Vibrational Properties in heterostructures

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This is a comprehensive path about theoretical approaches to the vibrational properties in periodic and multilayered structures. The phonons modes taking a large part of our work are detailed beyond the limit offered by the area targeted by this sort of paper. In fact, in many cases of this type of materials, metallic, semiconductor or insulator, these modes are investigated. Although, the electronic properties are devoted, generally, to the semiconductor ones as well as the optical properties will be derived in the second paper of this volume. Another topic can be touched which concerns the coupling effect between phonons and electrons or photons and electrons giving rise to interesting results; but it is not addressed here. Throughout this paper, we bring forth the theoretical model currently used by us, and the results obtained in consequence. This model is called the response function based on the Green function and its properties are stressed as well as the results obtained.

I. INTRODUCTION

The heterostructures and superlattices have emerged because of the need to produce new systems showing new properties in order to perform electronic and optoelectronic applications. At least, two ideas have led to the creation of the type of structures provided by such systems. The first one consists of searching for new properties by systems growing out of material of different nature which could be metallic, semiconductor or insulator layers. It can be viewed as well as a simple juxtaposition of layers showing differences at the level of the physical properties through its response to the external excitations. The second idea, involves the scheme of the lattice periodicity as a factor to which band structures are very sensitive. In other words, this second approach is imperative because of these implications of symmetry and periodicity considerations in the determination of the structures of every crystalline system, where they exist. One of these implications is the introduction of new periodic conditions related to growth.

The aim of this paper, therefore, is to provide the vibrational aspects related to the heterostructures studies which have been considered by us during the last period. The general studies of SL have been the object of a great deal of experimental and theoretical study throughout the last decade as reported in several journals[1-10]. An example of these would be the SL actual extended domain where the states are propagating in the whole structure associated with the form bulk bands separated by small gaps. Until then, all interests have been devoted to the bulk properties on the one hand; while only few efforts have been made for the surface properties on the other.

The theoretical and experimental aspects of vibrational properties[11-28] on the heterostructures as well as the homogenous medium are investigated generally by two models[29-36]. Each one of these models is related to the nature of the scale and of the wave length considered. At the atomic scale (few angstroms), the model which is currently provided is the Montroll-Pott model and which consists of regarding the interaction between the atoms and their nearest neighbours parametered by the constant forces. When the wave length considered is very long compared to the interatomic distances, one can adopt the continuum scale and then the elastic limit remains the best way to treat these media.

These two approaches can be overlooked when the phonons are regarded as well as the particles or the quasi-particles which come under the form of quantized fields. This leads us to change the guide for our calculations and to do with the method involving hypothesis of bosonic system. We will be dealing afterward with a system where a new treatment rises. It is the Hamiltonian function, which may be complicated furthermore by using second quantization process.

Our contribution to the debates of the issue brought forth above, will consist of devoting the greatest part of the phonons propagation which are investigated as assimilating the heterostructures layers as an elastic continuum medium. Different kinds of modes can be encountered in heterostructures system. The bulk, localised, and resonant modes which may be propagated, attenuated, or confined in layers, or mainly localised at boundaries between the constitutive layers. Through all these properties of behavioural modes existing, one can succeed to emphasise each of them and classify them by means of the dispersion curves (projected or complex) and by the local or total density of states analysis (DOSA). The localised modes are intimately brought by the semi-infinite media in general and by the semi-infinite SL in particular. In accordance with the existence of the surface (or interface), they occur if and only if they are associated with inhomogeneity or defect which may be planar or with another geometrical form. The resonant modes are induced by the capping layer (system 1D), or only by surface (system 2D); or by semi-infinite substrate in term of interface between SL and adsorbed system.

The theoretical method mentioned above, and added to the transfer matrix model enable us to determine the relation of dispersion. But on its own, the Green function method[46-48] enables us to study the resonant modes[49-51] by calculations of both local and total DOS. In addition to these characteristic functions, one can also obtain the spatial distribution of these modes, which may appear as defined peaks of the density of states inside the bulk bands.

This paper will be organised as follows: first, we present some general lines of the theoretical model ; second we gives some illustrations about four cases of heterostructures beginning with the simple interface case and moving to more complicated cases of semi-infinite SL

The geometrical case of symmetry considered is the hexagonal and cubic configurations, which involves very interesting simplifications which rise mainly as a decoupling between the modes in sagittal plane and the shear horizontal direction. The elastic proprieties derived, are associated with these two decoupled modes which are treated separately.

II. THE BASIC EQUATIONS

In this section, special attention is allocated to particular geometry case which concerns the hexagonal and cubic symmetry[40] with the grown layers the axis x_3 and the waves propagating along the (100) direction. As advanced before, this paper will focus on this type of geometry because it involves very interesting simplifications which rise mainly as decoupling form between modes polarised in sagittal plane (plane containing $k_{//}$ and x_3) and the shear horizontal waves. For instance, this happens also when the films are isotropic[38]. In this case, for example the transfer matrix becomes a juxtaposition of 2 x 2 and 4 x 4 matrices. Moreover, the eigenvalues problem for this last problem can be solved analytically by introducing an artefact which is the matrix 4 x 4 as a diagonalized block onto two 2 x 2 sub-matrices whose eigenvalues are $\mathrm{Cos}(k_3D)$.

On the other side, the complicated model based on Green function is viewed under general lines in order to elucidate briefly its content.

Let us consider an homogenous and infinite material defined in a space which is associated with an operator H. The Green function G of this material is defined by :

$$\mathbf{HG}=\mathbf{I} \tag{1}$$

when **I** is the identity operator.

With the help of the cleaving operator $\mathbf{V_s}$, we can obtain a material which is associated to the operator $\mathbf{h_s}$:

$$\mathbf{h_s}=\mathbf{H}+\mathbf{V_s} \tag{2}$$

and the corresponding response function $\mathbf{g_s}$ can be written :

$$\mathbf{h_s g_s}=\mathbf{I} \tag{3}$$

The response operator surface is then

$$\mathbf{A_s}=\mathbf{V_s G} \tag{4}$$

The knowledge of **G** and $\mathbf{A_s}$ enables us to determine the response function $\mathbf{g_s}$ of an homogenous medium with free surfaces :

$$\mathbf{g_s(I+A_s)=G} \tag{5}$$

which can be written :

$$\mathbf{g_s(DD)=G(DD)-G(DM)\Delta_s^{-1}(MM)A_s(MD)} \tag{6}$$

where D an M are respectively the whole space of the interfaces in the composite material.
One particular form of the equation (6) is

$$\mathbf{g_s(MM)=\Delta_S(MM)G^{-1}(MM)} \tag{7}$$

where $\mathbf{\Delta_s^{-1}(MM)}$, $\mathbf{g_s^{-1}(MM)}$ and $\mathbf{G^{-1}(MM)}$ are the inverted forms of

$\mathbf{\Delta_s(MM)}$ $\mathbf{[=I(MM)+A_s(MM)]}$, $\mathbf{g_s(MM)}$ and $\mathbf{G(MM)}$

A composite material is defined as an association of a big number of material with free surfaces or more precisely the interface space M is the space constitute i of j interfaces.
The response function of this material is :

$$\begin{aligned}\mathbf{g(DD)}&=\mathbf{G(DD)-G(DM)G^{-1}(MM)G(MD)}\\&+\mathbf{G(DM)G^{-1}(MM)g(MM)G^{-1}(MM)G(MD)}\end{aligned} \tag{8}$$

Let us consider a thin film of hexagonal crystal, the solution of elasticity equation enables us to deduce the Green function elements . In the case of the shear horizontal wave, this element G_{22} is written :

$$G_{22}(k_{//},\omega/x_3,x'_3)=-\frac{1}{2\alpha_2C_{44}}e^{-\alpha_2|x_3-x'_3|} \tag{9-a}$$

where

$$\alpha_2^2=k_{//}^2\frac{C_{11}-C_{12}}{2C_{44}}-\rho\frac{\omega^2}{C_{44}} \tag{9-b}$$

with C_{ij} and ρ the elastic constant and the density.
The components of G defining the sagittal modes are G_{11}, G_{31}, G_{13} and G_{33} given under matricial form :

$$G(k_{//},\omega/x_3,x'_3)=$$

$$\begin{bmatrix}-\frac{1}{F\xi_1}\left[-e^{-\alpha_1|x_3-x'_3|}+\xi e^{-\alpha_3|x_3-x'_3|}\right] & \frac{i}{F}\mathrm{sgn}(x_3-x'_3)\left[-e^{-\alpha_1|x_3-x'_3|}+e^{-\alpha_3|x_3-x'_3|}\right]\\ \frac{i}{F}\mathrm{sgn}(x_3-x'_3)\left[-e^{-\alpha_1|x_3-x'_3|}+e^{-\alpha_3|x_3-x'_3|}\right] & \frac{\xi_3}{F}\left[\xi e^{-\alpha_1|x_3-x'_3|}-e^{-\alpha_3|x_3-x'_3|}\right]\end{bmatrix} \tag{10-a}$$

with

$$F=\left[\frac{k_{//}(C_{44}+C_{13})}{2C_{44}C_{33}(\alpha_1^2-\alpha_2^2)}\right] \tag{10-b}$$

$$\alpha_1^2=\frac{1}{2}\left[x+(x^2-4y^2)^{1/2}\right] \tag{10-c}$$

and

$$\alpha_3^2=\frac{1}{2}\left[x-(x^2-4y^2)^{1/2}\right] \tag{10-d}$$

and

$$x=-\delta_1^2-\delta_3^2-\left[\frac{(C_{13}+C_{44})^2}{C_{33}C_{44}}\right]k_{//}^2 \tag{10-c}$$

$$y^2=\delta_1^2\delta_3^2 \tag{10-d},$$

$$\delta_1^2=\frac{(\rho\omega^2-C_{11}k_{//}^2)}{C_{44}} \tag{10-e},$$

$$\delta_3^2=\frac{(\rho\omega^2-C_{44}k_{//}^2)}{C_{44}}\ ,\ \xi=\frac{\xi_1}{\xi_3} \tag{10-f}$$

$$\xi_i=\frac{C_{11}k_{//}^2-C_{44}\alpha_i^2-\rho\omega^2}{(C_{13}-C_{44})k_{//}\alpha_i}\ ,\ i=1,3 \tag{10-g}$$

when $\mathbf{g}_s^{-1}(\mathbf{MM})$ is defined for any film, we can obtain the Green function $\mathbf{g}^{-1}(\mathbf{MM})$ as a linear superposition of $\mathbf{g}_s^{-1}(\mathbf{MM})$ elements.

III. ACOUSTIC PHONONS IN HETEROSTRUCTURES :

As mentioned before, the geometrical case and the growth axis involve the decoupling of the so called transverse waves from the sagittal waves. This enables us to treat separately these two modes in many cases of heterostructures. For the sagittal waves the calculations are more complicated than the transvers waves and this reason gives us the opportunity to study a large number of heterostructures and SL for the last case(transverse modes) In this section we begin with this mode in four cases of heterostructures : adlayer, bilayer on substrate ; infinite and semi-infinite SL.

A. Transverse wave: Adlayer, bilayer on substrate and superlattices.

i) Adlayer and bilayer:

We begin with a simple form of hetrostructure which is an adlayer deposited on semi-infinite substrate; which a system formed by a semi-infinite elastic medium bound by a planar surface supporting surface vibration modes. These waves are defined with the transverse velocity of sound $C_t = \sqrt{C_{44}/\rho}$. We consider the simple case of isotropic media Al-W, (Al : adlayer and W : substrate). When C_{ta} the velocity of the adsorbat is lower than the velocity C_{ts} of substrate ($C_{ta} < C_{ts}$), and the waves propagate with increasing the wave vector $k_{//}$ (parallel to the direction of propagation). The general aspect shown by figure 1 giving the velocity C as function of $k_{//}h$ (h : the thickness of the adlayer), is the fact that these modes emerge from the substrate bulk bands. Their extension in these bands corresponds to resonant modes also called leaky or pseudo-waves, radiating their energy into bulk bands (or modes) and, therefore, getting infinite lifetime. In opposite case of ($C_{ta} > C_{ts}$), the modification induced by the adlayer can only appear as a resonant or pseudo-modes falling inside the substrate bulk bands. In any case, the dispersion and lifetime of these waves are dependent upon the parameter $k_{//}h$, in addition to the material parameters.

An analysis is of the above localised and resonant surface modes have been done within the Green function formalism which enables to calculate both local and total DOS : localised modes appear as delta peaks outside the substrate bulk bands, whereas the positions and widths of the resonant modes which may be more or less pronounced features depending on material parameters and on $k_{//}h$.

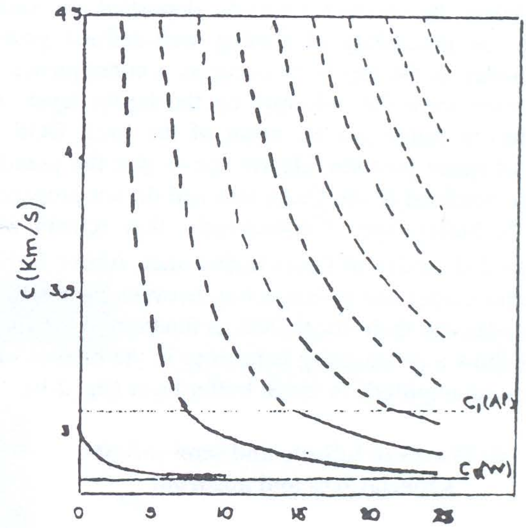

Figure 1. The dispersion of localised and resonant transverse modes for a W slab on an Al substrate. Full and broken curves respectively represent localised and resonant modes. c is the velocity.

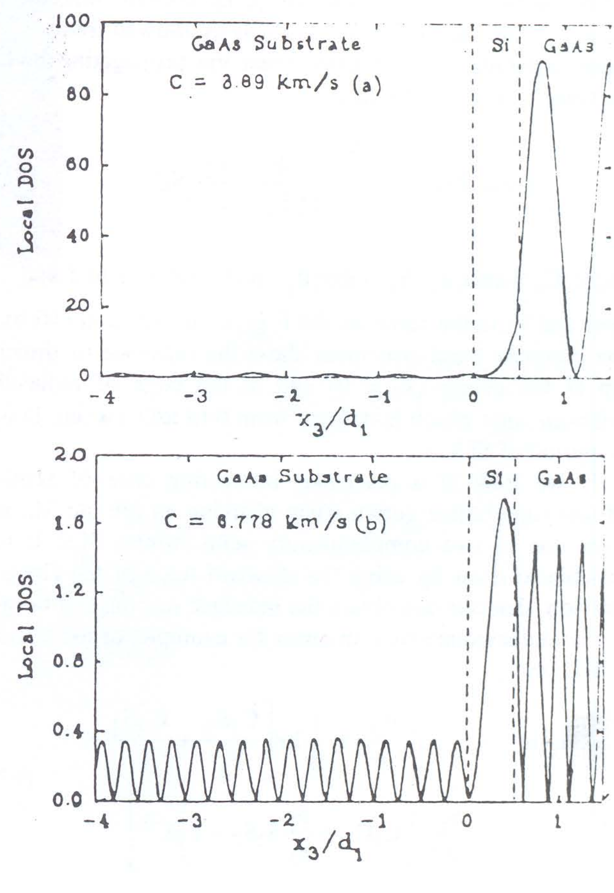

Figure 2. (a) Spatial representation of the local DOS for C=3.89 km/s and $k_{//}d_1$=7. (b) the same figure as (a) but for C=6.778 km/s and $k_{//}d_1$=7.

The same analysis can also be applied to the case of a bilayer grown on substrate. The problem considered here is related to recent work, where the surface modes and pseudo-modes of Si-SiO_2 bilayer grown on Si substrate[12-15]

are pointed out. The discussion of all possible combinations about the material parameters or velocities will not be considered in this paper. We would report one of the particular results not reported by any author yet. If one considers the bilayer GaAs-Si deposited on GaAs substrate, the possibility of finding well-defined guided pseudo-modes in the top layer occur as a consequence of its separation from the substrate by the buffer layer. As represented in figure 2.a by mean of the local DOS as function of space position, clearly shows that the pseudo-modes are confined in the GaAs slab and do not propagate into the Si buffer layer. Consequently, they remain well defined guided modes of GaAs higher slab. Above C_t(Si), the resonant modes due to interaction between the GaAs-Si bilayer modes and their local DOS as function of the space positions show a propagating behaviour in the bilayer with a pronounced amplitude in the Si buffer layer (fig. 2-b).

ii) Waves in infinite and semi-infinite superlattices and adsorbat :

This topic has been touched on early by the direct method[38-40] in the two symmetrical cases cited above and for isotropic layered media. Band structures projected along the $\mathbf{k}_{//}$ and complex along k_3 (k_3 is the component of the wave vector along the axis x_3) are emphasised in contrast with the bulk and surface modes. As indicated before, these band structures along $k_{//}$ present, therefore, the same characteristic which consists of allowed frequency bands separated by min-gaps when the propagating bulk phonons is given by the relation :

$$\cos k_3 D = C_1 C_2 + \frac{1}{2}\left(\frac{F_1}{F_2} + \frac{F_2}{F_1}\right) S_1 S_2 \tag{11}$$

where $C_i = \mathrm{ch}\alpha_i d_i$, $S_i = \mathrm{sh}\alpha_i d_i$ with i relative to 1 and 2 layer and F_i is the same as the F given by relation (10-b). The complex band structures show the presence of direct gap at the centre ($k_3 = 0$) and at the edge of reduced Brillouin zone which is defined from 0 to π/D (where D is the period of SL).

If we look at a particular interesting case of semi-infinite superlattice gotten when cleaving an infinite SL, it gives rise to two complementary semi-infinite SLs. It is possible to show by using the standard trace of the Green function, that one can obtain the interface response of these two complementary SLs, in terms for example, of local and total DOS :

$$n_s(\omega^2, k_{//}; 0, 0, \frac{d_0}{2}) = \frac{1}{\pi}\mathrm{Im}\left[\frac{C_1 S_2}{F_2} + \frac{C_2 S_1}{F_1} + \frac{S_0}{F_0 C_0}\left(C_1 C_2 + \frac{F_1}{F_2} S_1 S_2 - t\right)\Delta^{-1}\right] \tag{12}$$

Where Δ and t are defined in reference[44], and S_0, C_0, F_0 reported to the capping layer on the SL with thickness d_0.

The total DOS can be written as the addition of the variation of the DOS $\Delta_1 n(\omega^2)$ and $\Delta_2 n(\omega^2)$ of two SL layer and the DOS of the capping layer $\Delta_0 n(\omega^2)$. All these variations are calculated as integrals of the local densities of states over all the layer of SL. Also, then explicit relations are obtained and presented in reference[44].

The DOS is a function which is zero inside the bulk band and that all edges of these bulk bands $\Delta n(\omega^2)$ display (δ) function of weight (-1/4). This is demonstrated by the quantity :

$$\frac{1}{(t^2-1)^2} = \frac{1}{8}\left(\frac{d\eta}{d\omega}\right)^{-1}_{\omega_0}\left[P\left(\frac{1}{\omega-\omega_0}\right) - i\pi\delta(\omega-\omega_0)\right] \tag{13.a}$$

Which can give easily :

$$\Delta_1 n(\omega^2) + \Delta_2 n(\omega^2) = (1/4)\delta(\omega-\omega_0) \tag{13-b}$$

These facts assembled together with necessary conservation of the number of states conditions enable us to conclude that when one considers in compound form the two semi-infinite SL obtained by cleavage of infinite one, one has many localised surface modes in mini-gaps, for each value of $k_{//}$. These results remain valid when the thickness (d_0) of the capping layer is going to zero. On the contrary, when the limit of the capping layer has no zero thickness, but is of the same nature as that of the two layers of SL, we get the same results which are localised modes. In this case, we calculate the variation of the density of states between such a semi-infinite SL and the same amount of the bulk SL. If we assume that the cap layer is different from the two layers of SL, for example, Si deposited on the top of GaAs-AlAs; this cap-layer induces the dispersion of localised and resonant modes (figure 3-a) presented in reference[52]. For one case of $k_{//}D=3$, we give on figure 3-b the variation of the DOS where R_i are the resonant modes, L_i the localised ones and B_i , T_i are the peacks of weight (-1/4) lying at the bottom and at the top of bulk bands.

Depending on their frequencies, these modes may propagate along a perpendicular line to the interface in both the SL and the cap-layer. Another situation can be observed and which consists of the fact that these modes propagate in one and decay in the other; or decay on both sides of the SL-adlayer interface. This result depends on the nature of SL layer GaAs or AlAs on which it is deposited.

When the thickness of the adlayer goes to the infinite value, this means that we have a semi-infinite substrate instead of the adlayer. This case has been addressed through the transfer matrix method with which one cannot derive the resonant modes. Using the Green function method here, we show the possibility of occurrence of resonant modes, associated with this interface, which appeared as well defined features of the DOS. In reference[52], the existence of localized waves was discussed as a function of the parameter $\gamma = C_{44}^{SL} / C_{44}^{S}$ (when C_{44}^{S}, C_{44}^{SL} are the elastic constants of the substrate and the layer of SL in contact with the substrate). Two extremes case of γ value can be considered ; $\gamma = 0$ and $\gamma \to \infty$. In the first case, the localised modes are associated with the free surface of SL, furthermore in the second case the amplitude of vibration goes at the interface and remains very close in the substrate (rigid interface). Other intermediary cases of γ have been derived in order to discuss the occurrence or non occurrence of the resonant and localised modes but not presented here.

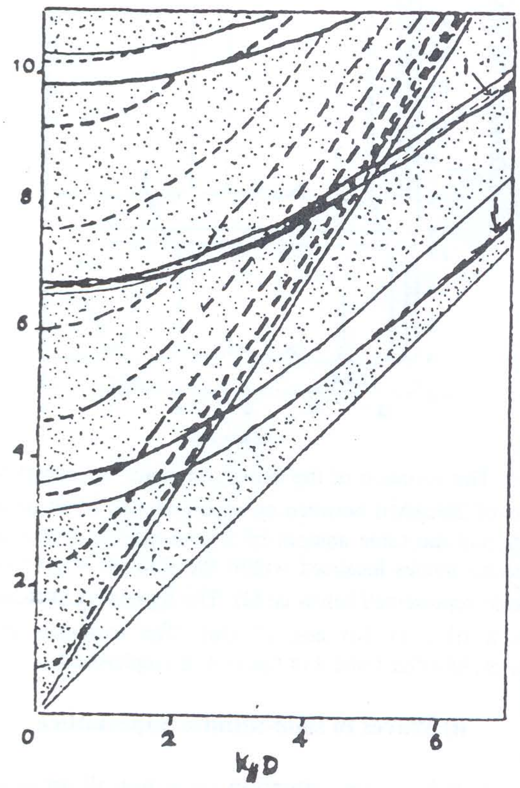

Figure 3-a. Dispersion of localised and resonant modes (dashed lines) induced by a Si cap layer of thickness d_0=4D, deposited on the top of the GaAs-AlAs superlattice terminated by a full GaAs layer. The shaded areas are the superlattice bulk bands. The heavy line indicates the bottom of the bulk band of Si. The branches labelled (i) correspond to modes localised at the superlattice-adlayer interface.

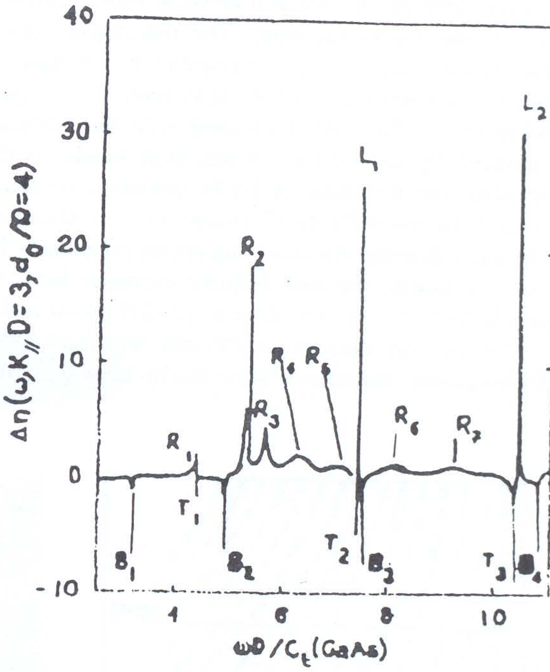

Figure 3-b. Density of states [in units of D/C_t(GaAs)] corresponding to the case depicted in figure 4, for $k_{//}$D=3. The contribution of the same amount of the bulk GaAs-AlAs superlattice was subtracted. B_i, T_i, L_i, R_i are respectively the bottom, the top, the localised and the resonant modes.

B. Sagittal Mode

Acoustic modes of sagittal polarisation have been investigated during the last few years using transfer matrix methods. In particular, surface localised modes have been obtained and discussed in detail[37-40]. However, to our knowledge, the variation of the total DOS associated with the above cited perturbation of the SL, and in particular the existence of surface resonant states have not been yet studied. Due to the coupling of two degrees of vibrations, the density of states deduced, becomes rather complicated as compared to the case of the transverse vibrations. For this reason these calculations performed, for the layer and the bilayer adsorbed on substrate on the one hand, and for the semi-infinite SL on the other will not be reported here. Throughout this paragraph, we restrict ourselves just to the case of isotropic media and particularity to the Al-W system when it does matter of layer adsorbed on semi-infinite SL. In the case of bilayer we illustrate our application with an example of GaAs-Si deposited on GaAs.

i) Adlayer and bilayer :

The dispersion curves of an Adlayer with 2h as thickness deposited on Al substrate is given in figure 4, the behaviour of the DOS is given on figure 5 for some values of $k_{//}h$. In the limit of $k_{//}h \rightarrow \infty$, the two lowest branches are given respectively, to the Raleigh wave (C_R) of the W crystal and to the Stonley wave at interface Al-W (C_S). The other branches go to the sound velocity of the transverse wave in W (C_t). Another type of evolution may occur in the analysis of DOS; it shows graduated change from character of transverse waves to longitudinal waves when increasing the frequency (or velocity). We can notice in this figure also an important interaction between these modes in the vicinity of the longitudinal sound velocity of W (C_l) accompanied by this change. A particular feature is also the arrangement of resonant modes into doublets in the range of the highest longitudinal velocity of W and Al. Due to their finite width , the resonant states can interact together giving rise to mixing of curves of the same doublets. This association into doublets is not related to arbitrary parameters of material.

For a given value of $k_{//}h$, we can observe in the spectre of DOS , when increasing the velocity, the resonance intensity decreases before increasing very significantly in the zone of longitudinal velocity. In this last region the most resonance have a longitudinal character when the velocity C falls between C_l(W) and C_l(Al). This component is attenuated in the substrate and consequently these resonances must correspond to the guided longitudinal waves . Otherwise, these well defined resonances may exist also for velocities just higher than the C_l(Al), where the waves have a propagating behaviour inside substrate (figure 5)

For the bilayer case, the type of the heterostructure studied is the same as the case of transverse wave; GaAs-Si deposited on the GaAs substrate. The dispersion curves show the lowest branch which correspond to the Raleigh wave velocity as a surface wave of GaAs layer. A new type of branches occur; they are associated with the resonant modes induced by the bilayer in the bulk bands of the substrate when the thickness of GaAs increases, resonant modes stretch to the velocity C_t (transverse) of GaAs as well as to the substrate. An other important point must be sorted out, it concerns the well-defined resonance between C_t (Si) and C_l (Si) that we can admit as guided waves in the bilayer GaAs-Si. An illustration through the local DOS shows the localised character of these modes belonging to

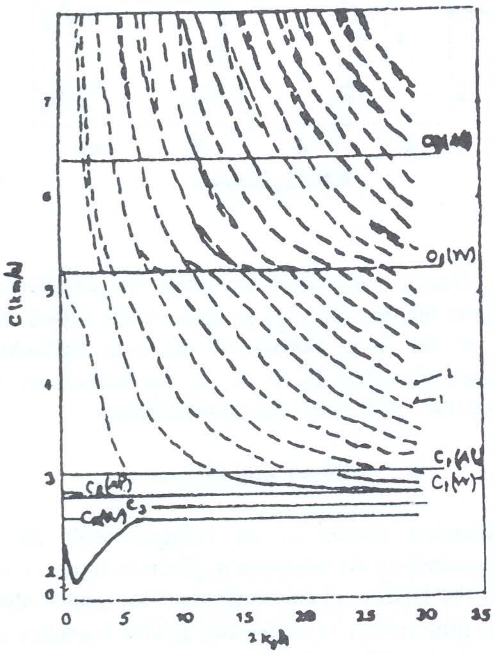

Figure 4. The dispersion curve for localised and resonant sagittal waves, for a W slab deposited on an Al substrate. The localised modes (full curves) below c_t(Al) extend as resonances (broken curves) into the bulk bands of the substrate. The asymptotic limits of the lowest two branches are respectively c_R(W) (the Rayleigh wave velocity of W) and c_s (the velocity of the Stoneley wave at the Al-W interface).

the zone velocity indicated before. This means that the two displacement components of sagittal polarisation remain coupled in the GaAs layer without propagation in Si layer.

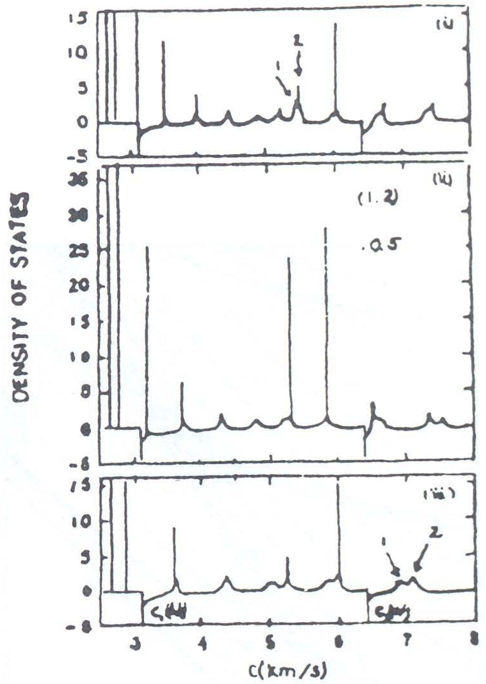

Figure 5. The variation of the density of states of sagittal waves (in units of $2h/c_t$(Al)) between an adsorbed slab of W on an Al substrate and the same amount of a semi-infinite crystal of Al. The Sezawa modes localised within the slab of W give rise to delta peaks represented below c_t(Al). The figures are sketched for $2k_{//}h$ = 8 (i) , 11 (ii) and 13 (iii). The evolution of two resonances, labelled 1 and 2 in figure 4, is emphasised.

ii) Waves in semi-infinite Superlattice:

We shall focus our attention on a few illustrations as indicated before with the example Al-W SL (made of Al and W). The thickness d_1 and d_2 of the two layers are assumed to be equal.

For given ω and $k_{//}$, the wave vector along the axis x_3 of the SL can be deduced from the bulk dispersion relations. In the case of sagittal modes involving two components of the displacement field, there are two pairs of k_3 associated with every value of (ω, $k_{//}$) point, which can be written[37-40] as $\pm [K_1 + iL_1]$ and $\pm [K_2 + iL_2]$.

Now, an elastic wave at the frequency ω, can propagate in the SL if only $L_1 = 0$ or $L_2 = 0$, while is attenuated if both L_1 and L_2 are different from zero. Each pair of k_3 can take four different forms; it can be:

(a) pure real($L_1 = 0$)
(b) pure imaginary ($K_1 = 0$)
(c) complex but with $K_1 = \pm \pi/D$
(d) complex with $K_1 \neq \pm \pi/D$

However, in the last case, the two pairs of k_3 necessarily become $K + iL$, $-(K + iL)$, $(K - iL)$, $-(K - iL)$.

The figure 6-a gives an example of the complex band structure in W-Al , showing the combinations of the above-mentioned cases . One can see the presence of direct gap at the centre and the edge of the reduced Brillouin zone but also the possibility of indirect gaps inside this zone (Fig. 6-b). Let us also mention that the imaginary parts of k_3 wave vectors give the attenuation of the possible localised waves in the gaps.

This situation, which can occur when the vibration involves at least two degrees of freedom, is of course without analogue in the case of transverse wave.

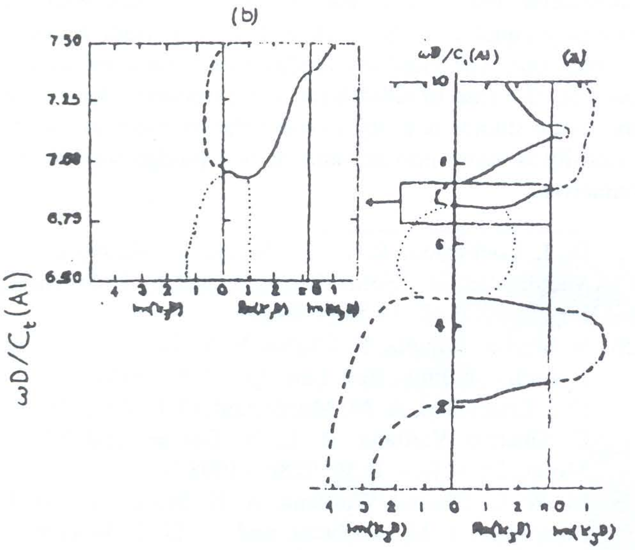

Figure 6. Complex band structure (ω versus complex k_3)in a W-Al SL with $d_1=d_2=D/2$ and $k_{//}D=3$. $\omega D/C_t(Al)$ is a dimensionless frequency where $C_t(Al)$ is the transverse velocity of sound in Al given by $(C_{44}/\rho)^{1/2}$. Solid curves are k_3 real (middle panel of the figure). Dashed-dotted curves are k_3 imaginary (left panel). Dashed curves are imaginary part of k_3 when its real part is equal to π/D (right panel). In addition, when k_3 is a complex quantity, the dotted curve gives both its real and imaginary parts ; in this case the imaginary part is presented in the left panel. (b) Same as in (a) enlarged in the range of frequencies where the indirect gap appears.

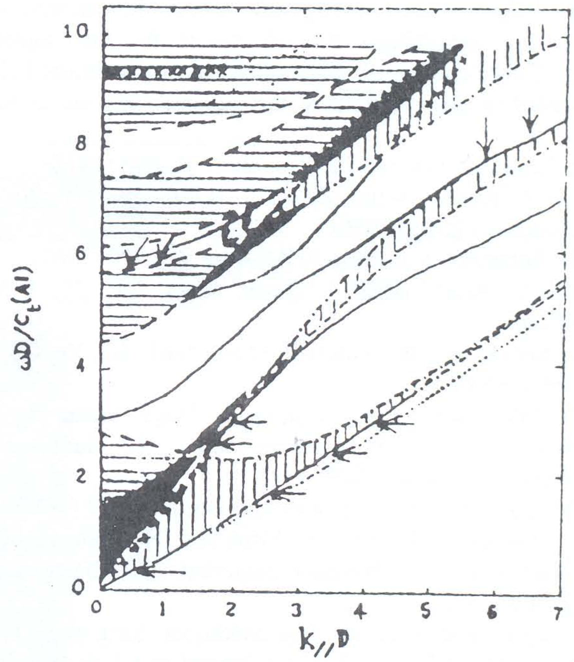

Figure 7. Bulk and surface sagittal elastic waves in W-Al SL. The curves give $\omega D/C_t(Al)$ as a function of $k_{//}D$, where ω is the frequency, $k_{//}$ the propagation vector parallel to the interfaces, $C_t(Al)$ the transverse speed of sound in Al, and $D=d_1+d_2$ the period of the SL. The horizontally and vertically shaded areas correspond to the bulk bands associated with each of the two polarisations of the waves. The range of frequencies belonging simultaneously to these two types of bands is represented in black. The surface modes associated with two complimentary SL's (ending, respectively, with a full W layer or a full Al layer) are represented by dashed lines (W at the surface) and solid lines (Al at the surface). Some of the surface modes are very close to the bulk bands and cannot be distinguished by arrows. The extensions of the localised modes into the bulk bands as resonances are indicated by crosses.

In figure 7, we have represented the projected band structure of the bulk and surface modes, namely, ω versus $k_{//}$. The bulk bands associated with each polarisation ($L_1 = 0$ or $L_2 = 0$) of the waves are , respectively represented by horizontally and vertically dashed lines. Due to the large difference between elastic parameters of W and Al , these gaps are rather large in contrast to the case of more usual systems likes GaAs-AlAs. Inside these gaps, we have represented surface modes corresponding to complementary semi-infinite SL obtained by cleaving the infinit W-Al SL in a way that one obtained one SL with a full W layer at the surface (dashed line) and its complementary with a full Al layer at the surface (solid lines). In these figures some of surface modes are very close to the bulk bands and cannot be distinguished from the latter on the scale of the figure.

Besides the localised modes which appear as δ -peaks inside the gaps (as well as the transverse case), the variational density of states also contains well-defined features falling inside the bulk band of the SL. These peaks can be considered as resonant states associated with the surface of the SL. Their dispersion is plotted in Fig. 7 by cross ; some dispersion curves seem to be a continuation of localised branches into the bulk bands of SL. Let us remark that these resonant modes may be localised with respect to one type of band and propagating with respect to other.

The behaviour of the localised and resonant modes in the DOS when the its variation is sketched when two complementary semi-infinite SL's are created by the cleavage of an infinite SL. The δ peak in the DOS are broadened by a small imaginary part to the frequency ω(i.e. $\omega \rightarrow \omega+i\varepsilon$).

When $k_{//}D = 0$, the sagittal modes is separated into decoupled longitudinal and transverse waves. When $k_{//}D$ departs from zero, these two components become both coupled, and some of the localised branches at $k_{//}D = 0$ may now fall inside a bulk band. Such modes can radiate their energy into the bulk modes and therefore become resonant (or leaky) waves.

IV. CONCLUSION

To conclude, we must indicate that other types of SLs have been studied and a large number of results have been obtained. Outermost of electronic properties which will be

proposed in second paper of this volume, there are other types of structures ; finites SLs, N-layered (N ≥ 3) SLs, sagittal modes with cap-layers or substrate etc...We have already finished to examine them and started to re-examine them on a broader perspective. Of great importance is that piezoelectric SL which presents very important effects of surface, in particular, the appearance of new types of modes called Bleustein-Gulyaev waves for transverse modes and generalised Raleigh waves for the sagittal modes. These can appear only when the displacement field is coupled to electric field of the material. We are in the stage of performing the numeric calculations of DOS which will be followed by the effect of cap-layer.

Another type of SL, which contains a fluid layer and a solid one by period, is studied. The simple situation considered until then is that the fluid is taken with the viscosity equal zero (μ = 0), and an important result is pointed out. The capillary modes which have no similar ones in the case of solid layer, are exhibited. Our aim in the future studies is to try to solve the problem where the viscosity is taken into account. It is a pledge we take on ourselves.

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