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Phonons at non-planar (III–V) semiconductor heterojunctions: II. GaSb/InAs (001)

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Abstract. We study the vibrational properties of the GaSb on InAs (001) single interface containing isolated narrow steps. We use a two-parameter valence force model and Green function techniques to obtain the phonon density of states at sites in the step region. Two types of interfaces are studied: with a Ga–As (light interface) or an In–Sb (heavy interface) bond; three types of interface modes have been identified, which serve as a signature of the type of interface. The presence of steps is shown to produce a boundary with mixed light–heavy characteristics. The interface phonons are confined within the step region and their frequency shifts from the planar boundary values due to confinement. Changes in the optical bands are qualitatively analysed by means of the atomic local environment.

1. Introduction

Interest in the vibrational properties of imperfect semiconductor heterojunctions and related layered systems has been motivated by the direct experimental evidence of the presence of interface steps and islands at all interfaces [1]; theoretical models for non-planar interfaces have been only recently been implemented in the analysis of the observed Raman [2–4] and photoluminescence [1b] spectra of quantum wells and superlattices. However, a systematic study of interface defects and their effect on the optical spectra is currently missing from the literature.

To this end, we have established in a previous paper [5] an atomic-scale formalism to study the vibrational properties of interfaces containing an isolated step and we have applied it to the GaAs/AlAs (001) interface with steps of various widths and orientations. Here, we use the same method [5] to investigate the role of steps on the vibrational spectrum of a GaSb/InAs (001) interface. High-quality GaSb/InAs (001) superlattices have been grown [6] and theoretical studies of their phonon states have been previously reported [7–9]. The GaSb/InAs layered structures have two qualitative differences with respect to the GaAs/AlAs (001) ones; namely, almost complete overlap of the optical bands, because of the unit cell masses being approximately equal, and the possibility of two new mass pairs (bonds) at the interface—Ga–As (light interface) or In–Sb (heavy interface). It has been demonstrated [7, 9] that the new interface bond can sustain vibrations with frequencies outside the two bulk continua, giving rise to interface localized modes. The frequencies of these modes are characteristic of the type of bond. We show here that the formation of interface steps causes mixing of the interface modes and produces a spectrum with the characteristic features of both types of interfaces; in addition, the bands arising from interface modes show modified shape and appear at different frequencies due to phonon confinement within the step.

The lattice dynamical model and the results for the planar interfaces are given in section 2; the stepped interfaces are studied in section 3, and finally, our conclusions are summarized in section 4.

2. Lattice model and planar interfaces

We describe the crystal dynamics by a two-parameter valence force field model [5, 9, 10] with bond stretching (f_s) and bond bending (f_b) force constants. We neglect the long-range Coulomb forces, which are expected to affect only in a minor way the interface modes of mechanical (microscopic) origin. Characteristics of the model are given in table 1. The bulk vibrational density of states (VDOS) is shown in figure 1, where the similarity between the two crystals is clear. Both semiconductors show an acoustic–optical gap around 5 THz.

For the new bonds that are present at the planar interface, namely Ga–As and In–Sb, the bond stretching force constants of the corresponding crystals have been used (see table 1). For the bond bending force constants for bonds of the type A–B–C, we use an arithmetic average of the values for A–B–A and C–B–C. In figure 2, the VDOS of the planar interfaces is given, projected on a

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Table 1. Model characteristics. Experimental values as in [10].

Force constants (N m^{-1})
f_s(Ga–Sb) = 101.0
f_s(In–As) = 102.0
f_s(Ga–As) = 115.0
f_s(In–Sb) = 95.0
f_b(Ga–Sb–Ga) = f_b(Sb–Ga–Sb) = 1.52
f_b(In–As–In) = f_b(As–In–As) = 1.33
f_b(Ga–As–Ga) = f_b(As–Ga–As) = 2.09
f_b(In–Sb–In) = f_b(Sb–In–Sb) = 0.78

Frequencies (THz) (model/expt.)		
	GaSb	InAs
LO Γ	7.2/7.2	7.1/7.1
TA X	1.7/1.7	1.6/1.6
LA X	4.41/4.9	4.52/4.9
LO X	5.82/6.2	5.59/6.1
TO X	6.85/6.2	6.80/6.4

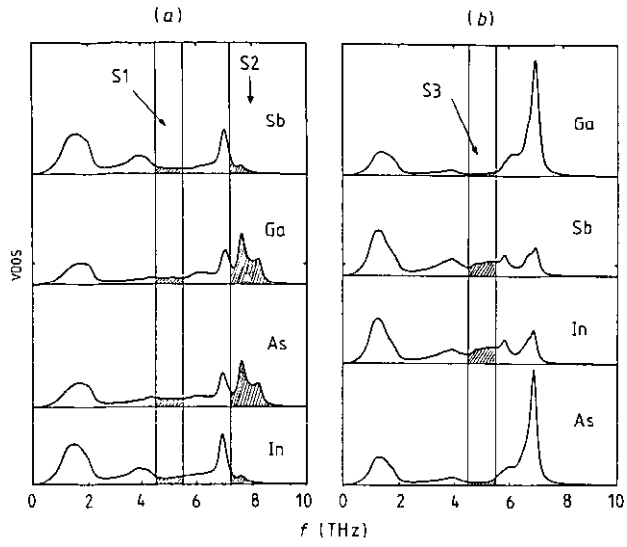

Figure 2. Vibrational density of states on two atomic planes on either side of the planar interface: (*a*) light interface, (*b*) heavy interface. The vertical lines indicate the main gap and the maximum frequency of the two crystals.

few layers around the interface plane. The light interface shows two peaks well above the maximum frequency of both crystals, which arise from interface modes of longitudinal (~7.6 THz) and transverse (~8.3 THz) character and they have also been found before [7, 9]. Their projection on the interface Ga–As layer only and their frequency position supports their character as local vibrations of the Ga–As pair. In the region of the main gap the VDOS shows a slight enhancement at the expense of the LA peak, which arises from longitudinal interface modes [9]. These modes are quite dispersive [9], which explains the rather uniform filling of the gap with no pronounced structure. On the other hand, the heavy interface shows a substantially enhanced VDOS in the main gap at the expense of the TO band, which arises from longitudinal (~4.75 THz) interface modes. These modes project mainly on the interface In–Sb layer and are enhanced as local optical vibrations of the In–Sb bond. This interface also supports transverse modes (~5.8 THz), which, however, fall within the LO continuum and behave as resonances away from the two-dimensional Brillouin zone centre. These states are responsible for the small peak around 5.8 THz.

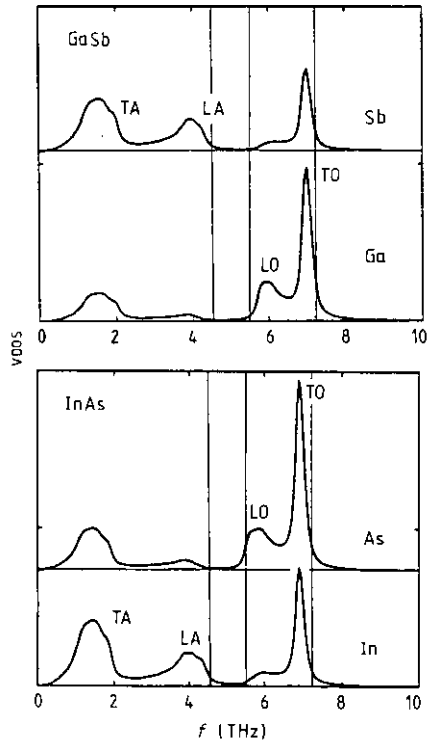

Figure 1. Vibrational density of states of GaSb and InAs crystals. The vertical lines indicate the frequency range of the acoustic–optical gap and the maximum frequency.

In summary, the high-frequency interface modes (denoted by S2) and the dispersive modes in the main gap (S1 modes) make up a feature characteristic of the light interface (Ga–As bond), while the less dispersive modes in the main gap with a peak around 5.8 THz (S3 modes) are the signature of a heavy interface (In–Sb bond).

3. Stepped interfaces

The different anions and cations of the two crystals give the possibility of three different types of interface steps of one monolayer height ($=a/2$); a single step, where substitution takes place only within the first plane of the interface layer; a double step, where both anions and cations of the first layer are substituted; and diffused atoms in the second plane of the interface layer. These defects are shown schematically in figure 3; in the following results both the masses and the force constants have been modified according to the nearest neighbours of each atom. Despite the fact that all these defects are

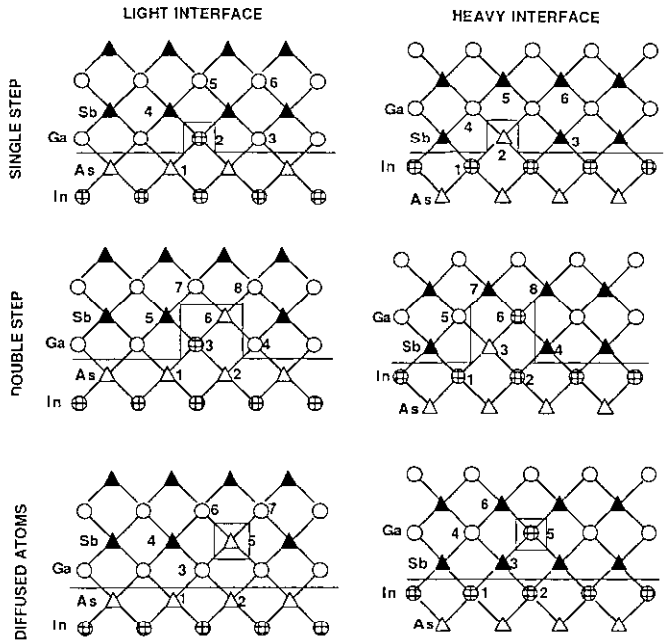

Figure 3. Profile of single-row steps along the [100] direction. The labelling of sites is the same as in figures 4 and 5.

confined within the first monolayer, which is the precision limit of modern growth techniques [1], we demonstrate below that the phonon states of the interface are substantially different in each case. This can be deduced from comparison of figure 4(*a*, *b*, *c*) which shows the VDOS of a GaSb on InAs(001) light interface with a single-row step in the [100] direction. The single and double steps produce localised states (S3) in the main gap, that are characteristic of a heavy interface and, as said earlier, correspond to vibrations of the In–Sb bond. These modes are absent from the spectrum of the interface with diffused As atoms, because this type of defect does not produce any In–Sb bonds. If, however, a Sb atom diffuses into InAs one should expect the S3 modes to be present. Similarly, for the heavy interface (figure 5), the single or double step and diffused Sb atoms produce S1 and S2 modes along the step axis that are characteristic of the light interface, while diffused In atoms simply enhance locally the S3 modes.

Furthermore, the step formation affects drastically the frequency position and lineshape of the interface modes. For example, an inversion of the height ratio of the S2 peaks, with respect to the planar interface, occurs in figure 3(*b*) site 4, which implies that transverse interface modes are more probable near the edge. At site 6 in the same figure the transverse interface modes show a broad structure, which can be attributed to the increased number of Ga neighbours. The same effect is more pronounced at site 5 in figure 3(*c*), where a bulk-like environment for the As atoms is formed. In the case that only one Ga–As bond is present the S2 modes show a single-peak structure, as is the case for example at sites 3, 5 in figure 5(*b*). The position of this peak is between the L, T peaks of the S2 modes, which indicates that step formation can indeed shift the Raman lines of the interface modes with respect to their position for a planar interface and modify their shape. The same conclusion

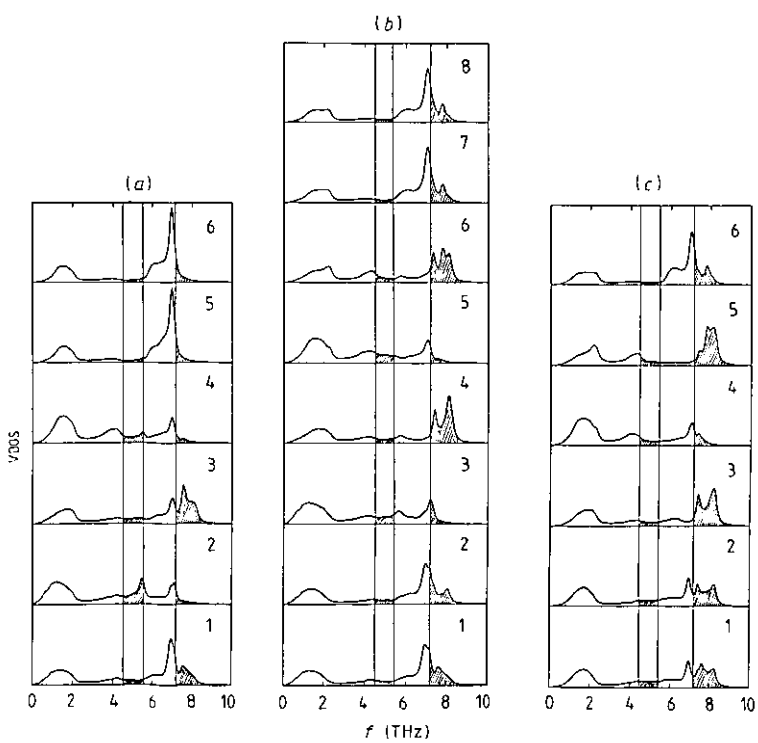

Figure 4. Vibrational density of states at a light interface with three types of [100]$_1$ steps: (*a*) single step, (*b*) double step, (*c*) diffused row of atoms. The labelling of sites is the same as in figure 3. The vertical lines indicate the main gap and the maximum frequency of the two crystals.

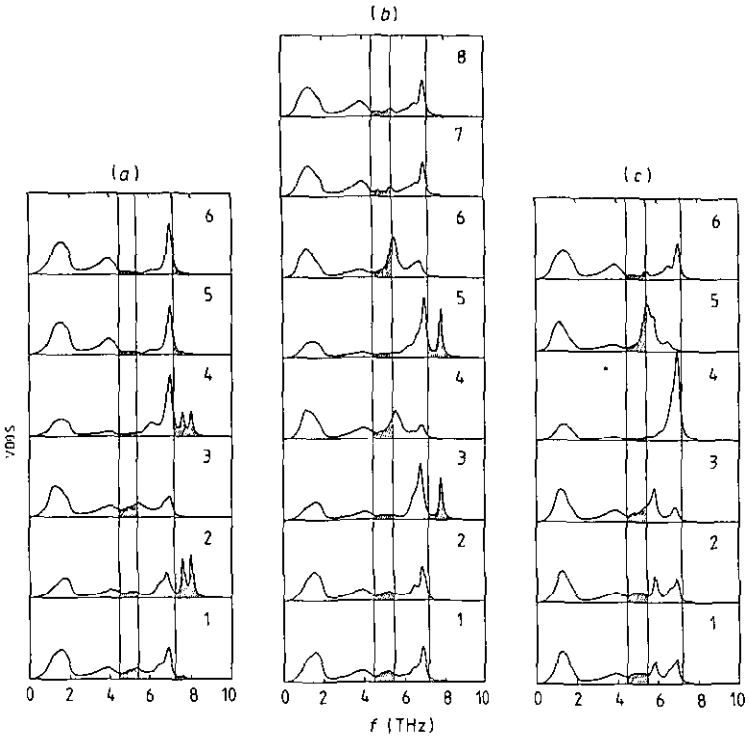

Figure 5. Vibrational density of states at a heavy interface with three types of $[100]_1$ steps: *(a) single step, (b) double step, (c)* diffused row of atoms. The labelling of sites is the same as in figure 3. The vertical lines indicate the main gap and the maximum frequency of the two crystals.

can be drawn by considering the following sequence of As sites: figure 5(*b*) site 3, figure 5(*a*) site 2, figure 4(*b*) site 6 and figure 4(*c*) site 5, where the four bonds sequentially change from As-In to As-Ga.

Another reason for frequency shift is the spatial confinement of the modes, while the local environment remains unchanged. Consider, for example, an In atom at the planar interface (figure 2) with the same atom in figure 4(*a*) site 2. Apparently, the peak in the main gap corresponds to the transverse S3 modes, as it only projects on the In-Sb bond; the downshift seen with respect to the planar interface is due to the confinement of the S3 modes within the step region. A combination of both confinement and increase of the number of Sb neighbours is shown in figure 5(*b*) site 6, where the resulting downshift and height of the peak are bigger.

4. Conclusions

We have presented detailed results on the vibrational density of states of the two types of GaSb/InAs (001) interface containing very narrow steps ($\sim 0.707a$) of one monolayer height and different atomic compositions. It has been demonstrated that the presence of these steps produces a 'hybridized' spectrum, containing local states characteristic of either of the planar interfaces, thus making the interface identification difficult. Certain step geometries, e.g. a single step at the light interface, has been shown to cause confinement of an interface mode within the step region, which then appears at a lower frequency. The transverse modes are more sensitive to step formation due to their dispersionless character. Further changes in the lineshape of the local optical modes are attributed to the local bonding.

Our results also indicate that interface steps should have an analogous effect on the confined modes of a superlattice structure. In particular, they can lead to parallel confinement of the confined phonons in the wide or the narrow regions of the well thus producing split peaks in the Raman spectrum, in the same way that the interface modes can be confined in the interface layer or the narrow step. Recent calculations in a supercell geometry have demonstrated that fact for a GaAs/AlAs superlattice [11].

Acknowledgments

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