CALCULATED LONGITUDINAL SUPERLATTICE AND INTERFACE PHONONS OF InAs/GaSb SUPERLATTICES

A. Fasolino International School for Advanced Studies, Strada Costiera 11,I-34014 Trieste, Italy
E. Molinari C.N.R., Istituto O.M. Corbino, Via Cassia 1216, I-00189 Roma, Italy
and
J.C. Maan Max-Planck-Institut für Festerkörperforschung, H.M.L., 166X, F-38042 Grenoble Cédex, France

(Received 18 August 1986)

The longitudinal phonon spectrum and the associated Raman strength of (100) InAs/GaSb superlattices are calculated along the growth direction. Apart from confined and extended modes, as found also in GaAs/AlAs superlattices, this system shows new modes localized at the interface. The energy and the Raman strength of these latter modes depend crucially on the nature of the interface (InSb or GaAs) and suggest that they are experimentally observable.

Molecular Beam Epitaxy permits the growth of very thin layers of different lattice matched materials with almost perfect interfaces at an atomic scale. Here we will focus on the lattice dynamical properties of InAs/GaSb superlattices[1], which can be grown with high crystalline quality[2] and which have extensively studied electronic properties[3].

This system, contrary to the most studied GaAs/AlAs[4-9] system does not possess a common anion in both materials and this makes the interface sharply localized. Furthermore 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 interfaces - either InSb or GaAs - have respectively much heavier and lighter masses. The peculiarity of this interface has been shown experimentally with ion beam channeling experiments[10] although no final conclusion could be drawn about the type of interface(s) present. In a previous paper[1], we have shown that these two facts, namely the presence of a different compound at the interfaces and the occurrence of almost overlapping ranges of frequencies for the optical vibrations of InAs and GaSb leads to a variety of possible phonon modes, namely phonons confined in either InAs or GaSb, phonons extending to both layers, phonons localized at the interface.

In this paper we concentrate on the behaviour of longitudinal optical and interface modes which are more accessible experimentally. In order to have a realistic description of these modes and of their observability, we have included third neighbour interactions plus long range Coulomb interactions in the spirit of Ref. 11 and we have evaluated the Raman strength associated with all optical and interface modes. However, we would like to point out that the essential features concerning the optical modes and, in particular, the presence and behaviour of the interface phonons are already accounted for by a simple, nearest neighbour, model as the one used in Ref. 1.

The lattice dynamics of a (100) stacking of atomic planes can be mapped onto that of a linear chain whose force constants are thought of as interplanar force constants, provided that different values are used for different polarizations. Since differences in the phonon spectra of III-V compounds are mainly due to their different masses and not to a different bond[12] we choose as a start the same force constants for both InAs and GaSb and scale their actual interactions according to their masses because this makes the superlattice geometry easy to be dealt with. In particular when considering further than first neighbour interactions, this assumption becomes very useful in order to treat the interfaces, since for instance there would be no easy way to guess the appropriate interactions between two different cations (In and Ga) or anions (As and Sb).

In order to reproduce the LO phonon dispersion of the two components we need to extend the range of interactions to third neighbours. As a

0749-6036/87/020117+04 $02.00/0

starting point we have used the interplanar force constants, calculated for GaAs[13], using of course the appropriate (InAs and GaSb) masses. We find that, using these force constants as they are, the LO phonon energies at Γ are higher than those experimentally observed, although their dispersion is fairly well reproduced. To obtain agreement with experiments for either one of the materials these values have to be reduced. For our convenience we reduce the GaAs force constants by 20% in order to obtain good agreement for the GaSb LO spectrum. However, within this "mass" approximation, the LO(Γ) phonon of InAs is bound to fall slightly lower than the one of GaSb, contrary to the experiments where it is 5 cm^{-1} higher[14,15]. In order to obtain the right relative position of the InAs and GaSb LO phonon at Γ, we include a corrective Coulomb term following Ref. 11, to account for the difference of the In and As effective charges with respect to Ga and Sb. This difference is taken to be .21|e|. This procedure means that, although the set of force constants we use are supposed to take into account both short range and long range Coulomb interactions, only the latter ones are corrected for, when going from GaSb to InAs, through a different effective charge localized on the site and, once more, not through a different pair interaction. Hence the conceptual and practical simplicity of dealing with a superlattice and its interfaces is preserved, although the superlattice is now represented not only as a given sequence of masses but also of effective charges. The bulk longitudinal phonon spectra of GaSb and InAs calculated in this way are shown in Fig. 1 together with the experiments[14,15]

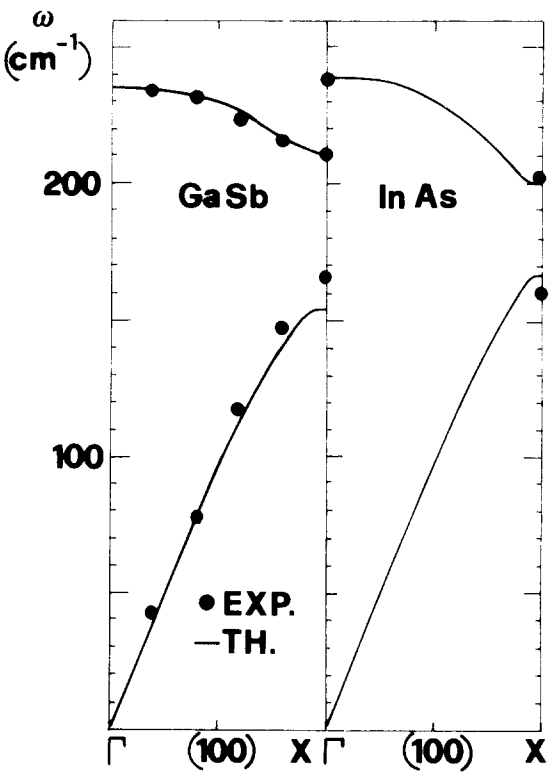

Fig. 1. - Calculated bulk phonon spectra of InAs and GaSb along the (100) direction (solid lines). Dots represent the experimental data of Ref. 14, 15.

In Fig. 2 we show the calculated longitudinal optical phonon spectrum at the Γ point of an InAs/GaSb superlattice with 8½ monolayers of each material and the two types of interfaces as mentioned before. It can be seen that almost all the discrete superlattice modes fall within the bulk LO continua of InAs and GaSb (also shown in the figure), and have similar energies for both types of interfaces. On the other hand the influence of the type of interface shows up clearly in the energy position of the interface modes, labelled 1, 2 and 3 in the figure, i.e. the ones falling outside the bulk continua. A clear discrimination between the two cases is the presence of two degenerate modes at energies above the bulk continua only in the case of GaAs interfaces, as a consequence of the light interface atoms. For the same reason a second interface mode of acoustical nature appears above the LA continua in this case. Correspondingly the two heavier In and Sb atoms give rise to an interface mode below the bulk LO continua.

From the normalized displacement patterns we have also calculated the Raman strength (R_{xy}) associated with all modes following Ref. 4 and 16, by assuming the same polarizability of the bonds for the two materials. The results are shown in Fig. 2 on top of the corresponding frequencies. For both types of interfaces we find two strong modes just below the upper LO edge of InAs and GaSb. These modes behave as confined modes. the upper being localized mainly in InAs, the lower in GaSb. While this behaviour was to be expected for the InAs-like mode, it is rather suprising to find a sharply localized GaSb-like mode at an energy where bulk continua overlap. The next two weaker observable modes, close to the strongest ones, are rather well confined in one or the other layer as well. This confined character gradually disappers for the modes in the centre of bulk continua, to reappear close to the lowest edge. Of course the modes

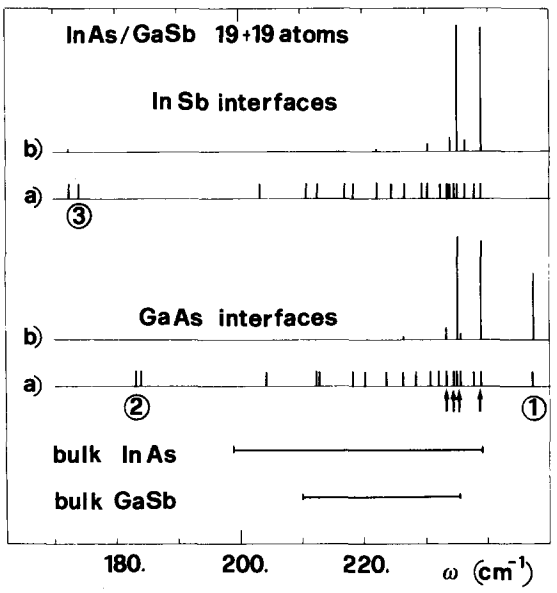

Fig. 2. - Calculated optical phonon spectrum of an InAs/GaSb superlattices of 8½ monolayer of each material and the two types of interfaces. a): energies at the point, b): corresponding Raman strength. The bulk optical continua of InAs and GaSb are also indicated. Interface modes are labelled 1, 2, 3.

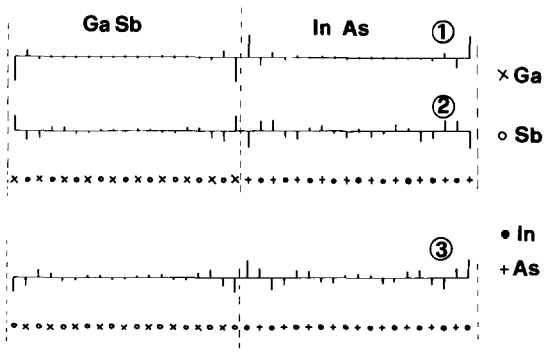

Fig. 3 - Displacement patterns of the B_2 interface modes for GaAs interfaces, modes 1 and 2, and for InSb interfaces, mode 3, corresponding to the frequencies shown in Fig. 2. The superlattice unit cell for the two types of interfaces is also shown.

with finite R_{xy} Raman strength are only the ones whose displacement pattern is even with respect to the centre of the layers, i.e. of B_2 symmetry. These modes bear a strong similarity to the ones observed in GaAs/GaAlAs superlattices.

Coming now to the interface modes we observe that the high energy GaAs interface mode (labelled 1) has a Raman strength comparable to that of the confined modes, while the one of the InSb interface mode (labelled 3) is much weaker. This fact can be understood by looking at the displacement pattern of the interface modes, shown in Fig. 3. There we can see that the interface mode 1 is sharply localized at the interface, whence its high Raman strength, while the other modes 2 and 3 have a much longer decay length. The very different decay lengths are related to their energy position; modes 2 and 3 are in fact close to the bulk acoustical continua, while mode 1 is far away from all other bulk modes. For the same reason, mode 1 is almost degenerate (one B_2 and one A_1 mode) and the degeneracy is lifted for 2 and 3 modes, as a consequence of the fact that the two interfaces are interacting, since their decay length is comparable with the layer thicknesses.

In conclusion we have calculated longitudinal optical confined and interface modes and the associated Raman strength of InAs/GaSb superlattices. The main conclusions can be summarized as follows: i) longitudinal interface modes outside the range of bulk LO continua are present, ii) the energy of these modes depends critically on the type of interface considered (GaAs or InSb), iii) their Raman strength, also strongly dependent on the type of interface, suggests that they should be observable.

Acknowledgement - We thank the AAE group of IDAC (CNR - Roma) for providing computer facilities and the GNSM-CISM for partial financial support.

1) A. Fasolino, E. Molinari, J.C. Maan, Phys. Rev. B33, 8889 (1986).
2) C.A. Chang, R. Ludeke, L.L. Chang and L. Esaki, Appl. Phys. Lett. 31 759 (1977).
3) See e.g.: L.L. Chang, J. Phys. Soc. Japan 49, Suppl. A, 997 (1980); J.C. Maan, in Infrared and Millimeter Waves, Vol. 8, Ch. 12, K.J. Button ed., Academic Press, 1982.
4) A.S. Barker, Jr., J.L. Merz and A.C. Gossard, Phys. Rev. B17, 3181 (1978).
5) J. Sapriel, B. Djafari-Rouhani and L. Dobrzynsky Surf. Sci. 126 197 (1983).
6) B. Jusserand, D. Paquet and A. Regreny, Phys. Rev. B30, 6245 (1984).
7) C. Colvard, R. Fischer, T.A. Grant, M.V. Klein, R. Merlin, H. Morkoc and A.C. Gossard, Superl. and Microstr. 1, 81 (1985).

8) A.K. Sood, J. Menendez, M. Cardona and K. Ploog Phys. Rev. Lett. 54, 2111 (1985); Phys. Rev. Lett. 54, 2115 (1985).
9) Sung-Kit Yip and Yia-Chung Chang, Phys. Rev. B 30, 7037 (1984).
10) W.K. Chu, F.W. Saris, C.A. Chang, R. Ludeke and L. Esaki, Phys. Rev. B 26, 1999 (1982).
11) E. Molinari, A. Fasolino, K. Kunc, Proc. 18th Conf. Phys. Semicond., Stockholm 1986; Proc. 2nd Int. Conf. on Superlattices, Microstructures and Microdevices (Göteborg, 1986).
12) K. Kunc and H. Bilz, Solid State Commun. 19, 1927 (1976).
13) K. Kunc and R.M. Martin, Phys. Rev. Lett. 48, 406 (1982); K. Kunc in Electronic Structure, Dynamics and Quantum Structural Properties of Condensed Matter, edited by J.T. Devreese et al. (Plenum Press, New York, 1985).
14) R. Carles, N. Saint-Cricq, J.B. Renucci, M.A. Renucci and A. Zwick, Phys. Rev. B 22, 4804 (1980).
15) M.R. Farr, J.G. Traylor and S.K. Sinha, Phys. Rev. B11, 1587 (1975).
16) B. Jusserand, D. Paquet, Superlattices and Microstructures 1, 61 (1985).