PRAMANA © Printed in India Vol. 45, No. 1,
— journal of July 1995
physics pp. 25–32

Phonon dispersion in quasiperiodic semiconductor superlattices

SUJATA RATH, PRAFULLA K JHA and SANKAR P SANYAL
Department of Physics, C V Raman Building, Bhopal University, Bhopal 462026, India

MS received 20 September 1993; revised 9 May 1995

Abstract. The phonon spectra of unstrained and strained quasiperiodic semiconductor superlattices (QSSL) have been calculated using one-dimensional linear chain model. We consider two types of quasiperiodic systems, namely cantor triadic bar (CTB) and Fibonacci sequences (FS), constituting of AlAs, GaAs and GaSb of which the latter two have a lattice mismatch of about 7%. The calculations have been made using transfer matrix method and also with and without the inclusion of strain. We present the results on phonon spectra of two component CTB and two as well as three component FS semiconductor superlattices (SSL), thickness and order dependence on LO mode of GaAs, effect of strain on LO frequency of GaAs. The calculated results show that the strain generated due to lattice mismatch reduces significantly the magnitudes of the confined optical phonon frequency of GaAs.

Keywords. Quasiperiodic; phonon; strained layer; transfer matrix.

PACS Nos 63·20; 63·90; 68·35

1. Introduction

In the recent years with the development of various crystal growth techniques, a great deal of interest has been generated towards the experimental as well as theoretical studies of the electronic and vibrational properties of semiconductor superlattices (SSL) [1–11]. This is mainly because of the potentiality of the applications of the SSL in various high speed semiconductor devices.

Although a lot has been studied on the binary SSL having perfect lattice matching between its components, only a few investigations have been reported on the periodic strained layer semiconductor superlattices (SLSL) [12–14]. The fabrication and study of the lattice vibrational properties of superlattices consisting of lattice mismatched materials are gaining interest because of their applications in various opto-electronic devices. The strain due to lattice mismatch of the constituting components of the SLSL is accommodated by each layer in such a way that the system is structurally and thermodynamically stable. The strain generated in such systems is isotropic in nature and in most of the cases, it changes the volume of each binary layer without affecting the crystal symmetry [15]. Due to this fact, it has now been possible to fabricate semiconductor heterostructures by avoiding misfit dislocations [14].

On the other hand, the discovery of icosahedral crystallographic symmetry has proved to be a new dimension to the study of the electronic and vibrational properties of quasi-periodic systems [16, 17]. Among the quasi-periodic superlattices, the Fibonacci superlattices (FSL) have been studied extensively both theoretically [18] as well as experimentally [19]. However, in the case of FSL, the main emphasis has been on the study of acoustic phonon propagation and their transmission [20–22]. Other types of quasi-periodic sequences are Thue-Morse, Cantor bar etc. Recently, some theoretical efforts have been devoted to investigate the vibrational properties in such semiconductor quasi-periodic systems [20].

In a recent paper, we have reported the calculated results of vibrational properties of $(GaAs)_{n_1}(GaSb)_{n_2}$ SSL [2]. In this investigation the effects of strain on the vibrational modes of a kind of quasiperiodic semiconductor superlattices, the cantor bar semiconductor superlattices (CBSSL) of one and three generations comprising of GaSb and GaAs as its components. In addition to this, we have also calculated the phonon spectra for two component GaAs, GaSb and three component GaAs, InAs and GaSb FSL of four generations. Also, we have studied the thickness dependence on the LO phonon modes of GaAs. The main objective in investigating this problem has been to understand the effect of strain on the phonon properties of quasiperiodic superlattices. The lattice mismatch in GaAs and GaSb is quite large ($\approx 7\%$) and these materials are ideal for observing the effects of strain on the vibrational properties of such quasi-periodic SSL. The phonon dispersion curves (PDC) in CBSSL have been calculated using a linear chain model [2] and the transfer matrix method. This method has already been applied to study the PDC in multicomponent SSL [1] and strained layer superlattice [2]. We present the structure and generation of the sequence of CBSSL in § 2 followed by a brief outline of the method of calculation of PDC. The results have been discussed in § 3.

2. Model structure and dispersion relation

The one-dimensional quasiperiodic semiconductor superlattices under consideration are generated recursively along Z-direction by two elementary media: media A and media B. The model structure prescribed in figure 1, maps the mathematical rule of the cantor triadic bar sequence infinitely as follows [23], $C_1 = B_1A_1B_1$, $C_2 = B_2A_2B_2, \ldots C_n = B_nA_nB_n = C_{n-1}A_nC_{n-1}$ where $B_n = C_{n-1}$, while A_n is the same medium as layer A_1 but with different thickness, $dA_n = (2+\alpha)^{n-1}dA_1$ where the parameter α is the thickness ratio of dA_n to dB_n. The total thickness of an nth generation one-dimensional quasiperiodic semiconductor superlattice (QSSL) is $dC_n = (2+\alpha)^n dB_1$ where dB_1 is the thickness of the layer B in the first generation.

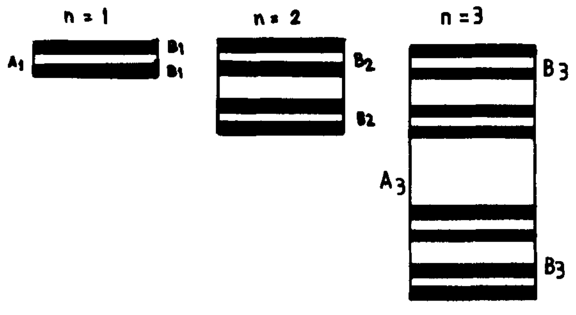

Figure 1. Geometry of a cantor bar triadic semiconductor superlattice of one and three generations.

The fractal dimension of present model [23] is given by $D = \ln 2/\ln(2+\alpha)$. It is easy to find that when $\alpha = 1$, the QSSL becomes usual CBSSL with $D = \ln 2/\ln 3$; when $\alpha = \Lambda = (\sqrt{5}-1)/2$, the structure of QSSL is somewhat like the Fibonacci superlattice. If we substitute, A_n by C_{n-2} and B_n by C_{n-2}, it is just the usual Fibonacci superlattice. Hence, the physical meaning of the quantity α can be found from the fact that it governs the formation of various sequences.

A Fibonacci superlattice comprises of an arrangement of individual building blocks of type A (each of thickness d_A) and type B (each of thickness d_B) following a concatenation scheme determined by the Fibonacci sequence $G_1 = A$, $G_2 = AB$, $G_3 = ABA, \ldots$, $G_r = G_{r-1}G_{r-2}$ [17]. The rth generation FSL G_r consists of F_r type A blocks and F_{r-1} type B blocks, where F_r are the Fibonacci numbers given iteratively $F_r = F_{r-1} + F_{r-2}$ for $r > 2$ with $F_0 = 0$ and $F_1 = 1$. In order that phonons may recognize the distinct interfaces spaced in Fibonacci manner, each building block should be subdivided into two or more layers with different elastic properties. In this paper, we have considered that both type A and B blocks consist of two and three layers.

In order to calculate the phonon dispersion curves for these QSSL, we have adopted a linear chain model in one-dimension, details of which have been given in our previous papers [1, 2]. The general equation of motion of any atom in either of the components of the QSSL can be written as [1]

$$m_j\omega^2 u_n = -C_i(u_{n-1} + u_{n+1} - 2u_n) \tag{1}$$

where $C_i (i = A, B)$ are the nearest neighbour force constants, u_n are the displacements, and m_j are respective masses of the atoms. By using the transfer matrix method as in our earlier papers [1, 2], we get

$$\cos QD = 1/2 \, \mathrm{tr}\, T \tag{2}$$

where T is a unimodular (2×2) transfer matrix which has the property of relating the coefficients of the displacement vectors in one cell $(l+1)$ to those in the previous one (l) and is given by

$$T = \prod K_1^{-1} H_n K_n^{-1} H_{n-1} K_{n-1}^{-1} \ldots H_2 K_2^{-1} H_1 \tag{3}$$

where H_i and K_i $(i = 1, n)$ are (2×2) unimodular matrices and defined in ref. [1].

In the present paper, we have calculated the dispersion curves for diatomic one and three generation CBSSL and two and three component four generation FSL. The transfer matrix in the case of one generation CBSSL reduces to

$$T = K_1^{-1} H_3 K_3^{-1} H_2 K_2^{-1} H_1. \tag{4}$$

This equation is similar to that which has been reported earlier by us in the case of multicomponent SSL [2], where there are only two components, the middle one being different than the two adjacent neighbours. The dispersion relation for three generation CBSSL as well for two and three component four generation FSL have been calculated using (2) and (3) [24].

The effect of strain due to lattice mismatch at the interface of the two components has been considered in the usual manner, as discussed in our previous paper [2]. We have calculated the phonon dispersion relation by considering the effect of strain also, to reveal its role in the dispersion of phonons in such systems. Also we have investigated the effect of change in layer thickness on the highest longitudinal optical mode of GaAs by varying the value of α.

3. Results and discussion

We have calculated the phonon dispersion curves (PDC) of unstrained and strained one, three generation CBSSL and two, three component four generation FSL. The constituents of CBSSL and two component FSL are GaAs and GaSb and that of three component FSL are GaAs, InAs and GaSb. The various parameters and force constants have been calculated in the usual way as explained in our earlier papers [1, 2]. The calculated bulk dispersion curves (longitudinal modes) for GaAs and GaSb, compared with the experimental values [25, 26] have been reported in ref. [1, 2].

In figures 2(a) and 2(b), we have plotted the PDC of one and three generation CBSSL with the components B and A as $(GaAs)_{n_1}$ and $(GaSb)_{n_2}$ respectively with the thickness $n_1 = n_2 = 10$. In this calculation, we have not considered the effect of strain. These figures reveal that they adequately explain the usual features of the superlattice vibrations. It is also seen from these figures that with the increase of the thickness of GaSb from one to three generations, the number of confined modes of GaSb increases. This fact is true in both one and three generation CBSSL. However, when the order of the components is reversed with a motivation to study the effect of increased thickness of one of the constituents, the number of GaAs layers increases as the number of generations increase resulting into the increase in the number of confined optical modes. It is observed from these figures that the self similarity nature increases with increase in the generation number. In addition to this, we have also calculated the

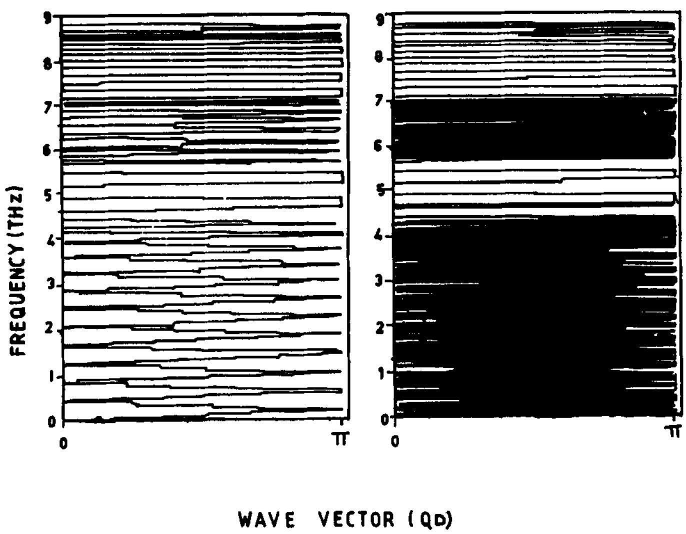

Figure 2. Phonon dispersion curves of CBSSL with layers A and B as $(GaSb)_{10}$ and $(GaAs)_{10}$ respectively for (a) one and (b) three generations.

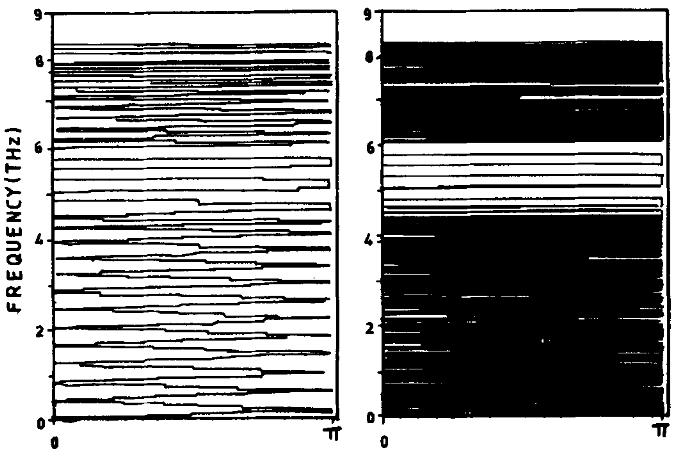

Figure 3. Phonon dispersion curves of strained CBSSL with components A and B as $(GaSb)_{10}$ and $(GaAs)_{10}$ respectively for (a) one and (b) three generations.

phonon dispersion curves in another quasiperiodic system, the two and multicomponent Fibonacci SSL. The results are quite similar to that of CBSSL.

In order to understand the effect of strain generated due to lattice mismatch, we have plotted in figures 3(a) and 3(b), the PDC of one and three generation CBSSL with the components GaSb and GaAs for the above mentioned order and thickness. It is observed from these figures, that in addition to the self similarity nature and other usual features observed in quasi-periodic SSL, there is a downward shift of the highest LO mode frequency of GaAs for both the cases and generations. This is attributed to the fact that the lattice mismatch is accommodated by tensile strain in GaAs and as compressive strain in GaSb. Thus, it reduces the lattice constant of GaSb and enhances that of GaAs. However, when the order of the components is reversed, the downward shift increases more because of the increase in the number of the GaAs layers. Our arguments can be justified from our earlier papers [1, 2] and Raman scattering measurements made on InGaAs/GaAs [13] and GaSb/AlSb [27] SLSL, respectively. To the best of our knowledge, we have calculated for the first time the PDC of a multicomponent four generation Fibonacci SSL without and with the effect of strain included. The FSL comprises of building blocks A as $(GaAs)_{10}(GaSb)_{10}(InAs)_{20}$ and that of B as $(GaAs)_{10}(GaSb)_{10}(InAs)_{4}$. The calculations here are carried out with the assumption that GaSb and InAs are perfectly lattice matched and there occurs a lattice mismatch between InAs and GaAs. The PDC have been plotted in figures 4(a) and 4(b). This figure reveals that there occurs a considerably large amount of frequency shift of the highest GaAs LO mode which is more prominent in this case than the two component FSL with all usual features observed in quasiperiodic systems.

To investigate the effects of strain on the LO phonon modes quantitatively, we plot in figure 5, the highest LO mode of GaAs for three generation CBSSL for cases

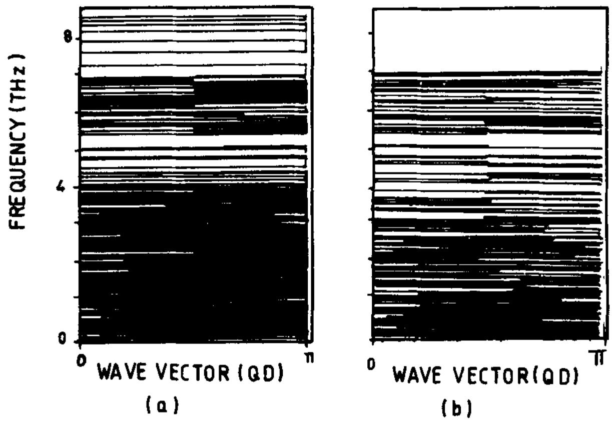

Figure 4. Phonon dispersion curves for FSSL of four generations with blocks $A = (GaSb)_{10}(InAs)_{20}(GaAs)_{10}$, $B = (GaSb)_{10}(InAs)_4(GaAs)_{10}$ for unstrained (a) and strained (b) systems.

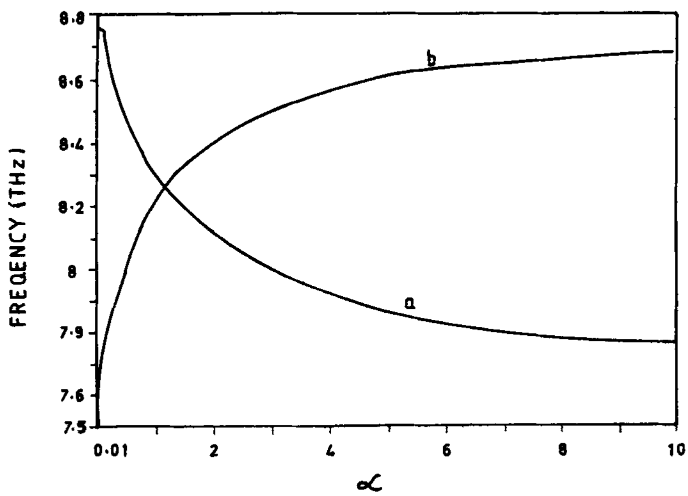

Figure 5. Thickness ratio α as a function of highest GaAs LO frequency of strained CBSSL for three generations with layers A and B as (a) $(GaSb)_{10}$ and $(GaAs)_n$; (b) $(GaAs)_{10}$ and $(GaSb)_n$ respectively.

(a) B = GaAs and A = GaSb, (b) B = GaSb and A = GaAs. Considering the first case in which the thickness of the GaSb layer is kept constant and that of GaAs is varied resulting into the variation of the parameter α from 0·01 to 10. It is observed that as the value of the parameter α increases from 0·01 to 10, the thickness of GaSb increases as compared to that of GaAs leading to the downward shift of the GaAs LO mode. At α = 10, the system behaves as bulk GaSb and the frequency is very near to that of GaSb

LO mode. But as α decreases to 0·01, the strain induced effect on the LO modes of GaAs relaxes thereby saturating at a frequency quite close to that of experimental zone centre value. This is due to the fact that around $\alpha = 0{\cdot}01$, the thickness of GaAs layers is very large as compared to GaSb and hence the system behaves as bulk GaAs. Similar arguments hold good when the order is reversed (case (b)) thereby showing reverse nature.

In conclusion, we have investigated the effect of built-in strain on the PDC of quasiperiodic CBSSL and FSL thereby observing that the change in the in-plane lattice parameter subsequently, enhances (or suppresses) the highest LO mode of GaAs. However, so far no efforts have been made from the experimental point of view on the phonon properties of such systems. We emphasize the need of Raman measurement for such systems.

Acknowledgements

The authors are grateful to the Department of Science and Technology for financial assistance. SR and PKJ are grateful to CSIR for the award of senior research fellowship and research associateship respectively. One of us (SPS) acknowledges the career award of UGC.

References

[1] S Rath and S P Sanyal, *Phys. Status Solidi* **B176**, 63 (1993)
[2] S Rath and S P Sanyal, *Pramana – J. Phys.* **41**, 21 (1993)
[3] C Colvard, T A Gant, M V Klein, R Merlin, R Fischer, H Morkoc and A C Gossard, *Phys. Rev.* **B31**, 2080 (1985) and references therein
[4] B D Rouhani, A A Maradudin and R F Wallis, *Phys. Rev.* **B29**, 6454 (1984)
[5] L Esaki, *Physics and applications of quantum wells and superlattices*, edited by E E Mendez and K Von Klitzing (Plenum Press, New York, 1989)
[6] A K Ramdas and S Rodriguez, *Semiconductor and semimetals*, edited by J K Furdyna and J Kossut (Academic Press, New York, 1988)
[7] J Sapriel and B D Rouhani, *Surf. Sci. Rep.* **10**, 189 (1989)
[8] M V Klein, *IEEE J. Quantum Electronics* **22**, 1780 (1986)
[9] M Cardona, *Spectroscopy of semiconductor microstructures*, (Plenum Press, New York, 1990)
[10] B Jusserand and M Cardona, *Light scattering in solids*, (Springer–Verlag, Heidelberg, 1989) Vol. V, p. 49
[11] M Cardona, *Superlattices and microstructures* 7, 183 (1990)
[12] E Friess, K Eberl, U Menczigar and G Abstreiter, *Solid State Commun.* **73**, 203 (1990)
[13] F Iikawa, F Cerdeira, C Vazquez-Lopez, P Motisuke, M A Sacilotti, A P Roth and M A Masut, *Solid State Commun.* **68**, 211 (1988) and references therein
[14] P Voisin, *Semiconductor Physics*, edited by C E T Gonsalves da Silva, L E Oliveiza and J R Leile (World Scientific, Singapore, 1987) p. 46
[15] T P Pearsell, *Semiconductors and semimetals*, (Academic Press, New York, 1990) Vol. 32, p. 1
[16] H Bottger and G Kasner, *Quasicrystals*, Edited by M V Jaric and S Lundqvist, (World Scientific, Singapore, 1990)
[17] R Merlin, *IEEE J. Quantum Electron.*, **QE-24**, 1791 (1988)
[18] S Tamura and J P Wolfe, *Phys. Rev.* **B36**, 3491 (1987)
[19] D C Hurley, S Tamura, J P Wolfe, K Ploog and J Nagle, *Phys. Rev.* **B37**, 8829 (1988)
[20] S Tamura and F Nori, *Phys. Rev.* **B40**, 9790 (1989)

[21] S Tamura and F Nori, *Phys. Rev.* **B41**, 7941 (1990)
[22] N Nishigushi, S Tamura and F Nori, *Phys. Rev.* **B48**, 2515 (1993)
[23] B B Mandelbrot, *The fractal geometry of nature* (Freeman, New York, 1982)
[24] Sujata Rath, *Phonons in semiconductor superlattices* Ph.D. Thesis, Barkatullah University, Bhopal (1993)
[25] D Strauch and B Dorner, *J. Phys.* **C2**, 1497 (1990)
[26] M K Farr, J G Traylor and S K Sinha, *Phys. Rev.* **B11**, 1587 (1975)
[27] P V Santos, A K Sood, M Cardona, K Ploog, Y Ohmori, M Okamoto, *Phys. Rev.* **B37**, 6381 (1988)