



HAL
open science

CALCULATED PHONON SPECTRA OF Si/Ge SUPERLATTICES: ANALOGIES WITH OTHER SYSTEMS AND NEW FEATURES

A. Fasolino, E. Molinari

► **To cite this version:**

A. Fasolino, E. Molinari. CALCULATED PHONON SPECTRA OF Si/Ge SUPERLATTICES: ANALOGIES WITH OTHER SYSTEMS AND NEW FEATURES. *Journal de Physique Colloques*, 1987, 48 (C5), pp.C5-569-C5-572. 10.1051/jphyscol:19875123 . jpa-00226707

HAL Id: jpa-00226707

<https://hal.science/jpa-00226707v1>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

CALCULATED PHONON SPECTRA OF Si/Ge SUPERLATTICES : ANALOGIES WITH OTHER SYSTEMS AND NEW FEATURES

A. FASOLINO and E. MOLINARI*

SISSA, Strada Costiera 11, I-34100 Trieste, Italy

**CNR, Istituto di Acustica "Corbino", Via Cassia 1216,
I-00189 Roma, Italy*

Resumé - Les spectres de phonons de superréseaux Si/Ge dans la direction de la croissance ont été calculés. A côté des modes pliés et confinés comme dans le cas du système GaAs/AlAs, dans la direction (001) les résultats montrent aussi des modes d'interface dans la polarisation transverse et des modes résonants dans la polarisation longitudinale au bord de la région des fréquences où les modes de volume de Si et Ge se recouvrent. La dispersion, les vecteurs propres et la dépendance en fonction de l'épaisseur des couches de ces derniers modes ont un comportement très semblable à celui des modes proprement confinés.

Abstract - The phonon spectra of Si/Ge superlattices are calculated along the growth direction. Besides folded and confined modes, as in the more studied case of GaAs/AlAs systems, along (001) they show interface modes in the transverse polarization and resonant modes in the longitudinal one at frequencies just below the edge where the Si and Ge bulk modes start overlapping. The thickness dependence, dispersion and displacement patterns of the latter modes show their similarities to proper confined modes.

The lattice dynamics of semiconductor SL's has been extensively studied both experimentally and theoretically in the last few years [1-15] mostly for the GaAs/AlAs system, for which the concepts of folding of the acoustical branches and confinement of optical modes have been introduced. Si/Ge superlattices (SL's) are now starting to be grown with high crystalline quality [16] despite their 4.2 % lattice mismatch. The Si/Ge (001) SL's are, on one hand, similar to GaAs/AlAs in that one component (Si) is much lighter than the other (Ge), with a consequent much higher upper edge of the frequency spectra; on the other hand there are two important differences: i) the Ge longitudinal bulk continuum is entirely contained in the Si bulk frequency range, and ii) the bonds present at the interface (Si-Ge) are different from those inside the layers (Si-Si and Ge-Ge). These two latter features make Si/Ge SL's much more similar to InAs/GaSb SL's, which have recently been studied theoretically [14,15] and where, in particular, the different bonds at the interfaces (In-Sb or Ga-As) have been shown to give rise to new modes localized at the interface. It is therefore worthwhile investigating to which extent the same behaviour can be expected for Si/Ge SL's.

We calculate the phonon spectra of Si/Ge superlattices along the (001) and (111) growth directions by means of a one-dimensional model with interplanar force constants, as done for GaAs/AlAs in [12,13]. We use the interplanar force constants (extending to third neighbour planes for longitudinal and fifth neighbour planes for transverse modes), calculated for bulk Ge [17] in the local density approximation, to describe both materials, the differences in their bulk spectra being accounted for by their different masses only. In Fig.1 we compare the resulting bulk Si and Ge phonon spectra along the (001) direction with the experimental data [18,19]. (Analogous results are obtained for dispersions along the (111) direction, for which Ge *ab initio* interplanar force constants are also available in Ref. 17.) The agreement is satisfactory. A further improvement could be achieved by *e.g.* abandoning the mass approximation and using force constants derived

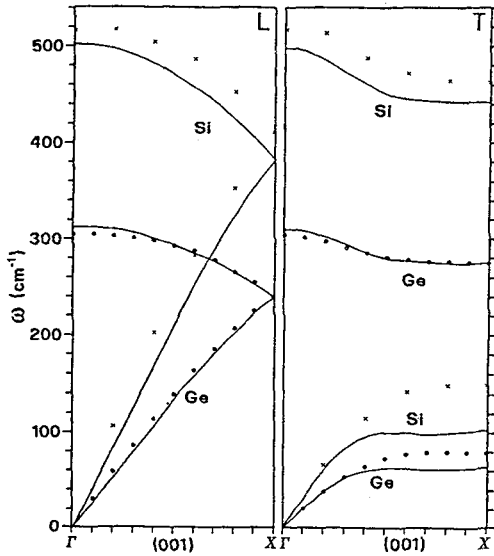
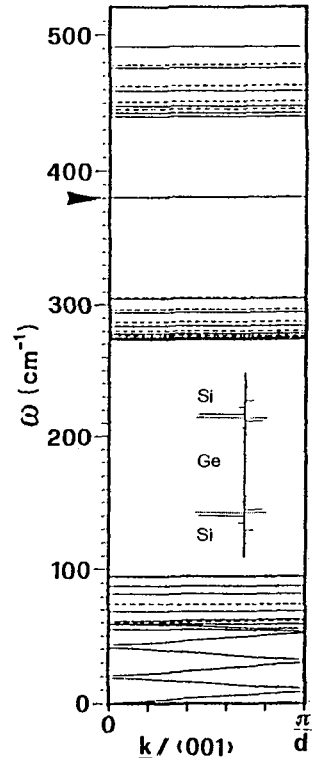


Fig.1. Longitudinal (L) and transverse (T) bulk phonon dispersions for Si and Ge along the (001) direction. Solid line: calculation with force constants from Ref. 17; circles: Ge neutron scattering data at 80°K, after Ref. 18; crosses: Si neutron scattering data at 296°K, after Ref. 19.

Fig.2. Dispersion of T modes for a (001)-grown Si/Ge superlattice with 14 atomic planes of Si and 14 atomic planes of Ge in the unit cell. Solid lines represent modes belonging to one T polarization direction; dashed lines represent the modes of the other T polarization which do not coincide with the first ones. The arrow shows the dispersionless interface modes; the corresponding amplitude of T displacements is displayed in the inset, where the dotted lines show the position of interfaces.



for both materials from a bond-charge-model calculation [20]. This procedure, however, when applied to SL's introduces further arbitrariness in the treatment of the interactions close to the interface. On the other hand all qualitative features are known to be preserved once the relative positions of the two bulk continua are reproduced, as is the case in our treatment. We also neglect at present the effect of the strain induced by the lattice mismatch, because it does not affect in any fundamental way the qualitative features of the spectrum. Furthermore the way strain affects the theoretical results depends on the details of the SL structure (thickness, substrate) [16] and is worth considering only at the stage of interpretation of experimental results.

In Fig.2 we show a typical transverse (T) SL phonon spectrum where two almost degenerate interface modes show up in between the high lying Si-like confined optical modes and the Ge-like ones. The presence of these interface modes is related to the fact that the frequencies of vibration of the Si-Ge bonds fall where no Si or Ge bulk modes are available. The vibration is then localized on the interface planes and decays exponentially in the layers as shown in the inset of Fig.2. In the longitudinal (L) spectrum, on the contrary, there are no gaps where an interface localized mode can exist. Moreover, as the Ge dispersion falls within the one of Si, proper confined modes, evanescent in the other layer, can exist only for Si.

The confined nature of the SL Si-like modes beyond the Ge longitudinal edge is confirmed by their dispersionless behaviour and their displacement patterns in Fig.3, and by their characteristic dependence on the thickness of the Si-layer and independence of the one of Ge (Fig.4). However we notice that also below the top edge of Ge there are modes which behave similar to (Ge-like) confined modes. In particular in Fig.4 this is evident for the mode at $\sim 309 \text{ cm}^{-1}$, whose dependence on the thickness of either layer is evidenced by the dashed lines. This mode is almost

dispersionless as shown in Fig.3a. Its displacement pattern (Fig.3d) is mostly localized in the Ge layer with the typical Raman active displacement pattern of a first confined mode, but – contrary to a proper confined mode – it is matched to a smaller but non-evanescent displacement in the other layer. This type of modes result from the matching of bulk solutions of Si and Ge of different (real) wavevectors and are the analogue of resonant modes in for impurity states in a continuum [21].

Lastly we briefly comment on the folding of acoustical modes. From Fig.3a it can be seen that the acoustical branches are folded with gap opening at zone center and zone edge. The size of the minigaps and their occasional vanishing can also be derived by means of a continuum theory for elastic waves as done in Ref. 11. Although this treatment applies only to the linear part of the acoustic dispersion (ω below $\sim 120 \text{ cm}^{-1}$ for Si/Ge SL's) we have found that stickings of the folded doublets occur also at higher frequencies and can be explained by the same reasoning: doublets with vanishing gap at the zone center occur when the two bulk dispersions, folded separately over a period π/d_i (d_i being the individual layer thickness), happen to fall at the same energy after having both been folded either an even or an odd number of times; while they occur at zone boundary if the coincidence of frequencies takes place after an even number of foldings in one material and an odd number for the other. The occurrence of such doublets is of course very sensitive to individual layer thicknesses.

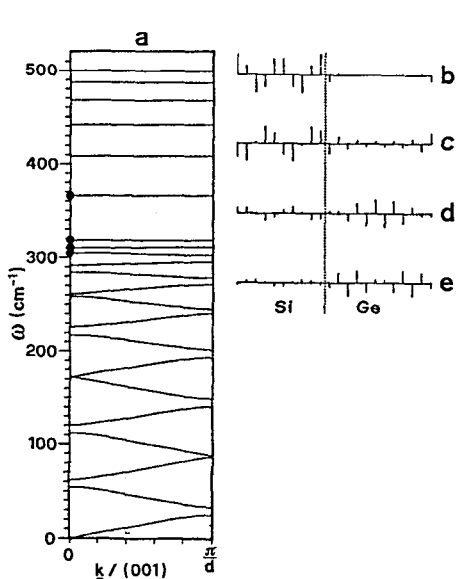


Fig.3. L modes of a (001)-grown Si/Ge superlattice with 10 atomic planes of Si and 14 atomic planes of Ge in the unit cell. a): dispersion along the (001) direction; b)-e): amplitude of L displacements for the four modes evidenced by circles in a), in order of decreasing frequency; the dotted lines show the position of interfaces.

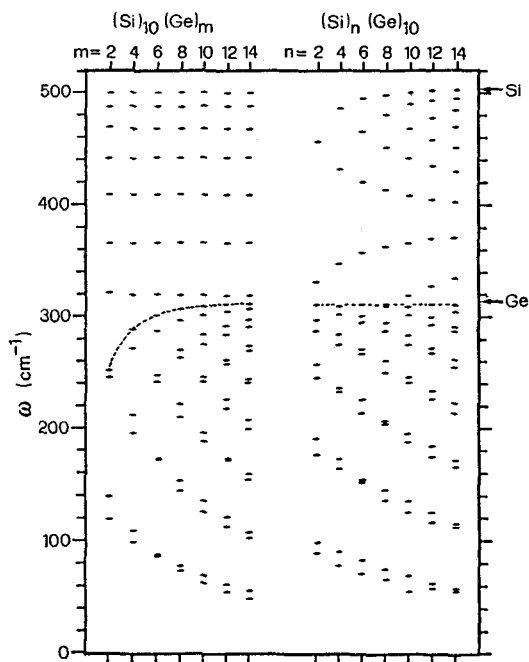


Fig.4. Dependence of zone-center longitudinal phonon frequencies on the thickness of Ge and Si layers. The dashed lines evidence the thickness dependence of the first mode below the edge of Ge bulk continuum. m and n represent numbers of atomic layers.

In summary we have shown that the spectra of Si/Ge (001) SL's should display a very rich structure, resulting from the folded acoustical modes, the Si-like and Ge-like Raman-active "optical" modes in the longitudinal spectrum, and by the same modes plus interface modes in the transverse polarization.

We acknowledge partial financial support by GNSM-CISM.

References

1. For reviews see: J. M. Worlock, in *Proc. 2nd Int. Conf. on Phonon Physics*, Budapest 1985, edited by J. Kollár, N. Kroó, N. Menyárd and T. Siklós, World Scientific (1985), p. 506; M. V. Klein, *IEEE J. Quantum Electron.* **QE22**, 1760 (1986); B. Jusserand and D. Paquet, in *Semiconductor Heterojunctions and Superlattices*, edited by N. Boccarda, G. Allan, G. Bastard, M. Lannoo and M. Voos, Springer (1986)
2. A. S. Barker, Jr., J. L. Merz and A. C. Gossard, *Phys. Rev.* **B17**, 3181 (1978)
3. G. Sai-Halasz, A. Pinczuck, P.Y. Yu and L. Esaki, *Solid State Commun.* **25**, 381 (1978)
4. J. Sapriel, J. C. Michel, J. C. Tolédano, R. Vacher, J. Kervarec and R. Regreny, *Phys. Rev.* **B28**, 2007 (1983)
5. B. Jusserand, D. Paquet and A. Regreny, *Phys. Rev.* **B30**, 6245 (1984)
6. J. E. Zucker, A. Piczuk, D. S. Chemla, A. Gossard and W. Wiegmann, *Phys. Rev. Lett.* **53**, 1280 (1984)
7. S. Yip and Y. C. Chang, *Phys. Rev.* **B30**, 7037 (1984)
8. C. Colvard, T. A. Gant, M. V. Klein, R. Merlin, R. Fischer, H. Morkoç and A. C. Gossard, *Phys. Rev.* **B31**, 2080 (1985)
9. A. K. Sood, J. Menéndez, M. Cardona and K. Ploog, *Phys. Rev. Lett.* **54**, 2111 (1985)
10. B. Jusserand, F. Alexandre, D. Paquet and G. Le Roux, *Appl. Phys. Lett.* **47**, 301 (1985)
11. B. Jusserand, D. Paquet, F. Mollot, F. Alexandre and G. Le Roux, *Phys. Rev.* **B35**, 2808 (1987)
12. E. Molinari, A. Fasolino and K. Kunc, in *Proc. 18th Int. Conf. Phys. Semiconductors*, Stockholm 1986, edited by O. Engström, World Scientific (1987), p. 663
13. E. Molinari, A. Fasolino and K. Kunc, *Superlattices and Microstr.* **2**, 397 (1986)
14. A. Fasolino, E. Molinari and J. C. Maan, *Phys. Rev.* **B33**, 8889 (1986)
15. A. Fasolino, E. Molinari and J. C. Maan, *Superlattices and Microstr.* **3**, 117 (1987)
16. J. Bevk, J. P. Mannaerts, L. C. Feldman, B. A. Davidson and A. Ourmazd, *Appl. Phys. Lett.* **49**, 286 (1986); G. Abstreiter, H. Brugger, K. Iberl and R. Zakai, in *Proc. SPIE Conf. "Advances in Semiconductors and Semiconductor Structures"*, Baypoint, Florida, 1987 and references therein. Several groups have grown Si/SiGe SL's; measurements of folded acoustic phonons in these systems are reported by: H. Brugger, G. Abstreiter, H. Jorke, H. J. Herzog and E. Kasper, *Phys. Rev.* **B33**, 5928 (1986); D. J. Lockwood, M. W. C. Dharma-wardana, J.-M. Maribeau and D. C. Houghton, *Phys. Rev.* **B35**, 2243 (1987)
17. K. Kunc and P. Gomes Dacosta, *Phys. Rev.* **B32**, 2010 (1985)
18. G. Nilsson and G. Nelin, *Phys. Rev.* **B3**, 364 (1971)
19. G. Dolling, in *Symposium on Inelastic Scattering of Neutrons in Solids and Liquids*, IAEA, Vienna (1963), vol. II, p. 37
20. A. Fleszar and R. Resta, in *Proc. 2nd Int. Conf. on Phonon Physics*, Budapest 1985, edited by J. Kollár, N. Kroó, N. Menyárd and T. Siklós, World Scientific (1985)
21. see e. g. D. W. Taylor, in *Dynamical Properties of Solids*, edited by G. K. Horton and A. A. Maradudin, North-Holland (1975), p.285.