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Phonon confinement in InAs/GaSb superlattices

D. Berdekas and G. Kanellis
Physics Department, University of Thessaloniki, 540 06 Thessaloniki, Greece
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Shell-model calculations of the zone-center phonons of InAs/GaSb superlattices reveal that their confinement characteristics depend on the direction of the atomic displacements and the relative orientation of the interface bonds. Similar behavior is found for certain modes even in the frequency range of bulk acoustic phonons. These findings are attributed to different elastic coupling between the two constituent layers. Interface modes localized at the two different interfaces Ga-As and In-Sb are discussed.

The electronic properties of InAs/GaSb superlattices (SL's) have been extensively studied over the past ten years,[1-3] while their dynamical properties are still under investigation. To our knowledge, these systems have not been studied either by infrared or Raman spectroscopy up to now. The phonon dispersion and confinement in long-period InAs/GaSb SL's was examined by Fasolino, Molinari, and Maan, using the linear-chain model.[4-6] Similar features have been observed by Akera and Ando[7] again using the linear-chain model but the envelope-function formalism for long-wavelength phonons. In all these cases only one type of interface is assumed, either Ga-As or In-Sb, which corresponds to higher-symmetry SL's in three dimensions than the more natural case where both types of interfaces appear alternately. Moreover, the ambiguities in the choice of force constants in Refs. 4–6 or the approximations involved in Ref. 7 may influence the accuracy of the eigenvectors more than the calculated frequencies. In particular, confinement and/or quasiconfinement of phonons in regions where the bulk continua of frequencies overlap has not been studied in detail. Other calculations, using three-dimensional models,[8,9] report on the phonon dispersion in short-period SL's. Their interest is mainly concentrated on the interface modes and on the anisotropy of the phonons propagating parallel and perpendicular to the SL axis.

In this paper we study the confinement of phonons in an 8/8 SL, for phonons at the center of the first Brillouin zone (BZ), for both longitudinal and transverse phonons. It is found that the confinement characteristics of transverse phonons depend on the relative orientation of the atomic displacements with respect to the direction of the interface bonds. These bonds provide either a weaker or stronger coupling between the eigenmodes of the two different layers, which results in a larger or smaller mutual transfer of energy, depending also on the eigenfrequencies of the modes.

The calculation is based on a ten-parameter valence-overlap shell model (VOSM),[10] with a slightly modified valence force field.[11] The model employs three electric parameters, Z, Y_1, and Y_2, to describe the long-range interactions, two core-shell coupling parameters, k_1 and k_2, and five valence-force-field parameters, λ, $k_{r_1\theta}$, $k'_{r_1\theta}$, $k_{r_2\theta}$, and $k'_{r_2\theta}$, to describe the short-range interactions. The values of the parameters are obtained by a least-squares fitting to the experimentally known phonon dispersion of the bulk compounds InAs (Ref. 12) and GaSb.[13] They are found to be for InAs (GaSb): $Z=2.00$ (kept constant for both compounds), $Y_1=4.930$ (4.277) and $Y_2=-2.513$ (-3.502) in proton charges, $k_1=13.790$ (15.111) and $k_2=4.829$ (4.448), $\lambda=1.718$ (1.717), $k_{r_1\theta}=0.116$ (0.171) and $k'_{r_1\theta}=-0.179$ (-0.195), $k_{r_2\theta}=-0.078$ (-0.052) and $k'_{r_2\theta}=-0.008$ (-0.003) in 10^5 dyn/cm. The mean standard deviation of the fitting procedure is 4.1 cm^{-1} for InAs and 3.3 cm^{-1} for GaSb.

The phonon frequency ranges of the two compounds partly overlap. Therefore, in a SL formed by the above compounds, the modes with frequencies inside the overlapping frequency ranges of the bulk constituent compounds are expected to be extended modes, but it turns out that this is not the case for all of these modes. Furthermore, two different interfaces, consisting of Ga-As and In-Sb bonds, respectively, appear alternately. The optic modes of the interfaces are found either above the optic frequency ranges of both layers (Ga-As interface modes), or in the gap between their optic and the acoustic modes (In-Sb interface modes).

The SL interactions are obtained from the bulk interactions of the constituent compounds using a method described in detail in Ref. 14. In this work, we follow a slightly different procedure in order to correctly introduce the necessary self-term corrections to the SL dynamical matrix. We calculate separately the short- and long-range interactions for the SL and combine them to obtain the SL dynamical matrix, before the elimination of the "electronic" degrees of freedom. The interlayer short-range interactions between the pairs In-Ga and As-Sb are taken equal to the average interactions of the corresponding pairs In-In and Ga-Ga, and As-As and Sb-Sb, respectively. Interactions between the pairs In-Sb and Ga-As are taken equal to the average of In-As and Ga-Sb interactions and the rest of the short-range interactions are taken equal to the corresponding ones in the bulk compounds.

The SL Coulomb coefficients are found from the transformation of the corresponding coefficients of the zinc-blende structure, calculated at the same points of the BZ as the short-range interactions. To obtain the core-core, core-shell, and shell-shell long-range interactions in the SL, we multiply the SL Coulomb matrix with the proper

core and shell charges of the corresponding ions. The lattice constant of the underlying zinc-blende lattice is assumed to be equal to 6.07 Å.

$(InAs)_n/(GaSb)_m$ SL's along (001) appear in two different orthorhombic space groups depending on the number of layers each compound contributes to the SL. If $n+m$ is even, the space group is C_{2v}^1 ($Pmm2$), while if $n+m$ is odd the space group is C_{2v}^{20} ($Imm2$). In both types the $0x$, $0y$ axes of the SL unit cell are along the $\mathbf{x}_0+\mathbf{y}_0$ and $\mathbf{x}_0-\mathbf{y}_0$ directions, respectively, of the underlying zinc-blende structure. The bonds of both types of interfaces lie on the $y0z$ plane. In the case where both interfaces are of the same type the symmetry is tetragonal and the interface bonds lie alternately on the $y0z$ and $x0z$ planes. To account for this fact, two different force constants are used alternately at the interfaces in Ref. 7 for transverse phonons.

Inside the unit cell of P-type lattices, cations occupy a and d Wyckoff sites while anions occupy b and c sites. In the I-type lattices, cations occupy a Wyckoff sites, while anions occupy b sites. All these sites have $mm2$ symmetry and each one contributes three modes to the vibrational degrees of freedom which belong to A_1, B_1, and B_2 irreducible representations.

For phonons propagating along the SL axis, the atomic displacements of A_1 modes are parallel to this axis, while for B_1 and B_2 the displacements are parallel to the $0x$, $0y$ axes of the unit cell, respectively. Therefore, A_1 and B_2 optic modes involve mainly stretching of the interface bonds, since in both cases the atomic displacements lie on the $y0z$ plane, while optic modes of B_1 symmetry involve mainly bending of the interface bonds. For the latter type of vibrations the characteristic frequencies of the interface layers fall much closer to or inside the frequency range of the bulk modes. Hence folded TO modes of B_1 symmetry are less influenced by the presence of the interface as compared to the corresponding modes of B_2 symmetry, for which the interface is rather "hard."

In Fig. 1, the frequency ranges of the longitudinal phonon branches of the constituent binary compounds are shown together with the corresponding ranges in GaAs and InSb calculated using both sets of model parameters. In the same figure the zone-center SL modes of A_1 symmetry are also shown and the values of frequencies of bulk LO modes in InAs and GaSb folded to the center of the SL BZ. The overlapping range of bulk LO phonons is defined from LO(Γ) and LO(X) frequencies of GaSb at 235.9 and 211.7 cm^{-1}, respectively. The corresponding phonons for InAs have frequencies 243.5 and 202.2 cm^{-1}, respectively. In order to compare the SL modes, we have calculated the sum of the squares of the displacements in each layer and divided it by the same sum in both layers. The resulting percentage for each layer is considered as a measure of the "energy" concentrated in the layer. It turns out that in some confined modes, whose atomic displacements evanescently decay into the second layer, a higher percentage of their energy is leaking into that layer than in modes with nondecaying atomic displacements into the second layer.

In the optic frequency range, the highest-frequency A_1 mode at 252.5 cm^{-1} (IF_1 in Fig. 1) is a sharply localized

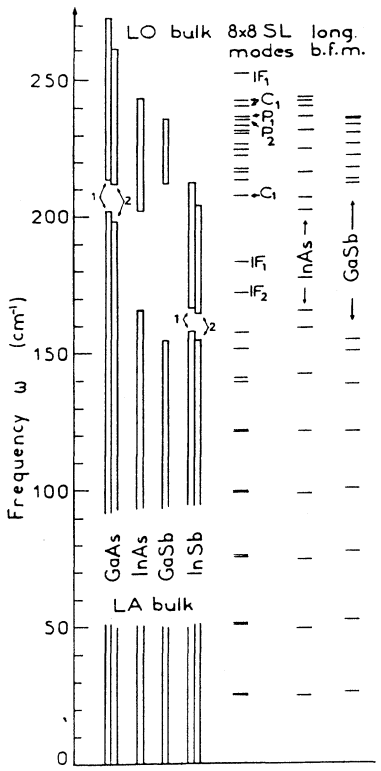

FIG. 1. Frequency ranges of the longitudinal bulk branches in the four binary compounds (left-hand side). For GaAs and InSb, these are calculated using both sets of force constants, those of InAs (column 1) and those of GaSb (column 2). SL mode frequencies for A_1 modes (middle) and frequencies of the longitudinal bulk folded modes (long b.f.m.) of InAs and GaSb (right-hand side). The labeling of the modes is explained in the text.

mode at the GaAs interface [the displacement pattern is shown in Fig. 2(a)]. The A_1 modes outside the overlapping range, at 242.6, 240.4, and 207.3 cm^{-1}, are well confined in the InAs layer (C_1 in Fig. 1). In these modes the energy percentages in the InAs layer are 99.6%, 98.5%, and 97%, respectively, while most of the remaining energy is concentrated at the interfaces. The mode labeled P_1, almost 0.5 cm^{-1} above the overlapping range, propagates with very small amplitude inside the GaSb layer. This situation is reversed for the mode at 235.3 cm^{-1}, labeled P_2 in Fig. 1, which possesses 99.4% of its energy in the GaSb layer, while the rest of it is distributed in the InAs layer. Its displacement pattern is shown in Fig. 2(b). Such modes, having almost all of their energy in one layer but not evanescently decaying displacements in the other, may be called quasiconfined or pseudoconfined modes.[15] The frequency of the P_1 mode is closer to that of the bulk InAs LO folded mode, while that of the P_2 mode is closer to the frequency of the corresponding GaSb mode. Similar observations have been reported in Refs. 5–7. In the bulk acoustic-phonon range, all A_1 modes of the SL are extended and their frequencies lie very close to the frequencies of the bulk folded modes of

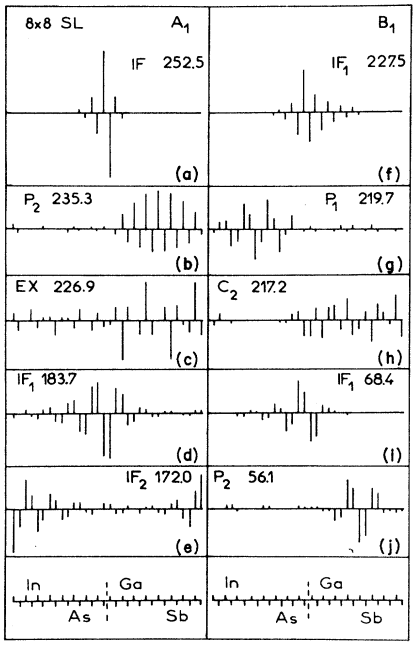

FIG. 2. Displacement patterns for some SL modes of A_1 and B_1 symmetries. The positions of the ions are shown in the lower part of the figure.

both compounds. At the top of this range we find two interface modes (Ga-As labeled IF_1 and In-Sb labeled IF_2). Their displacement patterns are shown in Figs. 2(d) and 2(e), respectively. All the unlabeled modes of Fig. 1 are extended modes.

Figures 3(a) and 3(b) show the results for the bulk and SL transverse modes. The overlapping range for bulk TO phonons [Fig. 3(a)] is extended from 225.0 to 219.3 cm^{-1}, which are the values of TO(Γ) and TO(X) for InAs. The corresponding frequencies for GaSb are 226.2 and 208.9 cm^{-1}. This range contains seven modes originating from InAs and only two from GaSb. In a total of eight B_2 SL modes with frequencies in this range, one is a true confined mode in the InAs layer, labeled C_1 in Figs. 3(a) and 4(c), and three of them may be characterized as pseudoconfined in the same layer, labeled P_1 in Fig. 3(a), as less than 0.5% of their energy is leaking into the GaSb layer. The frequencies of these SL modes are very close to frequencies of InAs bulk folded modes. The displacement pattern of one of them is shown in Fig. 4(d).

Above the upper end of this range a mode confined in the GaSb layer is found, labeled C_2 in Fig. 3(a). Its displacement pattern is shown in Fig. 4(b). Close to the lower end both B_1 and B_2 modes are P_1 in character [Figs. 2(g) and 4(e)]. The highest-frequency B_2 and B_1 modes are localized at the GaAs interface [IF_1 in Figs. 2(f), 3(a), and 4(a)]. The B_2 mode labeled IF_2, lies in the gap between optic and acoustic frequency ranges, and it is localized at the InSb interface [Figs. 3(a) and 4(f)]. The different confinement characteristics of these transverse modes with different symmetries reflect the anisotropy of the orthorhombic SL.

Finally, the results for the folded TA modes of both symmetries are presented in Fig. 3(b). For the B_1 mode,

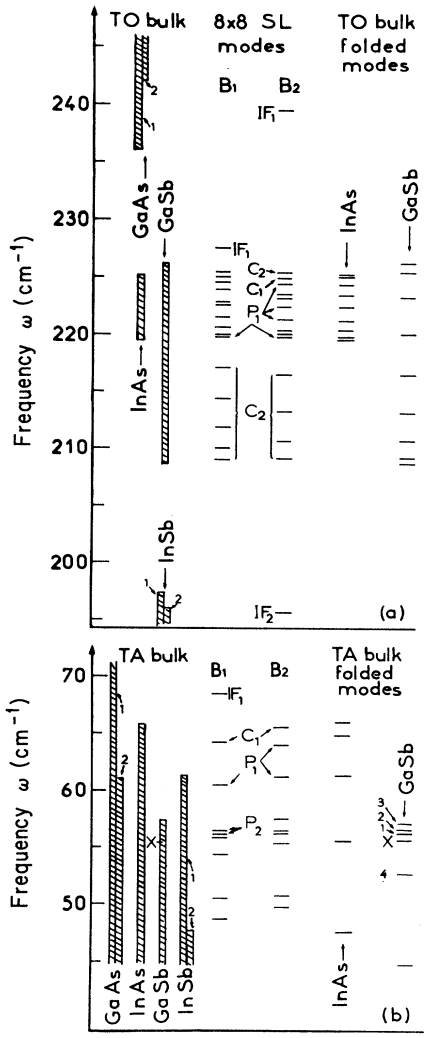

FIG. 3. (a) Frequency ranges of the TO bulk branches in the four binary compounds (left-hand side). For GaAs and InSb, these are calculated using both sets of force constants, those of InAs (column 1) and those of GaSb (column 2). Frequencies of the SL modes of B_1 and B_2 symmetry are in the middle, and frequencies of the folded TO modes of bulk InAs and GaSb on the right-hand side. (b) The same information as in (a) for the acoustic region. The numbers in the rightmost column indicate the sequence of folded modes from the X point towards the zone center. The labeling of the modes is explained in the text.

labeled IF_1 in Fig. 3(b), the motion is localized at the GaAs interface [Fig. 2(i)], and therefore has the higher frequency in this range (68.4 cm^{-1}). For the mode of B_2 symmetry at 61.0 cm^{-1} [Figs. 3(b) and 4(g)], a significant amount of energy, almost 30%, is concentrated at the GaAs interface. Both modes may be considered as originating from the doubly degenerate TA(X) of bulk GaAs which has been split into two modes of different symmetry.

It should be noted that transverse-acoustic modes of bulk GaSb along $(0,0,\xi)$, for the reduced wave vector $\xi=0.75$, 0.625, 0.875, have higher frequencies than TA(X) of the same compound. These points are labeled

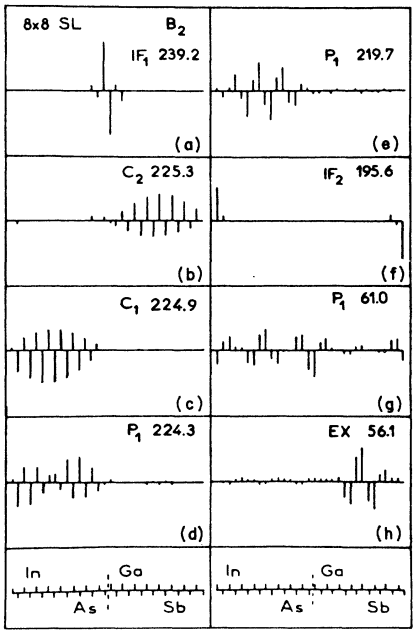

FIG. 4. Displacement patterns for some SL modes of B_2 symmetry. The positions of the ions are shown in the lower part of the figure.

3, 2, 1, and X at the right-hand side of Fig. 3(b). The higher frequency belongs to the bulk transverse-acoustic phonons at $\xi=0.75$ (56.8 cm^{-1}). All of the modes above this frequency originate from InAs, but only two of them, close to TA(X), are well confined in the InAs layer. In thicker SL all modes above 56.8 cm^{-1} are confined in this layer. At the upper limit of the acoustic overlapping range, we find two modes of B_1 symmetry with frequencies almost the same with those of GaSb at $\xi=0.625$. Both modes may be characterized as pseudoconfined in GaSb [P_2 in Fig. 3(a)]. One of them is shown in Fig. 2(j). The B_2 mode at 56.1 cm^{-1} is considered an extended mode [Fig. 4(h)].

All of these features could be explained by the following idealized model: The two layers of the SL may be considered independent oscillators with frequencies ω_1 and ω_2 which are weakly coupled through the interface layers by a force constant g. These frequencies may be taken to be the frequencies of the corresponding bulk branches folded to the center of the first BZ, as they are given in Figs. 1 and 3. This coupling slightly raises the eigenfrequencies of the two oscillator systems to ω_1' and ω_2'. Assuming that a mode of the SL has frequency ω_A coinciding with one of the latter two frequencies, the mode appears with maximum amplitude A into that layer (1 or 2) and a much smaller amplitude B into the other layer. It can be shown that, to second order in the coupling g, the ratio of the vibrational amplitudes is

$$\frac{B}{A}=\frac{2g}{m_A(\omega_A^2-\omega_B^2)}.$$

As can be seen in Fig. 3, the folding of the InAs TO branch in a narrow frequency range results in a dense spectrum for the oscillator InAs layer, as compared to the spectrum of the oscillator GaSb layer. Hence, SL modes in the overlapping frequency range have, in general, frequencies closer to InAs TO folded ones. As it has already been discussed, B_1 modes see "softer" interfaces, or for B_1 modes the coupling of the two layers is stronger than for B_2 modes. This explains the stronger localization of modes of the latter symmetry into the InAs layer in the high-frequency range. For folded TA modes the situation is reversed and B_2 modes show stronger coupling. The oscillator spectrum is more dense for the GaSb layer and B_1 modes localize stronger into that layer. For A_1 modes the oscillator spectrum is more dense for the GaSb layer too (Fig. 1), and modes localize preferably into that layer. In this case the coupling of the two layers is comparable to that for B_2 modes and, apart from the elastic properties of the interfaces, it must be also influenced by the electric macroscopic field in the SL. For SL with thicker layers, more optic modes of A_1 symmetry tend to localize into the GaSb layer, because of the more dense spectrum of the folded LO modes in that layer, while for B_2 symmetry modes, they tend to localize into the InAs layer. B_1 modes inside the overlap range remain extended.

In the case where both interfaces are of the same type as those in the systems studied in Refs. 4–7, transverse modes propagating along the SL axis are degenerate and their behavior, with respect to confinement, is analogous to the B_1 modes of the present case. Longitudinal modes for wave vectors in the same direction also show a behavior similar to the present case.

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