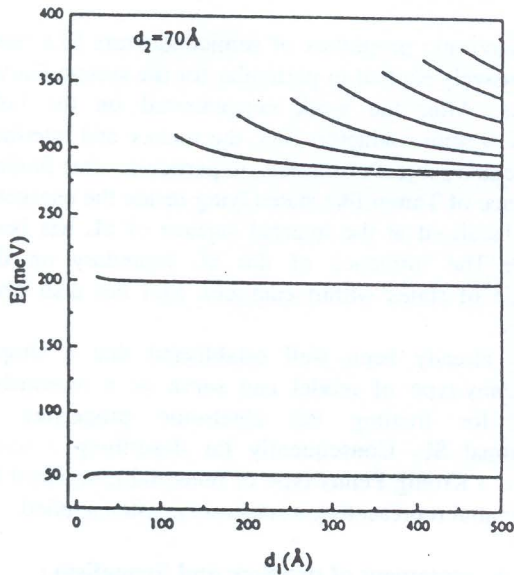


Figure 2. Variation of the energy levels of resonant states, for $d_2 = 70 \text{ \AA}$, as a function of d_1 where d_1 and d_2 are respectively the thickness of the $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ barrier and GaAs well. The horizontal full line indicates the position of the barrier height E_3 .

B. Results and discussion

The numerical calculations has been done on the basis of experimental data of Ohno et al^{12,13}, the effective mass of the electron inside the well and barrier are $0.067m_0$ and $0.0919m_0$, respectively, where m_0 is the mass of free electron. The barrier height is 283.2 meV .

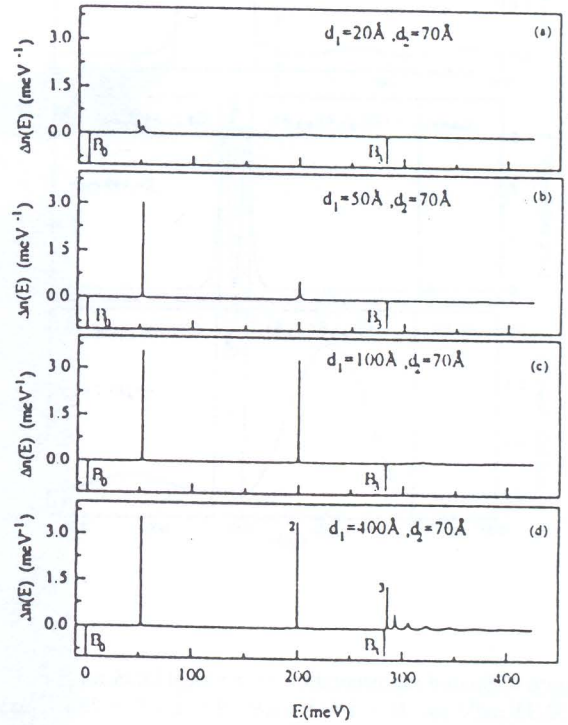


Figure 3. Variation of the DOS as explained in eq. (21) for $d_1 = 20 \text{ \AA}$, 50 \AA , 100 \AA and 400 \AA in Fig.2, while d_2 is kept constant ($d_2 = 70 \text{ \AA}$). The antiresonances appearing at $E_0 = 0 \text{ meV}$ and E_3 correspond to delta peaks of weight $-1/4$, resulting from the subtraction of the bulk bands of GaAs substrate and $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ barrier of infinite extent.

The figure 2 gives an illustration of the dispersion curves of energy levels when the thickness of the GaAs well is such that $d_2 = 70 \text{ \AA}$ and the thickness d_1 of the barrier layer is taken variable. All the branches in Fig. 2 represent resonant states induced by the $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}/\text{GaAs}$ bilayer in the continuum of the bulk bands of GaAs substrate and $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$ barrier of infinite extent. These resonant states are obtained from the maxima of the DOS, shown in Fig.3. The full horizontal line in Fig. 2 represents the position of the energy level $E_3 = E_1$. The two curves situated below E_3 represent resonant waves of the well, and appear as well-defined peaks in the DOS of Fig. 3, even though they are in resonance with the bulk states of the GaAs substrate, the corresponding energies of these resonances present a very small variation with d_1 . The resonances are enlarged by adding a small imaginary part ϵ to the energy E and the intensity of the resonances below E_3 increases by increasing the thickness d_1 of $\text{Ga}_{0.7}\text{Al}_{0.3}\text{As}$.

barrier. For large values of d_1 , the resonances appear as delta functions of weights 1 as the interaction between the GaAs well and the GaAs substrate becomes very weak.

delay motion of the electrons to appear on the right and left sides of the GaAs-Ga_{0.7}Al_{0.3}As double layers.

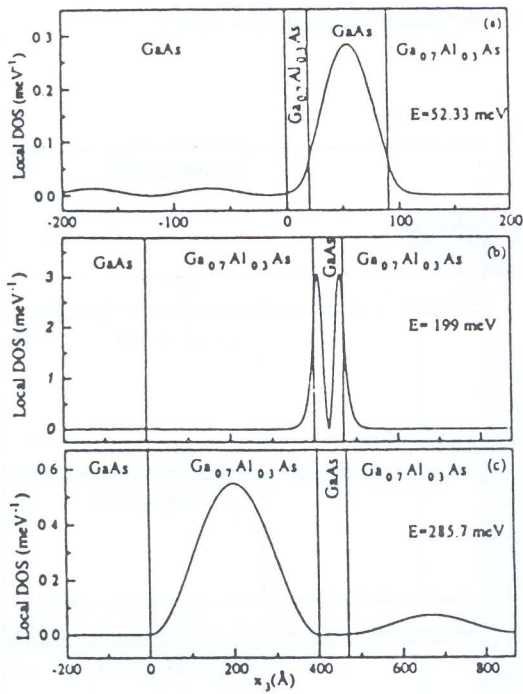


Figure 4. Spatial representation of the local DOS for $E = 52.33$ meV (a), $E = 199.8$ meV (b) and $E = 285.7$ meV (c). These resonances are respectively labelled 1, 2 and 3 in Figs. 3(a) and 3(b). The space positions of the different interfaces are marked by vertical lines.

It is well established that DOS is much better characteristic of resonant states than transmission rate. However, to our knowledge, there has been no comparison between the DOS and the reflection and transmission phase times up to date. In Figs. 4 and 5, we give a comparison of all the quantities cited above for two different values of the barrier layer : $d_1=20$ Å (Fig. 4) and $d_1=400$ Å (Fig. 5) , while the well thickness is kept constant ($d_2=70$ Å).

In figure 4(a), two resonances appear below E_3 in the DOS and give the same behaviour as the reflection phase time. Indeed, the intensity of the peaks in the DOS gives the weight of the resonances, while the intensity of the peaks in the reflection phase time gives the time needed for electron to complete the reflection process.

For the energy range $E > E_3$, the resonant states depend strongly on the Ga_{0.7}Al_{0.3}As barrier thickness and their intensity decreases with increasing the energy. On the other hand, the transmission rate (Fig.5(b)) shows sharp peaks with energy positions corresponding to the resonances in Fig. 5(a), however at high energies, the peaks in the DOS vanish, while the peaks in the transmission rate oscillate before they reach unity. An analysis of the phase times of the transmitted and reflected electrons from the GaAs / Ga_{0.7}Al_{0.3}As bilayer, shows that the transmitted and reflected phase times (Figs. 5(c),(d)) have the same behaviour as the DOS for energies lying above E_3 . Reflected and transmitted phase times are interpreted as the

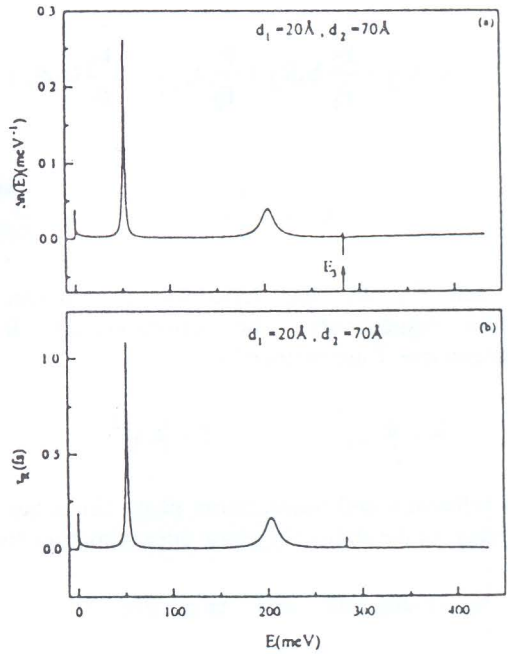


Figure 5. Energy dependence of the DOS (a) and reflected phase time τ_R (b) for $d_1=20$ Å and $d_2=70$ Å. The arrows indicate the positions of E_0 and E_3 energy levels.

III. SEMI-INFINITE SUPERLATTICE²³⁻²⁸:

The electronic properties of semiconductors SLs have been extensively studied in particular for the system GaAs-Ga_{1-x}Al_xAs. After the work concentrated on the bulk properties of semiconductors SLs, the surface and interface effects became subject of interest, in particular after finding the existence of Tamm-like states lying inside the energetic MG and localised at the internal surface of SL has been examined. The influence of the SL boundary on the distribution of states within energetic MG has also been studied.

It has already been well established that a simple Kronig-Penny-type of model can serve as a reasonable approach for treating the electronic properties of compositional SL. Consequently for describing a semi-infinite SL a Kronig-Penny-type of potential terminated by a step potential representing a substrate is often applied.

A. statement of problem and formalism :

The effect of an internal surface is taken into account by changing substrate parameters like the substrate parameters potential V_s or the substrate effective-mass m_s , while SL parameters are kept constant. For an investigated GaAs-Ga_{1-x}Al_xAs SL being in contact with Ga_{1-y}Al_yAs as substrate, this situation corresponds to a fixed x and varying y ($V_s = V_s(y)$, $m_s = m_s(y)$).

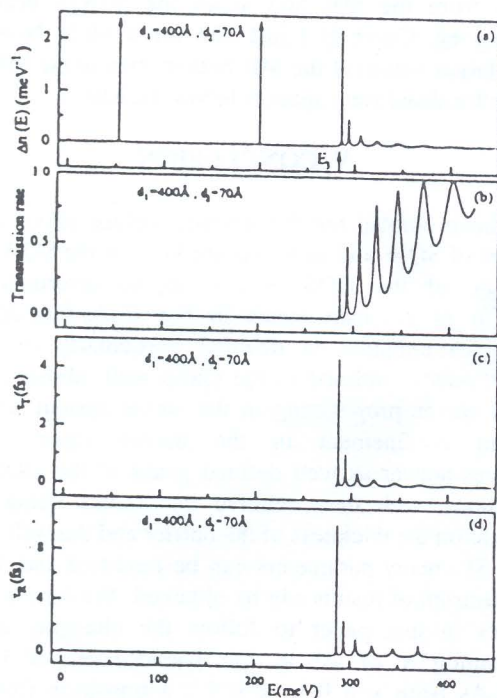


Figure 6. Energy dependence of the DOS (a), transmission rate (b), reflected phase times τ_R (c) and transmitted phase times τ_T (d) for $d_1=400 \text{ Å}$ and $d_2=70 \text{ Å}$.

It is interesting also to examine the opposite case, i.e., to keep substrate parameters unchanged ($y=ctse$) and to modify SL bulk parameters. The concentration x of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ barrier domain is variable leading to a variation of barrier potential $V_b(x) = V_b$ and the corresponding effective-masse $m_b = m_b(x)$.

This enables us to turn from the case of strongly coupled SL for $x \ll 1$ to the case of the weakly coupled SL for $x=1$ the interface response theory is utilised.

Within this approach the variational DOS is easily obtained as the total DOS of the whole substrate/SL system from which the DOS of a corresponding infinite SL and an infinite substrate integrated over the space occupied by the semi-infinite SL and the semi-infinite substrate respectively, are subtracted. The details of this calculations are reported in the paper of phonon of this volume and prevision section of simple quantum well where the transposition of vibrational properties to the electronic properties is described.

B. Results and discussions

For numerical results the system chosen is constituted of $\text{GaAs-Ga}_{1-x}\text{Al}_x\text{As}$ SL being in contact with $\text{Ga}_{0.4}\text{Al}_{0.6}\text{As}$ substrate. The data for which the calculations are performed are the same as those used by Ohno et al.^{12,13}, $m_s=0.1166$, $V_s = 556.4 \text{ meV}$, $a = b = 40 \text{ Å}$, $m_a = 0.067$, $m_b = 0.067 + 0.083x$, $V_b = 944x \text{ meV}$ and $x \in [0,1]$.

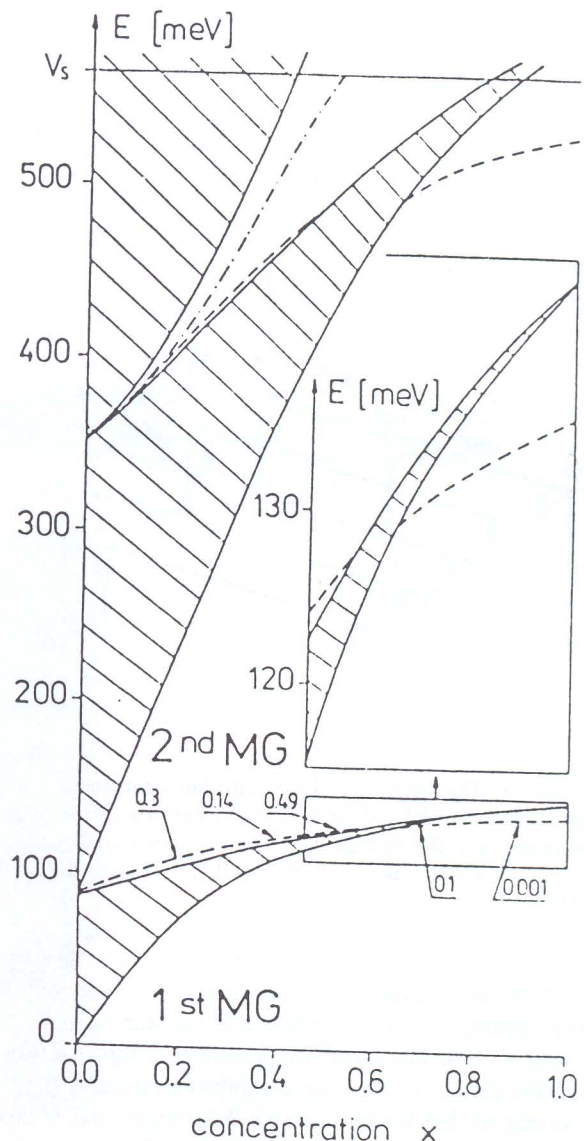


Figure 7. The electronic structure of a $\text{GaAs/ Ga}_{1-x}\text{Al}_x\text{As}$ SL being in contact with a $\text{Ga}_{0.4}\text{Al}_{0.6}\text{As}$ substrate for a varying concentration x of Al in the SL barriers. Hatched areas correspond to MBs while the dashed and dashed-dotted lines describe the position of surface levels inside MGs for the well- and barrier-termination of the SL, respectively. Underlined numbers give the values of localisation factor R .

The figure 7 shows the bulk bands (hatched areas) and the surface states (dashed and dashed-dotted lines) for either a GaAs -well-layer or a $\text{Ga}_{1-x}\text{Al}_x\text{As}$ barrier directly in contact with the substrate when the surface layer of SL is made of GaAs (the called well-termination-fig.6). The states localised at the intensity surface appear for $x \leq 0.5$ in the second as well as the 3rd MG (see the dashed in fig. 7), i.e., above the 1st and the 2nd MB respectively; since $V_b(x) < V_s$. For the values of x around $x = y = 0.6$, these two cross the corresponding MBs leading to an absence of term localised states because of $V_b(x) \approx V_s$. For still increasing x ($x \geq 0.65$) surface states appear again, however, they are present in the 1st and the 2nd MG. The crossing of surface states with the corresponding bulk bands exhibits similar features.

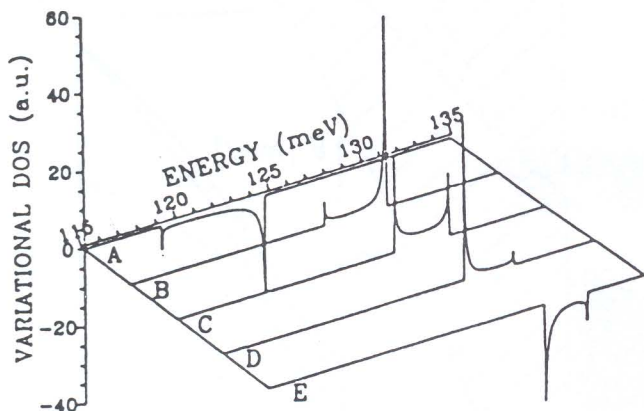


Figure 8. The variational DOS calculated for energy range comprising the 1st MB and for different values of x corresponding to the crossing of the surface state with this MB (see the inset in Fig. 2) — A : $x = 0.5$, B : $x = 0.58$, C : $x = 0.6$, D : $x = 0.62$, and E : $x = 0.65$.

In order to follow the behaviour of surface states when cross MB, the variational DOS has been computed for energy corresponding to the first MB and for some values of x near $x=0.6$. The result are presented in figure 8. For $x = 0.5$, the variation DSO curve exhibits a typical $(\Delta E)^{-1/2}$ like divergent behaviour near the MB edges and it takes negative values (eg. Curve A). For $x = 0.58$ the surface states already merges into the MB and this modifies drastically the VDOS distribution which becomes positive and broader at the MB top (eg. Curve B). For still increasing, the movement of the VDOS masses center to

the bottom of the MB is appearing (eg. Curve C and D), while the area under the corresponding VDOS curves remains almost constant. For $x = 0.65$ the surface states emerges from the MB and again the VDOS becomes negative (eg. Curve E) just like for $x = 0.5$. Now, it reaches larger values at the MB bottom than at the MB top since the localised state appears below the MB.

V. CONCLUSION

We have pointed out the internal surface effect in the two cases of SQW and semi-infinite SL. For the SQW, the expression of the DOS enables us to determine the dispersion of resonant states in the GaAs-Ga_{0.7}Al_{0.3}As bilayer. An attention is devoted particularly to sharp resonant waves confined in the GaAs well, above-barrier resonant waves propagating in the whole system with an important confinement in the barrier layer. These resonances appear as well defined peaks of the DOS and phase times, with their relative importance being very dependent on the thickness of the barrier and the well layer. For the SL, many parameters can be modified and a very large spectrum of results can be obtained. We have limited ourselves in this paper to follow the changing of the concentration x of Al in the barrier-layer of GaAs-Ga_{1-y}Al_yAs from $x = 0$ to $x = 1$, a transition from the strongly coupled SL to the weakly coupled one is obtained. The states localised at the interface move from above to beneath the corresponding MB so that the crossing of surface states with bulk bands occur. When the localised surface states merges into MB, the distribution of extended states inside the bulk band is significantly modified.

Between the SQW and the semi-infinite SLs, many other intermediary heterostructures exist, we can hold one particular type of structure which is the finite SL sandwiched between two substrates (or buffer layers) which can reveal very important results. More sophisticated calculations have been done and the found results will be published in close future.

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