

## Effect of strain on vibrational modes in strained layer superlattices

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**Abstract.** We have investigated the lattice vibrational properties of a two-component strained layer semiconductor superlattice  $(\text{GaAs})_{n_1}(\text{GaSb})_{n_2}$  using a one-dimensional linear chain model and transfer matrix method [1]. Effect of strain, arising due to the lattice mismatch ( $\approx 7\%$ ) has been considered explicitly in the equation of motion. We show for the first time that the optical vibrational frequency increases (in the case of  $(\text{GaAs})_4(\text{GaSb})_n$ ) or decreases (in the case of  $(\text{GaAs})_n(\text{GaSb})_4$ ) with increase of layer thickness  $n$ , in either type of superlattices. Raman scattering measurements on some other similar systems support our findings.

**Keywords.** Vibrational modes; strained layer; superlattices; linear chain model; transfer matrix.

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### 1. Introduction

The electronic and lattice vibrational properties of the semiconductor superlattices (SSL) have been investigated with great interest in the past few years. This is mainly because of the possible applications of these materials in electronic devices. However, these SSL are quite interesting from the fundamental physics point of view and can be realized from the fact that they show diverse physical properties, particularly some of which cannot be observed in the bulk materials (e.g. confinement of optical phonons). A sizable amount of work on the phonon and optical properties of SSL, using both experimental and theoretical techniques is now available in literature [2–10].

Fabrication of a perfect SSL, however depends on the matching of the lattice constants of the components. The most celebrated and extensively studied compound SSL is GaAs–AlAs in which lattice mismatch is the smallest ( $\approx 0.13\%$ ) [11]. However, Raman measurements on InGaAs/GaAs strained layer superlattices (SLSL) where the lattice mismatch is nearly  $\approx 7\%$  have also been reported [12]. It is now well established that during the growth, each of the atomic layers of the constituents of the lattice mismatched (or strained layer) SSL accommodates strain in order that such systems are structurally and thermodynamically stable [13]. In most of the systems, the strain generated due to lattice mismatch is isotropic and gives rise to change in the volume without affecting the crystal symmetry. In view of this fact, the SLSL allow the use of lattice mismatched materials without the generation of misfit dislocations, thereby providing freedom from the need for precise lattice matching and widens the choice of compatible materials for device fabrication.

Some of the consequences of the generation of strain at the interfaces of the

heterostructures are that they change the energy gap, effective mass and shift of the phonon frequencies. The changes in vibrational modes are extremely useful for characterization of the distribution of strain in the components of the superlattices. The effect of such strain on electronic structure in SLSL has been reviewed in ref. [14]. Despite the fact that the SLSL are the 'would be' materials for the future electronic devices, very little is understood as far as their vibrational properties are concerned. So far, only limited efforts have been made to study the changes in the vibrational energy levels using Raman scattering [12, 15].

In the present paper, we investigate the effect of strain on the vibrational properties of SLSL using a simple theoretical approach which essentially contains the features that one can expect in such systems. Such a theoretical model has already been successfully applied to study the phonon dispersion in multicomponent SSL [1, 8]. For this purpose, we choose GaAs–GaSb SLSL in which the amount of lattice mismatch is quite large ( $\approx 7\%$ ), and also the vibrational modes for bulk constituents are already analysed by using neutron scattering technique. However, our theoretical approach is general and can be applied to any SLSL system. In §2, we present the theory and in §3, we discuss our calculated results.

## 2. Model and method of calculation

In order to understand the role of strain arising from the lattice mismatch on the phonon dispersion curves in a two component compound SLSL, we have made use of a linear chain model which depicts qualitative features such as folding of acoustic and confinement of optic phonons in SSL [1].

The equation of motion of any atom in either of the components can be written as

$$m_j \omega^2 u_n = -(C_i + \Delta C_i)(u_{n-1} + u_{n+1} - 2u_n), \quad (1)$$

where  $m_j(j=1,2)$  are the masses of the respective atoms,  $u_n$  the displacements of various atoms at site  $n$ ,  $C_i(i=1,2)$ -components) the nearest neighbour force constants.  $\Delta C_i$  is the change in force constants due to the strain generated by the lattice mismatch and can be expressed as

$$\Delta C_i = [p_i(\varepsilon_{zz}^i) + q_i(\varepsilon_{xx}^i + \varepsilon_{yy}^i)]m_j, \quad (2)$$

with

$$p_i = k_{11}^i \omega^2; \quad q_i = k_{12}^i \omega^2.$$

Here  $k_{ij}$  are dimensionless fourth rank tensors and  $\varepsilon_{\alpha\beta}(\alpha, \beta = x, y, z)$  is the strain tensor whose non-zero components are given by

$$\varepsilon_{xx}^i = \varepsilon_{yy}^i = \frac{a_{\parallel} - a_i}{a_i}; \quad \varepsilon_{zz}^i = \left[ \frac{2C_{12}^i}{C_{11}^i} \right] \varepsilon_{xx}^i, \quad (3)$$

with  $a_{\parallel}$  as the inplane lattice parameter,  $a_i$  are the lattice constants of various constituents,  $C_{11}^i$  and  $C_{12}^i$  are the elastic constants of the corresponding components.

With the assumption that the lattice mismatch is accompanied by uniform deformation and minimization of the elastic energy, the inplane lattice parameter  $a_{\parallel}$  is given by [16]

$$a_{\parallel} = a_i \left[ 1 \pm \frac{\delta S_i d_i}{S_1 d_1 + S_2 d_2} \right], \quad (4)$$

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with  $d_i = 2n_i a_i$  as the layer thickness,  $S_i$  is the bulk shear modulus given by

$$S_i = 2 \left[ C_{11}^i + C_{12}^i - \frac{2(C_{12}^i)^2}{C_{11}^i} \right], \quad (5)$$

and the mismatch

$$\delta = \frac{a_1 - a_2}{\langle a \rangle},$$

with  $\langle a \rangle = 1/2 (a_1 + a_2)$ .

The solutions of the equations of motion [eq. (1)] for atoms *A* and *B* in component 1 for *l*th cell can be written as

$$\begin{aligned} u_i^A(z) &= a_i \exp[ik_1(z - lD)] + b_i \exp[-ik_1(z - lD)], \\ u_i^B(z) &= \alpha_1 u_i^A(z), \end{aligned} \quad (6)$$

where *z* is the position of the atom in the unit cell *l* along the growth direction,  $k_1$  is the wave vector and *D* is the periodicity of the SLSL. Similarly, the solutions for the second component are

$$\begin{aligned} u_i^{A'}(z) &= c_i \exp[ik_2(z - lD)] + d_i \exp[-ik_2(z - lD)], \\ u_i^{B'}(z) &= \alpha_2 u_i^{A'}(z). \end{aligned} \quad (7)$$

Substitution of (6) and (7) in (1) leads to

$$\alpha_i = \frac{2(C_i + \Delta C_i) - m_j \omega^2}{2(C_i + \Delta C_i) \cos k_i a_i} = \frac{2(C_i + \Delta C_i) \cos k_i a_i}{2(C_i + \Delta C_i) - m_j \omega^2}. \quad (8)$$

The bulk dispersion relation of any component can be obtained from (8).

Use of equation of motion of the atoms on either side of the interface within cell *l* and between cells *l* and (*l* + 1) results in

$$\begin{aligned} f_1 a_l + \bar{f}_1 b_l - c_l - d_l &= 0, \\ -\alpha_1 \bar{s}_1 f_1 a_l - \alpha_1 s_1 \bar{f}_1 b_l + \alpha_2 \bar{s}_2 c_l + \alpha_2 s_2 d_l &= 0, \end{aligned} \quad (9)$$

$$\begin{aligned} -a_{l+1} - b_{l+1} + f_2 c_l + \bar{f}_2 d_l &= 0, \\ \alpha_1 \bar{s}_1 a_{l+1} + \alpha_1 s_1 b_{l+1} - \alpha_2 \bar{s}_2 f_2 c_l - \alpha_2 s_2 \bar{f}_2 d_l &= 0, \end{aligned} \quad (10)$$

with

$$\begin{aligned} f_i &= \exp(ik_i d_i); \quad \bar{f}_i = \exp(-ik_i d_i), \\ s_i &= \exp(ik_i a_i); \quad \bar{s}_i = \exp(-ik_i a_i). \end{aligned}$$

We introduce two column vectors one for each component [17]

$$|u_i\rangle = \begin{pmatrix} a_i \\ b_i \end{pmatrix}; \quad |v_i\rangle = \begin{pmatrix} c_i \\ d_i \end{pmatrix}, \quad (11)$$

and four ( $2 \times 2$ ) unimodular matrices  $H_1$ ,  $H_2$ ,  $K_1$  and  $K_2$ , given by

$$H_i = \Delta_i^{-1/2} \begin{bmatrix} 1 & 1 \\ \alpha_i \bar{s}_i & \alpha_i s_i \end{bmatrix},$$

$$K_i = \Delta_i^{-1/2} \begin{bmatrix} f_i & \bar{f}_i \\ \alpha_i \bar{s}_i f_i & \alpha_i s_i \bar{f}_i \end{bmatrix}, \quad (12)$$

with

$$\Delta_i = \alpha_i (s_i - \bar{s}_i)$$

such that (9) and (10) replace the boundary condition for a continuum theory. Use of (11) and (12) in (9) and (10) leads to

$$H_1 u_l = K_2 v_l, \quad (13)$$

$$H_2 v_l = K_1 u_{l+1}. \quad (14)$$

Elimination of  $v_l$  from (13) and (14) results in

$$|u_{l+1}\rangle = T|u_l\rangle, \quad (15)$$

where  $T$  is a  $2 \times 2$  unimodular transfer matrix which has the property of relating the coefficients of the displacement vectors in one cell to that in the previous one and is expressed as

$$T = K_1^{-1} H_2 K_2^{-1} H_1. \quad (16)$$

The dispersion relation for two component diatomic SLSL can now be obtained from (16) and is given by

$$\begin{aligned} \cos QD &= 1/2 \text{Tr } T, \\ &= \cos(k_1 d_1) \cos(k_2 d_2) - 1/2 \left[ \frac{(C_2 + \Delta C_2) \tan(k_1 a)}{(C_1 + \Delta C_1) \tan(k_2 a)} A \right. \\ &\quad \left. + \frac{(C_1 + \Delta C_1) \tan(k_2 a)}{(C_2 + \Delta C_2) \tan(k_1 a)} A^{-1} \right. \\ &\quad \left. - \left( \frac{(C_2 + \Delta C_2)^2 A + (C_1 + \Delta C_1)^2 A^{-1} - 2(C_1 + \Delta C_1)(C_2 + \Delta C_2)}{(C_1 + \Delta C_1)(C_2 + \Delta C_2) \tan(k_2 a) \tan(k_1 a)} \right) \right] \\ &\quad \sin(k_1 d_1) \sin(k_2 d_2) \end{aligned} \quad (17)$$

where

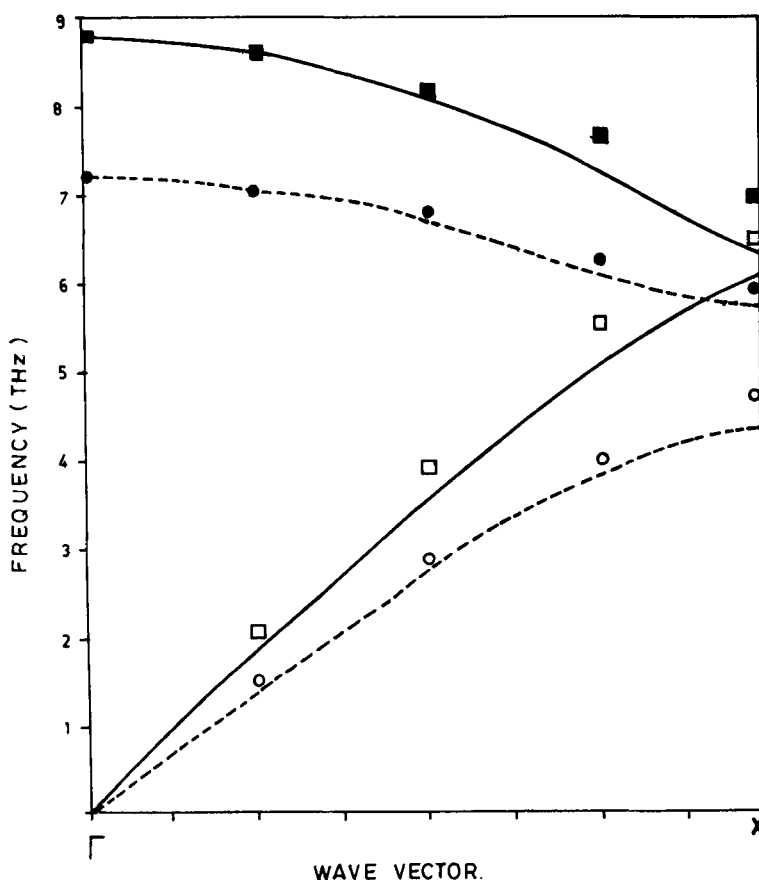
$$A = \frac{2(C_1 + \Delta C_1) - m_j \omega^2}{2(C_2 + \Delta C_2) - m_j \omega^2}.$$

### 3. Results and discussion

In the present model, we have considered only the nearest neighbour interaction. The force constants  $C_i$  can be calculated from the zone centre LO phonon mode for both GaAs and GaSb. The strain energy introduces a small change in the force constant (see (1)), which has been evaluated from the measured data on elastic constants and parameters of deformation potentials [14]. The calculated values of force constants ( $C_1$  and  $C_2$ ) are 2.310 and 2.200 N/m for GaAs and GaSb, respectively. The parameters used to calculate the change in force constants due to change in layer thickness are given in table 1. The calculated phonon dispersion curves (PDC)

**Table 1.** Inplane lattice constant ( $a_{||}$ ), strain components and change in force constants for  $(\text{GaAs})_{n_1}(\text{GaSb})_{n_2}$  SLSL.

No. of layers $n_1$	$n_2$	$a_{  }$ (Å)	$\epsilon_{xx}$ (dimensionless)	$\epsilon_{zz}$	$\Delta C_1$ (N/m)
4	4	5.800	0.0265	-0.0240	-0.270
4	8	5.870	0.0392	-0.0354	-0.398
4	12	5.910	0.0466	-0.0422	-0.474
4	16	5.940	0.0574	-0.0466	-0.523
4	20	5.960	0.0549	-0.0496	-0.558

**Figure 1.** Calculated phonon dispersion curves of GaAs (—) and GaSb (--) compared with experimental data taken from [18] and [19] respectively.

for GaAs and GaSb are presented in figure 1 and compared with neutron scattering results [18,19]. For simplicity, in the present calculations, we have considered the longitudinal modes only. It is worth pointing out that the present simple one-dimensional model can reproduce adequately the gross features of the measured PDC of these compounds along the  $\Delta$  direction. In figure 2 we have plotted the variation of lattice constant of  $(\text{GaAs})_4(\text{GaSb})_n$  and  $(\text{GaAs})_n(\text{GaSb})_4$  as a function of layer thickness for each component. The variation of lattice constants with layer thickness

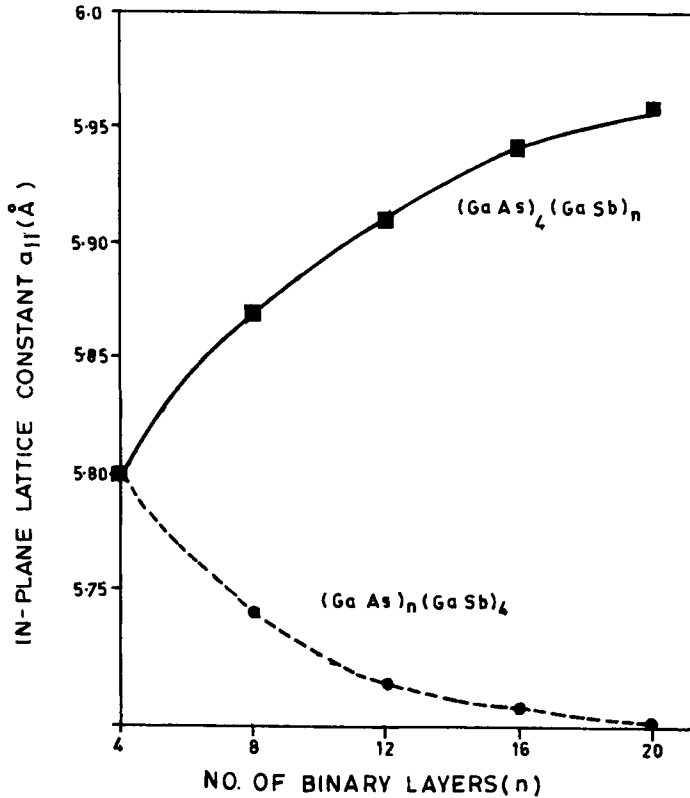


Figure 2. Inplane lattice constant as a function of number of binary layers for  $(\text{GaAs})_n(\text{GaSb})_4$  and  $(\text{GaAs})_4(\text{GaSb})_n$  SLSL.

can easily be explained from the fact that with the increase of layer thickness of GaSb, the volume of the unit cell increases. This results in the increase in inplane lattice constant. Similar argument holds for the decrease in lattice constant for  $(\text{GaAs})_n(\text{GaSb})_4$ .

Figure 3 depicts the PDC of  $(\text{GaAs})_{12}(\text{GaSb})_{12}$  strained and unstrained SLSL. The phonon dispersion curves for  $(\text{GaAs})_{12}(\text{GaSb})_{12}$  have been calculated from (17) which show the dispersion relation (frequency  $\omega$ ) as a function of reduced wave vector (QD). These curves are plotted in figures 3(a) and (b) for unstrained and strained SSL respectively. For unstrained SSL,  $\Delta C_i$  has been taken to be zero. The interesting feature, as can be noted from figure 3(b), is that the inplane strain substantially suppresses the confined optical GaAs-like LO mode, but does not affect much the propagating acoustic modes. In general, the nature of the PDC of the SLSL remains unchanged due to strain, except lowering of the highest LO frequency.

In order to understand the above aspect quantitatively, in figure 4 we have plotted the variation of the highest GaAs LO frequency, as a function of layer thickness. In doing such analysis, we have started with  $(\text{GaAs})_4(\text{GaSb})_4$  and increased the number of binary layers in one component, keeping the other constant. The figure 4 shows nearly similar trend in variation as in figure 2. A comparison of these two figures reveals that the change in volume, associated with the change in lattice constants increases (or decreases) the highest LO mode of GaAs. It is also expected that after a certain critical value of the number of binary layers, (or thickness) the constituents

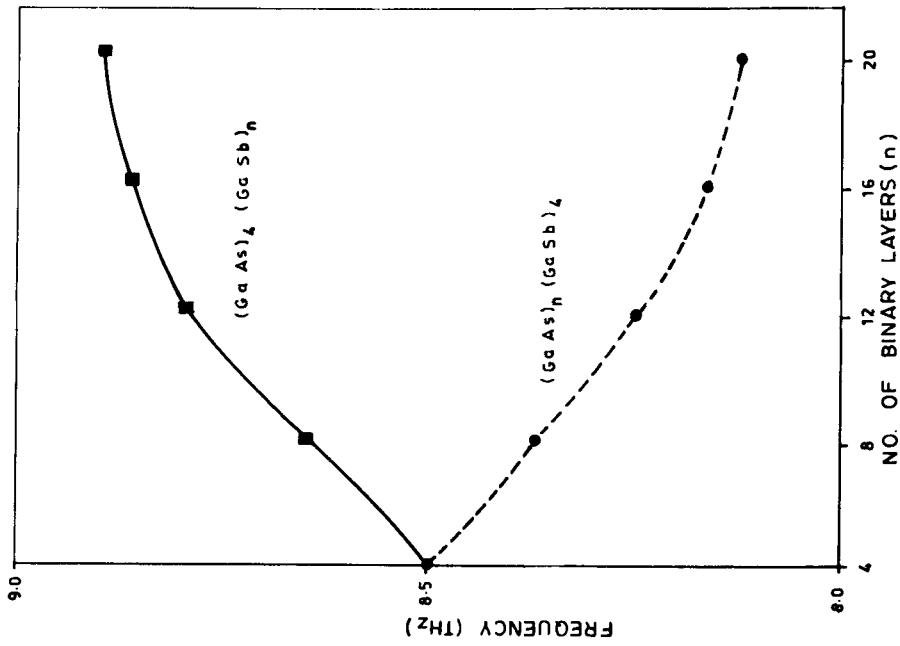


Figure 4. Highest GaAs LO frequency as a function of number of binary layers for  $(\text{GaAs})_n(\text{GaSb})_4$  and  $(\text{GaAs})_4(\text{GaSb})_n$  SLSL.

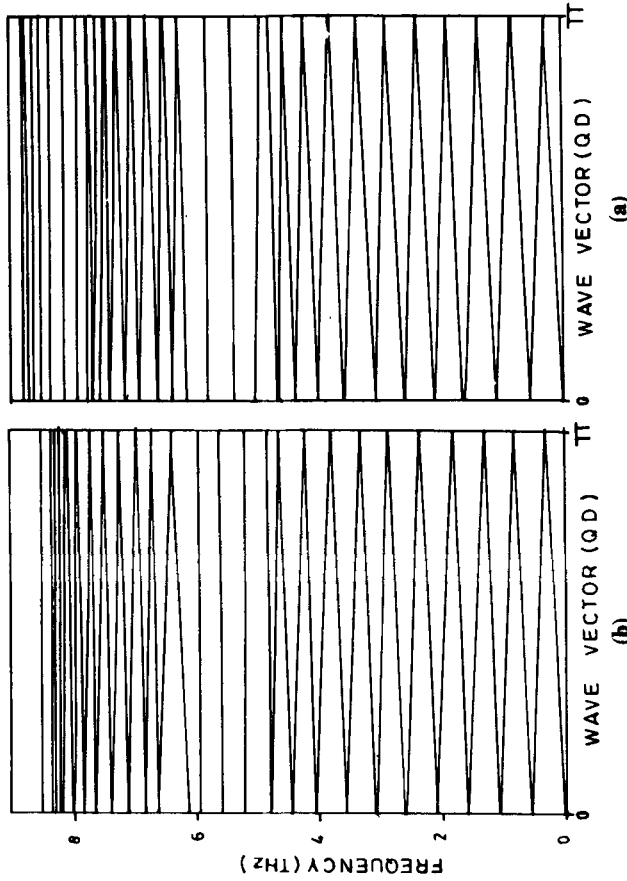


Figure 3. Phonon dispersion curves of  $(\text{GaAs})_{12}(\text{GaSb})_{12}$  unstrained (a) and  $(\text{GaAs})_{12}(\text{GaSb})_{12}$  strained (b) SLSL.

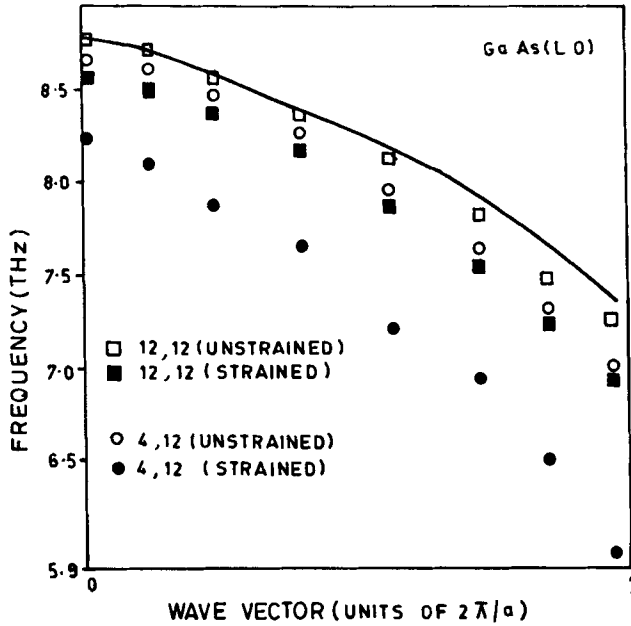


Figure 5. Dispersion curve for GaAs LO mode for different layer thicknesses. Solid line: bulk GaAs.

will behave like bulk materials, thereby no further depression (or increase) in this mode will be observed.

In figure 5, we have plotted the highest LO mode frequency of GaAs as a function of reduced wave vector. The LO dispersion curve for GaAs in unstrained  $(\text{GaAs})_{12}$   $(\text{GaSb})_{12}$  is quite similar to the bulk material. However, inclusion of strain substantially reduces the frequency. In addition, to understand the effect of strain generated due to unequal binary layers, we have also plotted the GaAs-LO mode for  $(\text{GaAs})_4(\text{GaSb})_{12}$  superlattices. It is clearly seen that the strain due to unequal binary layers is also significant and affect the PDC of SLSL. The lowering of the GaAs-LO mode, obtained from the present investigation can be justified from the arguments already given for InGaAs/GaAs superlattice [12]. However, for the GaAs-GaSb SLSL no measurement of zone-centre phonon has been reported so far. We emphasise the need of measurement of the phonon properties of such systems for a quantitative verification of our results.

In conclusion, we have reported, for the first time, the results of our investigations on the phonon properties in SLSL, using a simple theoretical model. The strain energy, in general increases (or reduces) the volume, thereby affecting the highest GaAs like LO mode.

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