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Calculated superlattice and interface phonons of InAs/GaSb superlattices

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The phonon spectrum of InAs/GaSb superlattices is calculated with a linear-chain model with interplanar force constants. Apart from confined and extended modes, as found also in GaAs/GaAlAs superlattices, this system shows new modes localized at the interface. These latter modes depend crucially on the nature (InSb or GaAs) of the interface and some of them do not coincide with any other possible superlattice mode. This fact would make them easily experimentally identifiable.

Molecular-beam epitaxy permits the growth of very thin layers of different lattice matched semiconductor materials with interfaces almost perfect at an atomic scale. This allows for the creation of systems with both new electronic and lattice dynamical properties. Here we will focus on the latter properties, which have been studied up to now almost exclusively for GaAs/GaAlAs layered structures.[1-6] This system possesses a common anion in both materials, which at the interface is shared between successive layers, and makes the interface in some sense not "sharply" localized. Intrinsically new phonon modes should arise for systems where this is not the case. As an example we will concentrate here on InAs/GaSb (100) superlattices, which can be grown with high crystalline quality[7] and which have well-established electronic properties.[8] This system is particularly interesting from the lattice dynamical point of view, since the mass of the unit cell of InAs and GaSb is roughly the same, while the pairs of atoms which may be present at the interface—either InSb or GaAs—have, respectively, much heavier and lighter masses.

In the following we will investigate theoretically the consequences of this fact and point out the essential differences with respect to GaAs/GaAlAs. In particular, we will show that the presence of almost overlapping ranges of frequencies for the optical bulk modes of InAs and GaSb, together with rather well separated ranges of frequencies for the vibrations of the atoms at the interface, produces a wealth of possible phonon modes, namely (i) phonons confined in one of the two constituents, (ii) phonons extending through both constituents, and (iii) phonons localized at the interface.

The lattice dynamics of a (100) stacking of atomic planes can be mapped onto that of a linear chain[1] whose force constants are thought of as interplanar force constants (Fig. 1), provided that different values are used for different polarizations and directions of propagation. Since it has been

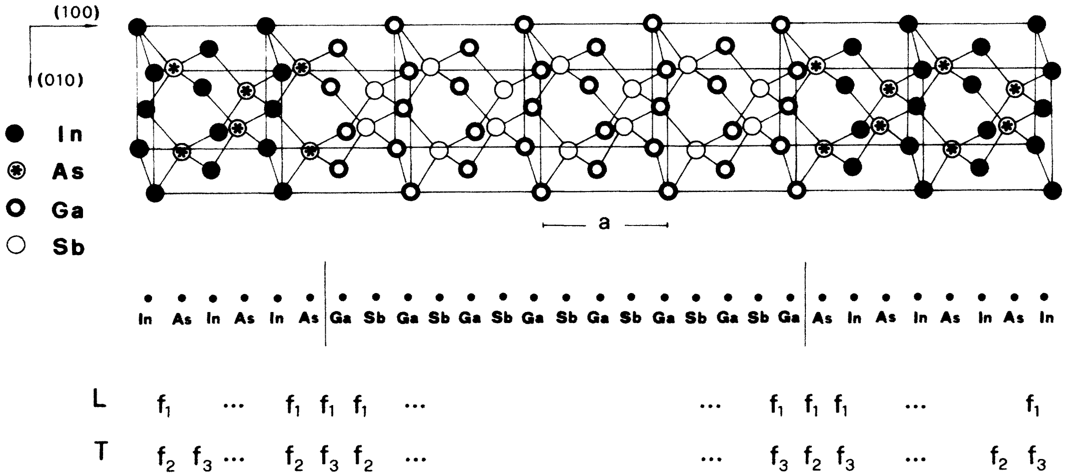

FIG. 1. Mapping of a three-dimensional (100) grown superlattice onto a linear chain for the case of a GaSb/InAs (15/13 atomic planes) superlattice (GaAs at all interfaces). The corresponding force constants for longitudinal (L) and transverse (T) vibrations (in 10^5 dyn/cm) are $f_1 = 0.800$, $f_2 = 1.250$, $f_3 = 0.120$. Note that InSb at all interfaces is obtained by moving the interfaces by $\frac{1}{4}a$, where a is the lattice constant.

pointed out[9,10] that the differences in the phonon spectra of III-V compounds are primarily due to their different masses and not to a different bond, we assume the same value for the force constants of the materials we are dealing with, and only scale their actual interactions according to their masses. This assumption makes it very easy to deal with the superlattice geometry. Taking the same force constants also at the interface, where either InSb or GaAs bonds can be present, means implicitly assuming that these bonds have the same length as they would have in bulk InSb or GaAs, even though the lattice constant is 7% longer (shorter) than that of InAs and GaSb. It has been shown that this assumption is not incompatible with ion-beam channeling experiments.[11]

We then solve the usual dynamical problem

$$\sum_j [(M_i M_j)^{-1/2} D_{ij} - \omega^2 \delta_{ij}] = 0 \ ,$$

where D_{ij} is the dynamical matrix; M_i, M_j are the masses of the atoms in the ith, jth planes and $i,j = 1, \ldots, N$ with N equal to the number of planes in the new superlattice unit cell. Within the nearest-neighbor approximation the mapping of the three-dimensional problem onto a linear chain requires one force constant for the longitudinal modes and two for the transverse. The nonequivalence of the nearest-neighbors force constants for transverse vibrations reflects the fact that along (100) each plane has two neighboring planes with different atomic arrangements (Fig. 1). In particular, one force constant is much stronger than the other.

Since it is not our main interest at this stage to provide a detailed description of the bulk phonons, we use first-neighbors force constants similar to those used in the past[1] for GaAs/AlAs superlattices. Our results describe the transverse modes better than the longitudinal ones, insofar as the relative position of the observed edges of allowed bulk phonon frequencies is reproduced. The correspondence between calculated and observed absolute energies is less good, as can be seen by a comparison of Fig. 3 with Table I.

TABLE I. Experimental longitudinal and transverse phonon frequencies at the high symmetry points along the (100) direction for the four bulk compounds. Unless specified, measures are taken at 300 K.

	InAs[a] ω (cm^{-1})	GaSb[b] ω (cm^{-1})	InSb[c] ω (cm^{-1})	GaAs[d] ω (cm^{-1})
LA (X)	160	166.2	143.2	226.4
LO (X)	203[e]	211.4	158.2	240.4
LO (Γ)	238.6	233.1	196.5	284.7
TA (X)	53	56.5	37.3	78.6
TO (X)	216	211.8	179.2	251.7
TO (Γ)	217.3	228.8	184.5	267.1

[a] First- and second-order Raman scattering, from Ref. 12.
[b] Neutron scattering, from Ref. 13.
[c] Neutron scattering, from Ref. 14.
[d] Neutron scattering, from Ref. 15.
[e] $T = 100$ K.

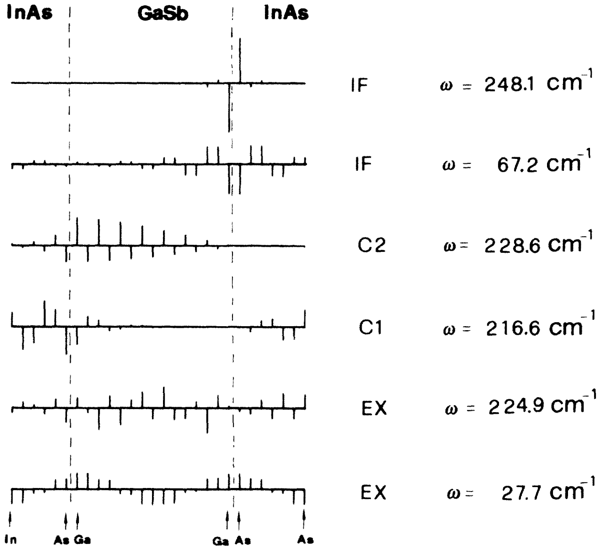

FIG. 2. Displacement patterns of some characteristic transverse phonon modes with the corresponding energies for the superlattice of Fig. 1: confined in InAs (C1), confined in GaSb (C2), localized at the interface (IF), extended through the superlattice (EX).

In Fig. 2 the transverse displacement patterns at Γ are shown for the superlattice with GaAs at all interfaces (Fig. 1). The three classes of modes previously mentioned can be seen: confined (C1, C2), extended (EX), and localized at the interface (IF). The corresponding frequencies are shown in Fig. 3(b) together with the windows of allowed bulk transverse phonons [Fig. 3(a)] obtained within our model for constituents and interface compounds. The bulk optical continua reduce to almost dispersionless discrete modes, which have extended or confined character depending on whether their frequency is allowed for both InAs and GaSb or just one of them. The acoustical modes are extended and are grouped in almost degenerate doublets at Γ as a consequence of folding. The number of modes at Γ and their energies depend of course on the thickness of the layers. Besides these features that are common to GaAs/GaAlAs superlattices, two additional interface modes show up in the spectrum. One falls in the region of allowed optical frequency of GaAs and is sharply localized on the atoms forming the interface, as shown in Fig. 2. The other falls in the acoustical range of frequency of bulk GaAs which ends higher than the edges of InAs and GaSb. The corresponding displacement pattern is mainly localized at the interface, but falls off slowly in InAs and GaSb, being still close in energy to the allowed bulk continua. For layer thicknesses large compared with the spatial extension of the interface modes, their frequency is strictly independent of the layer thickness. Note that for a given polarization only one interface corresponds to tightly bound planes and generates transverse interface modes. If we put InSb at all interfaces, we get the phonon spectrum displayed in Fig. 3(c). The "optical" interface mode has moved to a frequency inside the InSb TO continuum range with analogous displacement pattern, while the "acoustical" interface mode has disappeared, since the InSb acoustical continuum fully overlaps with the ones of InAs and GaSb. In the case of alternate GaAs and InSb interfaces, the results for a given polarization depend on which ones involve tightly bound planes in that polarization direction.

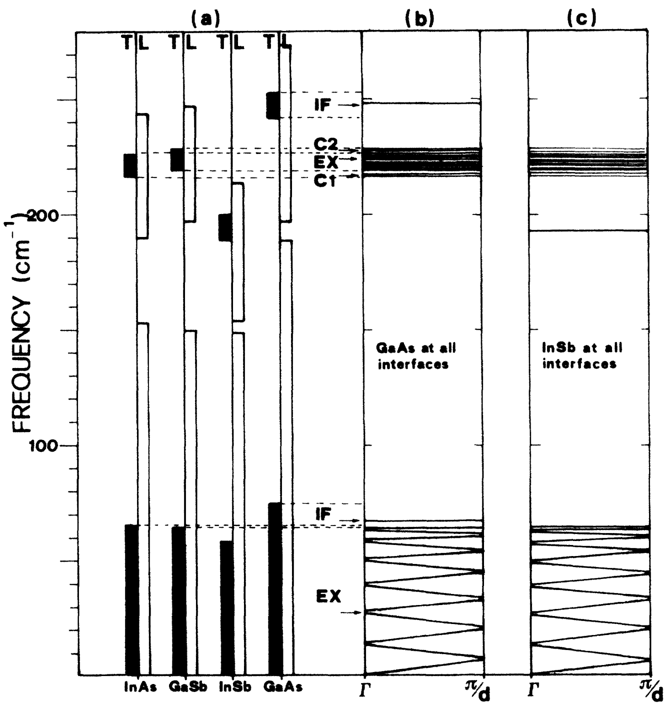

FIG. 3. (a) Calculated bulk transverse and longitudinal phonon continua for the four compounds, (b) transverse phonon spectrum of the GaSb/InAs (15/13) superlattice shown in Fig. 1 (GaAs at all interfaces), (c) same as (b) for a InAs/GaSb (13/15) superlattice with InSb at all interfaces. The arrows in (b) label the frequency of modes whose displacement patterns are shown in Fig. 2. The dashed lines illustrate how the character of the superlattice modes (C1, C2, IF, EX of Fig. 2) is strictly related to their energy with respect to the four bulk continua.

The appearance of interface modes is a mass effect peculiar to a situation in which the interface is intrinsically different from both constituents. It is indeed striking that the presence of just two atomic layers of a different compound at the interface is sufficient to give a sharply localized phonon mode in the window of allowed frequency of the corresponding bulk; the detection of such modes can give information about the interface atomic arrangement.

It should be noted that besides these "real" interface modes, other superlattice modes of macroscopic origin can appear, as has been reported[5] for GaAs/AlAs. These too have been referred to as interface modes because they are *originated* by the interface between two macroscopic media of different dielectric function, but they are not *localized* at the interface, as shown by the thickness dependence of their frequency. Since these macroscopic modes are bound to fall in the range of the bulk LO and TO phonons[16] (of InAs and GaSb in this case), they should not mask the localized interface modes.

Our calculation cannot directly be used to predict phonon energies in real superlattices because of the limited correspondence between the bulk experimental spectra and the calculated ones, which is a consequence of the approximations we adopted. However, we can use our results together with the existing bulk experimental data to attribute possible ranges of energies of the superlattice modes, i.e., propagating modes for energies which overlap with both InAs and GaSb bulk modes; confined phonon modes for energies at which bulk-phonon modes are allowed only in one of the two; localized interface modes in the range allowed for GaAs and/or InSb bulk phonons, depending on the nature of the interfaces. For easy reference in Table I we give the available experimental data for both bulk transverse and longitudinal phonons, even if they are not completely consistent as far as temperature and measuring technique are concerned.

In conclusion, we have shown that novel interface modes should exist in InAs/GaSb superlattices and that their frequency depends crucially on the nature of the interface. We have provided a physical picture that helps to identify these modes through their possible ranges of frequency and their thickness independence. In particular, if the interface is between In and Sb atoms, these modes have energies within the range of bulk InSb phonon spectra, and similarly for a GaAs-type interface. In both cases modes exist which are energetically distinct from any other superlattice mode and should therefore be experimentally observable.

Hence, standard phonon spectroscopies should be able to provide additional information for the characterization of interfaces on the atomic scale.

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