

Resonant quasiconfined optical phonons in semiconductor superlattices

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We point out that resonant phonon modes with quasiconfined behavior may arise in semiconductor superlattices in the continuum frequency range, i.e., where both constituents have allowed bulk frequencies with real wave vector. With reference to the cases of Si/Ge and InAs/GaSb (001) superlattices, we show that such modes appear close to the edge of overlapping optical frequencies, with displacement patterns and Raman strengths comparable to those of true confined modes. However, their degree of confinement and their actual number and frequency location are found to be more sensitive to the adjacent layer and to the details of the interfaces. Their study can therefore yield additional structural information on the interface region with respect to the study of true confined modes.

Folding and confinement in the phonon spectra of semiconductor superlattices¹ (SL's) are usually understood in terms of matching of (complex) bulk solutions at the interfaces.² Dispersive folded modes result in the frequency range where the bulk dispersions of the two constituents overlap [as in the longitudinal acoustical region of GaAs/AlAs (001) SL's, where both bulk GaAs and AlAs have Bloch oscillatory solutions with real wave vectors], while flat branches—corresponding to modes confined in one layer and evanescent in the other—result where the allowed bulk ranges do not overlap (as in the optical region of GaAs and AlAs).

GaAs/AlAs SL's are, however, representative of a limited class of materials in which only the acoustical branches overlap and the optical branches of the two constituents fall in separate energy ranges. Already the case of GaAs/Al_xGa_{1-x}As presents a different situation. There, below the top of the longitudinal-optical (LO) GaAs-like band of the alloy [which is lower than the LO(Γ) frequency of bulk GaAs], the two optical frequency ranges overlap. By a naive application of the above reasoning, confined modes would be expected only between the top of the LO continua of the two materials, and folded dispersive modes would be expected in the overlap region below. The observed disappearance of the Raman peaks associated to GaAs-like confined modes when passing below the edge of overlap has been taken as a confirmation of this picture.³ Overlap of the optical branches of the SL constituents is a quite common feature, which is encountered for instance also in InAs/GaSb and Si/Ge SL's, the vibrational properties of which are recently receiving increasing attention.⁴⁻¹⁰

In the following we will discuss the behavior of SL phonons in cases where the bulk dispersions of the two constituents overlap. In particular, we will show that, as in the electronic case,¹¹ strong resonances can appear just

below the edge of overlapping frequencies with behavior (thickness dependence, Raman activity) similar to that of true confined modes. These resonant quasiconfined modes result from the matching of two bulk solutions with different real wave vectors. However, the amplitude is mostly localized in one layer and matched to an oscillatory, nonevanescing wave of smaller amplitude in the other layer. The detailed properties of these modes—like their degree of confinement, their actual number and frequency location—depend strongly on the underlying bulk dispersions and are obviously more sensitive to the adjacent layer and to the details of the interfaces than those of true confined modes. This fact may be of relevance for interface characterization.

In order to illustrate these points we will focus, in particular, on the Si/Ge and InAs/GaSb systems, which clearly show a different behavior than GaAs/AlAs. To study this type of mode realistically, we need a detailed description of the superlattice lattice dynamics, capable of accurately treating at the same time the relative frequency position of the bulk continua and the bonds near the interface in the superlattice. In the case of InAs/GaSb SL's, these two requirements are of particular importance because the LO(Γ) of InAs falls only a few wave numbers above the LO(Γ) of GaSb, and because different types of bonds (between In and Sb or between Ga and As atomic planes) may occur at the interface. In the following, we will present results calculated with a one-dimensional approach [exact for wave vectors parallel to the (001) growth direction];¹² we will use the same interplanar force constants for the two materials and different masses and effective charges to describe the differences between InAs and GaSb,⁹ and only different masses to describe the differences between Si and Ge.¹⁰ Indeed the bulk experimental results are well reproduced, particularly for InAs/GaSb, with the same set of force constants: This

gives confidence in the reliability of the method in describing the main features of the band also at the interfaces.¹³

In Fig. 1 we show the displacement and frequency position of longitudinal Si-like confined modes and of resonant quasiconfined Ge-like modes. This figure illustrates the analogy of phonon displacements with the wave functions of a particle in a finite well.¹⁴ In this context the upper (lower) edge of the phonon barriers is given by the edge of the Si (Ge) bulk continuum. The modes shown are the Γ -point phonons of a Si_6/Ge_6 SL. Note that below the edge of Ge, which represents the edge of the continuum, the displacements in the Ge layer are quite similar to the ones of true confined modes (such as the topmost Si-like modes), but matched to an oscillatory nonevanescing wave in the Si layer. For some of these modes (for example for the highest one) the displacement amplitude in Si is much smaller than in Ge. This is why we call these modes resonant, quasiconfined Ge-like modes. Furthermore, as the displacement is similar to that of true confined modes, the corresponding Raman intensity should be comparable. Indeed, well-defined Ge-like peaks have been observed in light scattering experiments on Si/Ge SL's.⁴⁻⁸ Moreover, we find that their frequency approximately coincides with that of the modes actually confined in an isolated Ge slab. Notice also that resonances in the layer representing the well (Si in the present case) may occur; we will see later on that this aspect is even more evident in the case of InAs/GaSb. The full dispersion of the Si_6/Ge_6 SL is shown in the central part of Fig. 2. By comparison with $\text{Si}_6/\text{Ge}_{10}$ (left) and $\text{Si}_{10}/\text{Ge}_6$ (right) it is clear that the dispersion and energy

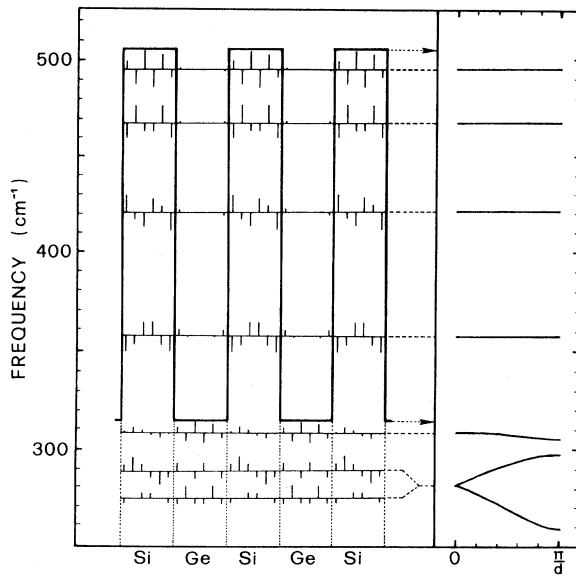


FIG. 1. Confined and resonant longitudinal modes in a Si_6Ge_6 superlattice. Right-hand side: phonon dispersion along (001) in the superlattice Brillouin zone. Left-hand side: amplitude of the Γ point longitudinal displacements vs position of the atomic layers along (001). The upper and lower edges of the barriers are given by the edges of the Si and Ge bulk continua, respectively, as marked by the arrows.

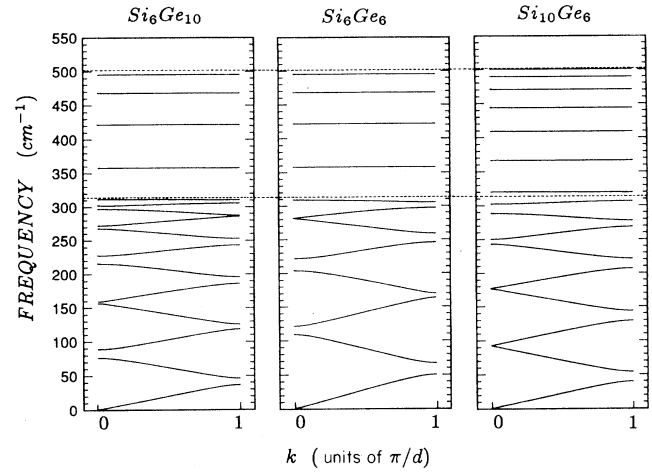


FIG. 2. Dispersion of longitudinal modes along (001) for the $\text{Si}_6\text{Ge}_{10}$, Si_6Ge_6 , and $\text{Si}_{10}\text{Ge}_6$ superlattices. The dashed lines represent the edges of the longitudinal continua of bulk Si and Ge. d is the superlattice period.

position of resonant modes are indeed somewhat affected by the thickness variation of the adjacent layer, contrary to what happens for the proper Si-like confined modes.

Resonant modes are also sensitive to the details of the interface. To illustrate this point we now consider InAs/GaSb superlattices, which may have either light (Ga and As) layers or heavy (In and Sb) layers at the interface,¹⁵ as sketched in Fig. 3. In Fig. 4 we show the dispersions of InAs₁₉/GaSb₁₃ SL's with "heavy" (left) and "light" (right) interfaces, together with the bulk InAs (solid line) and GaSb (dashed line) longitudinal phonon spectra.¹⁶ Besides the modes localized at the interface (denoted by IF in Fig. 4), which fall at very different frequencies depending on the interface composition,^{9,15} also

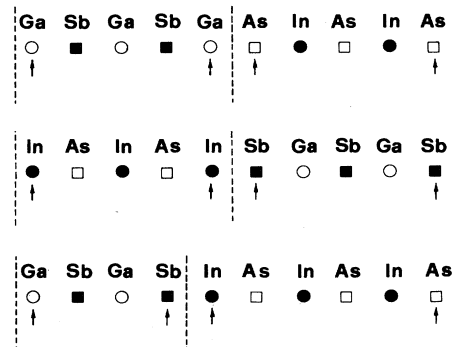


FIG. 3. Possible geometries of ideal InAs/GaSb (001) superlattices. Filled symbols correspond to "heavy" atomic planes (In and Sb), while open symbols correspond to "light" atomic planes (Ga and As). The arrows indicate the atomic planes involved in the interface bonds. Top: odd number of atoms per layer; two light interfaces per unit cell. Center: odd number of atoms per layer; two heavy interfaces per unit cell. Bottom: even number of atoms per layer; alternated heavy and light interfaces.

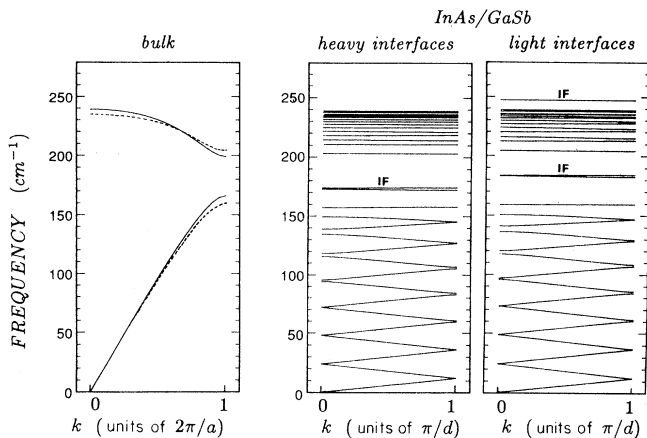


FIG. 4. Longitudinal phonon dispersion along the (001) growth direction for $\text{InAs}_{19}/\text{GaSb}_{13}$ superlattices with heavy and light interfaces (right-hand side), together with the (001) dispersion of their bulk constituents (left-hand side): InAs (solid line) and GaSb (dashed line). a is the bulk lattice parameter. Interface modes are marked by IF. For the displacement patterns of confined and resonant modes see Fig. 5.

the overall optical spectrum changes when the interface composition changes. In both cases, flat branches result for the InAs-like confined modes: These are the only true confined modes allowed in this case, as the optical bulk range of GaSb is entirely contained in the one of InAs. Several flat resonant SL modes are also present in the continuum frequency region of overlap of optical bulk branches. (The number of confined plus resonant modes is not the same in the two cases because the number of interface modes is not the same.) Resonant modes, however, appear to have a rather different behavior in the two interface configurations: For In-Sb interfaces, they become dispersive only well inside the region of overlap, while for Ga-As interfaces they always show a non-negligible dispersion.

By looking at the displacement patterns (Fig. 5) these differences are easily understood: for heavy In-Sb interfaces, modes remain well confined in either layer even inside the region of overlap, while for light Ga-As interfaces the displacement amplitude is non-negligible in both layers. The nature of resonant quasiconfined modes is, however, evident in both cases.

It is interesting to notice that resonant modes, quasiconfined in either the GaSb or the InAs layer, successively appear. In order to understand the sequence of occurrence of these GaSb-like and InAs-like modes, one has to recognize that when the quasiconfinement is well pronounced, resonant GaSb (InAs)-like modes fall on the bulk dispersion of GaSb (InAs) at wave vectors $m\pi/d_i$, as for true confined modes:¹² d_i is the confinement length in the InAs (GaSb) slab, which may depend itself on the particular interface geometry (see Fig. 5). The number of resonant modes to which this rule applies also depends on the type of interfaces, as well as on the thicknesses of the individual layers: For thick layers and heavy interfaces it holds accurately for several modes.

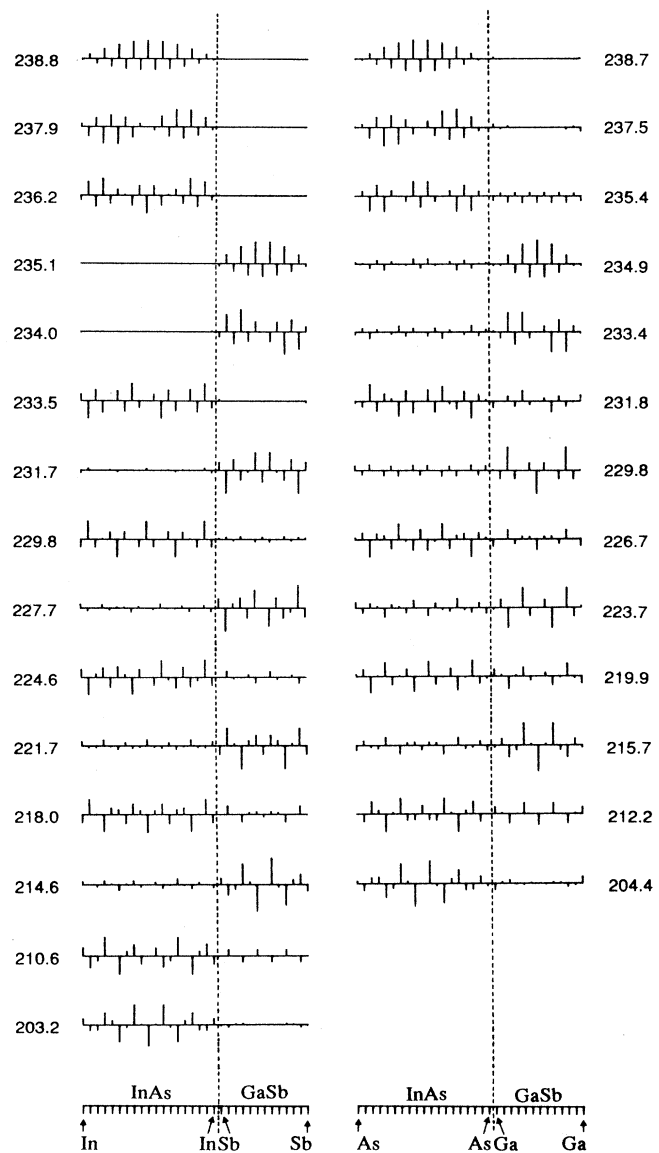


FIG. 5. Amplitude of the longitudinal Γ -point displacements of confined and resonant modes for $\text{InAs}_{19}/\text{GaSb}_{13}$ (001) superlattices with heavy (left-hand side) and light (right-hand side) interfaces. The corresponding dispersions are given in Fig. 4.

The study of resonant modes can, therefore, yield additional information with respect to the study of true confined modes. In particular, it is crucial for the interpretation of the Ge-like peak in Raman spectra of Si/Ge (001) superlattices.^{4-8,10} Although we have explicitly considered here the cases of Si/Ge and InAs/GaSb only, the presence of strong, Raman-active resonances is expected in several situations including $\text{GaAs}/\text{Ga}_{1-x}\text{Al}_x\text{As}$ superlattices.

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