Strained α-Sn/Ge superlattices: Geometrical structures and phonon spectra

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The geometrical structures and phonon spectra of strained α-Sn/Ge superlattices grown pseudomorphically on (001)-oriented substrates are studied using a generalized Keating model. It is found that symmetrically strained α-Sn/Ge superlattices grown on properly chosen substrates can be approximately achieved, which renders the growth of superlattices with large thickness possible. The general features of phonon spectra are discussed. Ge-like confined LO modes can be well described by the bulk dispersion with the confinement length taken as $d_{\text{eff}}=(n+1)a/4$, where n is the number of Ge layers and $a/4$ is the Ge-Ge interplanar distance. The Sn-like LO modes are resonant and quasiconfined. No interface modes are found in the longitudinal polarization; however, such modes do appear in the transverse polarization around 232 cm^{-1}.

I. INTRODUCTION

The possibility of combining and manipulating components of materials has attracted much interest. One of the ultimate goals in semiconductor physics has been the hope to combine and manipulate different semiconductors to synthesize a new material with a fundamental direct gap, which may have many technical applications. Extensive attention and great efforts along this direction have been made by the growth of appropriate alloys, quantum wells, and superlattices (SL's). Since a large number of degrees of freedom for tailoring the electronic and other properties can be provided by controlling variations in composition, strain, growth orientation, and thickness of layers, semiconductor SL's have attracted particular attention.

Recently, the α-Sn/Ge system has received much interest because of its potential applications in devices, which might serve as alternatives to Hg-Cd-Te systems,[1] opening fascinating possibilities in band-structure engineering based on group-IV semiconductors. Semimetallic α-Sn is a zero-gap semiconductor, exhibiting a very high electron mobility owing to its small electron mass and the absence of polar phonon scattering. Therefore, the combination of zero-gap α-Sn and indirect-gap Ge may yield different electronic band structures. Unfortunately, bulk tin undergoes a structural phase transition[2] from the semimetallic α phase to the metallic β phase even at room temperature, which has made the growth of α-Sn difficult for years. However, thin films of pure α-Sn grown on CdTe (Ref. 2) and InSb (Refs. 2–5) substrates by molecular-beam epitaxy (MBE) have been shown to be stable at temperatures well above room temperature. The incorporation of Ge is expected to raise the transition temperature even further.[6,7]

In spite of the very large lattice mismatch of 14.7% between α-Sn and Ge, short-period strained α-Sn/Ge SL's have been successfully grown pseudomorphically on a Ge(001) substrate by Wegscheider *et al.*[8] by a modified MBE technique. Because of the very large lattice mismatch between α-Sn and Ge, it has been found that on a Ge substrate, the critical thickness of α-Sn layers for the pseudomorphic growth is less than two monolayers.[8] Misfit defects might be introduced if the critical thickness of Ge layers were exceeded. It is expected that on an α-Sn substrate, the critical thickness of Ge layers must be even smaller, since the elastic constants of Ge are larger than those of α-Sn. Kasper *et al.*[9] indicated that the thickness of a strained SL strongly depends on the strain distribution. The unsymmetrical strain distribution can produce an energy instability, which imposes restrictions not only on the thickness of the sublattices but also on the total thickness. On the other hand, symmetrically strained SL's could be stable up to a much larger overall thickness. These suggestions have been shown by Zi, Zhang, and Xie[10] in the case of Si/Ge SL's. Thus, it can be expected that with an appropriate substrate, symmetrically strained α-Sn/Ge SL's could be also obtained.

In the present work, a generalized Keating model[10,11] is used for calculating geometrical structures and phonon spectra of α-Sn/Ge SL's. This model is a modified version of the Keating model,[12] which has been widely used to investigate the lattice-dynamical[12–14] and structural[15–17] problems. The detailed description of the theoretical method may be found in Refs. 10 and 11 and will not be repeated here. Structural and growth properties of α-Sn/Ge SL's are discussed in Sec. II. General features of phonon spectra of α-Sn/Ge SL's are presented in Sec. III. Section IV gives conclusions.

II. GEOMETRICAL STRUCTURES AND GROWTH

For bulk Ge and α-Sn there are only two Keating parameters α and β, describing the bond-stretching and bond-bending interactions, respectively. The values of the Keating parameters α and β for Ge are taken from Ref. 13, and for bulk α-Sn these parameters are determined by fitting the calculated optical-phonon-dispersion

curves to the experimental data, given in Table I. Figures 1 and 2 show the calculated phonon-dispersion curves by the Keating model for bulk Ge and α-Sn, respectively. For comparison, the experimental results are also given. Obviously, the Keating model can give a reasonable description of the lattice dynamics for both Ge and α-Sn. It is not totally unexpected that the calculated results do not fit well with the experimental transverse-acoustic (TA) phonon dispersion since it is difficult to describe the TA modes without taking the long-range interactions into consideration.

Because of the very large lattice mismatch between Ge and α-Sn, layers in an α-Sn/Ge SL experience a biaxial strain. The elastic strain energy can be reduced both by deforming the cell tetragonally and by relaxing the interplanar distances in the growth direction. The geometrical structures of strained α-Sn/Ge SL's grown pseudomorphically on a (001)-oriented substrate are determined by minimizing the total elastic strain energy. To assure commensurability in the (001) plane, the in-plane lattice constant of the pseudomorphic α-Sn/Ge SL's is taken to be equal to that of the substrate selected. In the following discussions, the lattice constant of the substrate $a_{\parallel}$, varying from that of Ge to that of α-Sn, takes the form

$$a_{\parallel}=(1-x)a_{\mathrm{Ge}}+xa_{\mathrm{Sn}},\quad 0\le x\le 1\ , \tag{1}$$

where a_{Ge} and a_{Sn} are the lattice constants of bulk Ge and α-Sn, respectively.

A. Ge(001) substrate ($x=0$)

Table II shows the calculated interplanar distances and axial ratio for strained $(\alpha\text{-Sn})_n/(\mathrm{Ge})_n$ $(2\le n\le 4)$ SL's grown pseudomorphically on a Ge(001) substrate. In this case, the in-plane lattice constant is equal to that of Ge. It can be clearly seen from Table II that on a Ge(001) substrate, Sn layers experience a tensile strain along the growth direction, i.e., the [001] direction. Ge layers, on the other hand, are nearly unstrained. Virtually all the strain is taken up by Sn layers. Obviously, for all SL's with different periodicity n, the Ge-Sn interplanar distance is identical within very small deviation. Moreover, this distance is close to the average of Ge-Ge and Sn-Sn distances.

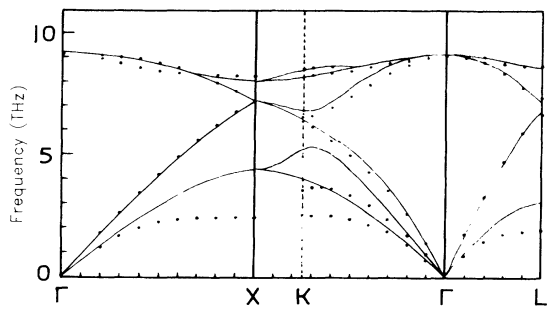

FIG. 1. Calculated phonon-dispersion curves for Ge by the Keating model. Dots are the experimental results taken from Ref. 18.

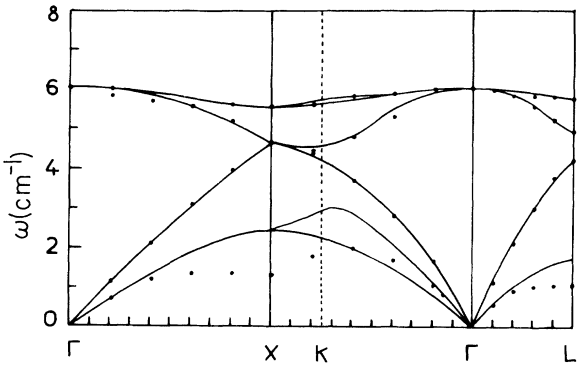

FIG. 2. Calculated phonon-dispersion curves for α-Sn by the Keating model. Dots are the experimental results taken from Ref. 19.

For an $n=4$ SL on a Ge substrate, the Ge-Ge distances next to the Ge-Sn interface are slightly larger than the other Ge-Ge distances; however, on the Sn sublattice the Sn-Sn distances next to the interface are smaller. Similar situations have also been found in the Si/Ge system.[10,11] Obviously, the difference of Ge-Ge distances on the Ge sublattice is very small, less than 0.009 Å. On the Sn side, the difference is less than 0.012 Å. Therefore, it can be reasonably assumed, for simplicity, that the interplanar distances in one sublattice are identical.

The calculated Sn-Sn interplanar distances in the case of the Ge substrate are found to be in good agreement with the experimental result[8] of 1.80±0.03 Å and the theoretical prediction of 1.801 Å based on the macroscopic theory.[20]

B. α-Sn(001) substrate ($x=1$)

It is expected that on an α-Sn(001) substrate, Sn layers in an α-Sn/Ge SL are unstrained, whereas Ge layers are fully strained. This can be clearly seen from Table III. All the SL's ($n=2$–4) are deformed approximately by the same amount. The strains is virtually wholly taken up by Ge layers which causes the contraction of Ge-Ge distances. The Ge-Sn distances for all the SL's are nearly the same, close to the average of Ge-Ge and Sn-Sn distances. This rule is found to be valid also for other substrates.

C. Proper substrate

On a substrate with lattice constant between Ge and α-Sn, both Sn and Ge layers are strained. It is found that the elastic strain energy for an α-Sn/Ge SL on this substrate is smaller than that in the case of the Ge or Sn sub-

TABLE I. Values of the Keating parameters (in eV/Å^4) for bulk Ge and α-Sn. The parameters of Ge are taken from Ref. 13 and those of α-Sn are obtained by the best fit to the experimental data.

	α	β
Ge	0.1508	0.0443
α-Sn	0.0882	0.0171

TABLE II. Interplanar distances (Å) and axial ratio $c/a_{\parallel}$ for strained $(\alpha\text{-Sn})_n/(\text{Ge})_n$ $(2 \le n \le 4)$ SL's grown pseudomorphically on a Ge(001) substrate. R(Ge-Ge), R(Ge-Sn), and R(Sn-Sn) denote Ge-Ge, Ge-Sn, and Sn-Sn distances, respectively.

	R(Ge-Ge)	R(Ge-Sn)	R(Sn-Sn)	$c/a_{\parallel}$
$n=2$	1.4008	1.5999	1.8141	1.1337
$n=3$	1.4083[a]	1.5994	1.8118[a]	1.1357
$n=4$	1.4076[a]	1.5996	1.8120[a]	1.1367
	1.4159		1.8092	

[a]This distance occurs twice.

strate due to the fact that both Ge and Sn layers are involved in relieving the elastic strain energy. If an appropriate substrate is chosen, it can be shown that the elastic strain energy for an α-Sn/Ge SL is not only minimal but its distribution is nearly symmetrical, i.e., uniformly distributed at each layer. This can be obviously seen from Fig. 3, which shows the elastic-strain-energy distribution for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL grown on different substrates. As pointed out by Kasper *et al.*,[9] the thickness of a strained SL strongly depends on the strain distribution. The unsymmetrical strain distribution can produce an energy instability, which restricts not only the thickness of the sublattice but also the total thickness. On the other hand, symmetrically strained SL's could be stable up to a much larger thickness. The appropriate values of x which ensure the minimal elastic strain energy for $(\alpha\text{-Sn})_n/(\text{Ge})_n$ $(1 \le n \le 6)$ SL's are given in Table IV, rendering the growth of a SL with a large thickness possible. This is very meaningful to experimentalists.

For Si/Ge systems, the symmetrically strained SL's can be achieved by growing on a properly chosen $Si_{1-x}Ge_x$ alloy substrate; however, for α-Sn/Ge SL's, this is not the case owing to the fact that crystalline $\alpha\text{-}Sn_xGe_{1-x}$ alloys can only be prepared in a small range of x values on a given substrate and their stability is still an open problem.[1] However, symmetrically strained α-Sn/Ge SL's can also be obtained by growing on a substrate (e.g., III-V or II-VI semiconductors) with lattice

TABLE III. Interplanar distances (Å) and axial ratio $c/a_{\parallel}$ for strained $(\alpha\text{-Sn})_n/(\text{Ge})_n$ $(2 \le n \le 4)$ SL's grown pseudomorphically on an α-Sn(001) substrate. R(Ge-Ge), R(Ge-Sn), and R(Sn-Sn) denote Ge-Ge, Ge-Sn, and Sn-Sn distances, respectively.

	R(Ge-Ge)	R(Ge-Sn)	R(Sn-Sn)	$c/a_{\parallel}$
$n=2$	1.2188	1.4242	1.6393	0.8794
$n=3$	1.2278[a]	1.4243	1.6304[a]	0.8800
$n=4$	1.2271[a]	1.4241	1.6311[a]	0.8802
	1.2367		1.6211	

[a]This distance occurs twice.

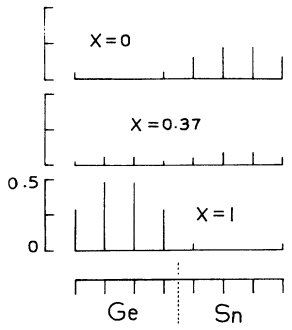

FIG. 3. Elastic-strain-energy distribution for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL grown on a different substrate. The case of $x=0.37$ corresponds to the proper substrate which ensures the SL with minimal elastic strain energy.

constant close to the values suggested in Table IV.

Note that the appropriate values of x given in Table IV decrease with the increasing periodicity n. This can be understood by the fact that the total elastic strain energy per unit cell can be divided by three contributions: bulklike Sn layers (not involving the interface Sn layers), bulklike Ge layers (not involving the interface Ge layers), and interface layers

$$E_{\text{tot}}=(n-2)e_{\text{Ge}}+(n-2)e_{\text{Sn}}+4e_{\text{Sn-Ge}} , \tag{2}$$

where e_{Ge}, e_{Sn}, and $e_{\text{Sn-Ge}}$ denote the elastic strain energy per layer for Ge, Sn, and interface layers, respectively. The fractional contribution from the bulklike Ge layers to the total energy is the factor

$$\left[1+\frac{e_{\text{Sn}}}{e_{\text{Ge}}}+4\frac{e_{\text{Sn-Ge}}}{(n-2)e_{\text{Ge}}}\right]^{-1} . \tag{3}$$

The Sn and Ge layers tend to adopt their bulk lattice constants. The interface layers, on the other hand, favor the average lattice constant. It can be seen from Eq. (3) that with an increase of periodicity the fractional contribution from the Ge layers becomes larger, leading to a decrease of appropriate values of x in order to relieve the elastic strain energy since Ge is more elastic than Sn. It can be expected that for large n ($\gg 6$) the fractional contribution from Ge layers will approach a constant, which can be treated by the macroscopic elastic theory of Ref. 20.

III. PHONON SPECTRA

It can be expected that general features of the phonon spectra of α-Sn/Ge SL's are similar to those of Si/Ge SL's. The confined modes are expected for the lighter

TABLE IV. Values of x for the minimal elastic strain energy of $(\alpha\text{-Sn})_n/(\text{Ge})_n$ $(1 \le n \le 6)$ SL's.

n	1	2	3	4	5	6
x	0.5	0.4	0.39	0.37	0.36	0.35

material and the quasiconfined modes for the heavier ones. In Si/Ge SL's the confined modes are confined to Si layers and the Ge-like modes are quasiconfined since the longitudinal-optical (LO) continuum of Ge overlaps with the longitudinal-acoustic (LA) continuum of Si, whereas in α-Sn/Ge SL's, Ge confined modes are truly confined to Ge layers and Sn confined modes are expected to be quasiconfined. No interface modes are expected in the longitudinal polarization since there are no gaps in the superposition of the longitudinal spectra of Ge and α-Sn. However, the lattice mismatch between Sn and Ge (14.7%) is much larger than that of Si and Ge (4.2%). Hence, strain plays a more important role in the α-Sn/Ge system.

A. General features

Figure 4 shows the calculated longitudinal-phonon-dispersion curves for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL grown pseudomorphically on a Ge(001) substrate along the [001] direction. The modes at 298 and 272 cm^{-1} are Ge-like confined LO modes with vibrations confined to the Ge layers and with very small vibrational amplitudes in the neighboring Sn layers. The mode around 233 cm^{-1} has finite dispersion. Since the frequency of this mode lies within the LA continuum of bulk Ge, there is a significant acousticlike excitation of Ge atoms. It is found from the displacement patterns that this mode is not an interface mode since the vibrations of Ge atoms away from the interface remain considerable. Moreover, the frequency of this mode is thickness dependent, depending mainly on the thickness of the Ge layers. Hence, a layer-thickness-dependent mode observed in experiments cannot be due to the mode around 233 cm^{-1}. The two modes below 230 cm^{-1} are Sn-like quasiconfined LO modes. The frequencies of these modes overlap with the LA continuum of bulk Ge. Therefore, the finite dispersion of these modes is due to a strong LA excitation existing in the Ge atoms. As a result of the finite thickness of Sn layers, the confinement always produces a downward shift of frequency for a Sn-like mode. However, grown on a Ge(001) substrate, the Sn layers experience a tensile strain along the growth direction and an in-plane compressive strain. Because of the very large lattice mismatch of 14.7% between Ge and Sn, frequencies of Sn-like modes are shifted upward considerably.[21] For an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL on Ge(001), the frequency shift due to the strain is larger than that induced by the confinement,[22] which makes the frequency of the first Sn-like quasiconfined LO mode (205 cm^{-1} at the zone center) slightly higher than that of the LO phonon of the bulk at the zone center. The three modes in the low-frequency range are the extended modes resulting from the folding procedure due to the reduction in the Brillouin zone in SL's. The minigaps at the zone center and boundary come from the difference in the sound velocities of bulk Ge and Sn. The observation of such folded doublets at $q \approx 0$ yields a precise determination of the overall thickness of SL's.

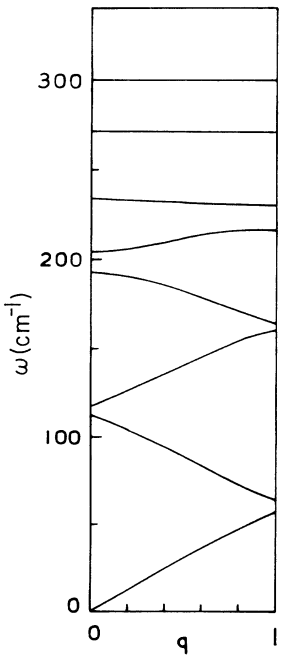

FIG. 4. Calculated longitudinal-phonon-dispersion curves along the [001] direction for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL grown pseudomorphically on a Ge(001) substrate.

No interface modes are found in the longitudinal polarization because of the absence of gaps in the phonon continua of Ge and α-Sn, similar to the observations in the Si/Ge system.[11,23–25]

For transverse polarization, the calculated phonon-dispersion curves of an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL on Ge(001) along the [001] direction are given in Fig. 5. There are two kinds of transverse modes, [110] and [1$\bar{1}$0] polarized, respectively. The three modes in the range 270–300 cm^{-1} are the Ge-like confined transverse-optical (TO) modes. In the range 160–180 cm^{-1}, there are three modes, one [1$\bar{1}$0] polarized and two [110] polarized. These modes are the true Sn-like confined TO modes since the frequencies of these modes lie within the gap of the phonon continua of bulk Ge. Between the Sn-like and Ge-like confined modes, two interface modes at 235 and 228 cm^{-1} appear. The frequencies of these modes lie within the gap of the phonon continua of bulk Ge and α-Sn, so that neither Ge layers nor Sn layers can sustain the vibrations. These modes are sharply localized at the interface and their vibrational amplitudes decay exponentially with the distance away from the interface. No interface modes are expected in the [110] polarization because the Sn—Ge bonds are all along the [1$\bar{1}$0] direction for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL. The two modes in the range 100–120 cm^{-1} are found to be thickness dependent. Frequencies of these modes are mainly dependent on the thickness of the Ge layers, since their frequencies lie in the Ge TA continuum, just in the gap of the α-Sn phonon continua. Therefore, strong TA excitations of Ge atoms exist.

B. Confinement

In Si/Ge SL's, the Ge-like LO modes are quasiconfined owing to the overlapping with the LA continuum of bulk

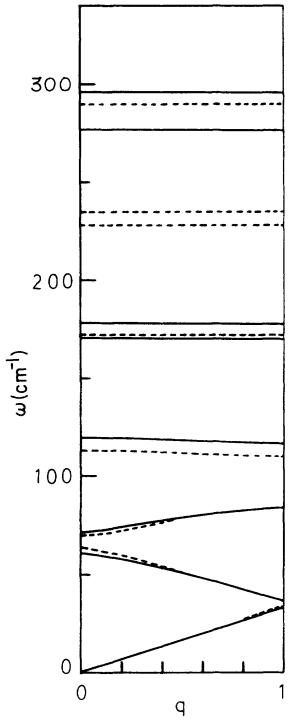

FIG. 5. Calculated transverse-phonon-dispersion curves along the [001] direction for an $(\alpha\text{-Sn})_4/(\text{Ge})_4$ SL grown pseudomorphically on a Ge(001) substrate. The solid curves are [110] polarized and the dashed curves are $[1\bar{1}0]$ polarized.

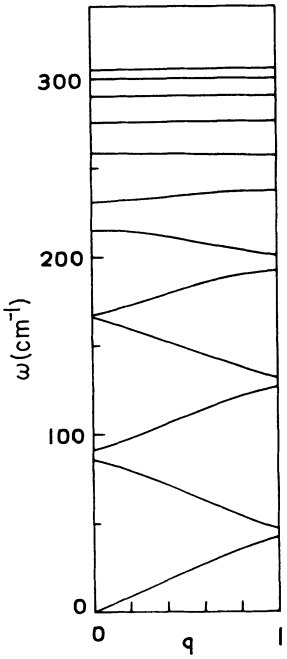

FIG. 6. Calculated longitudinal-phonon-dispersion curves along the [001] direction for an $(\alpha\text{-Sn})_2/(\text{Ge})_{10}$ SL grown pseudomorphically on a Ge(001) substrate.

Si.[26] However, in α-Sn/Ge SL's, Ge-like LO modes are truly confined to Ge layers, whereas Sn-like modes are quasiconfined. To assess the degree to which the LO phonons are confined, an $(\alpha\text{-Sn})_2/(\text{Ge})_{10}$ SL grown on a Ge(001) substrate is studied. The calculated results are shown in Fig. 6. The top five modes, which show almost no dispersion through the Brillouin zone, belong to the Ge-like confined modes. The corresponding displacement patterns are given in Fig. 7. It can be seen that for the higher-order (numbered in the order of decreasing frequency) Ge-like confined modes, vibrations of Sn atoms are more noticeable. This seems to indicate that vibrations of the neighboring Sn layers cannot be neglected for these modes. In other words, the effective layer thickness "seen" by the higher-order modes becomes larger than the lower-order modes. This is not surprising since vibrations of lower-order modes, with wave vector nearer to the zone center, are small for Ge atoms at the interface. On the contrary, vibrations of Ge atoms near the interface for higher-order modes are large and significant vibrations on the neighboring Sn atoms are excited.

Based on the idea of Sood *et al.*[27] that a confined mode can be described by a single slab mode, the dispersion of a Ge-like confined mode corresponds to the appropriate bulk dispersion at an effective wave vector, defined as a dimensionless quantity (in units of $2\pi/a$, a being the lattice constant)

$$q_{\text{eff}} = ja/2d_{\text{eff}} , \tag{4}$$

where j is the order of a confined mode and d_{eff} is the thickness of an effective slab to which the vibrations of the confined mode actually extend. It is found that an effective confinement length $d_{\text{eff}}=(n+1)a/4$ can be used to describe all Ge confined modes, where n is the number of Ge layers. This relationship is similar to that of Si-like confined LO modes found in Si/Ge SL's.[28,29]

For Sn-like modes, the confinement is very complex since their frequencies overlap with the LA continuum of bulk Ge. Strong LA-like excitations in Ge layers are expected. An $(\alpha\text{-Sn})_{10}/(\text{Ge})_2$ SL grown on an α-Sn(001) substrate is investigated in order to study the confinement

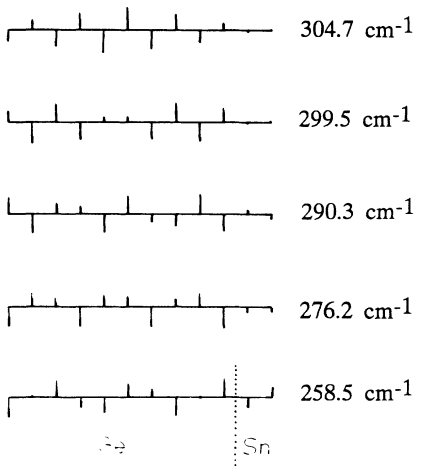

FIG. 7. Displacement patterns of the top five modes in Fig. 6.

of Sn-like modes. The reason for using an α-Sn substrate is to rule out the effect of strain on Sn-like modes. The calculated longitudinal-phonon-dispersion curves along the [001] direction and the corresponding displacement patterns for some selected modes are shown in Figs. 8 and 9, respectively. The mode at 256 cm^{-1} is a Ge-like confined mode. The frequency shift with respect to the bulk phonon at the zone center is due to both the strain and confinement. On an α-Sn substrate, the Ge layers suffer an in-plane tensile strain and a compressive strain along the growth direction, which causes a downward frequency shift in the Ge-like modes. The mode at 205 cm^{-1} (at the zone center) is an extended mode with a strong LA-like excitation in Ge atoms. The five modes at 202, 192, 188, 165, and 160 cm^{-1} (at the zone center) are the Sn-like quasiconfined modes. It can be seen from the displacement patterns that the odd-order modes (202, 188, and 160 cm^{-1}) are more confined than the even-order modes. Hence, the confinement length of the odd-order modes is smaller than that of the even-order modes. Since there exists a strong LA-like excitation of Ge atoms in these modes, their frequencies are somewhat dependent on the thickness of Ge layers, especially for the higher-order modes. The confinement on the Sn-like modes is quite complex and cannot be described simply by the bulk dispersion.

C. Interface modes

No interface modes are found in the longitudinal polarization since there are no gaps in the phonon continua of bulk Ge and α-Sn. However, two proper interface modems appear in the transverse polarization. For a SL

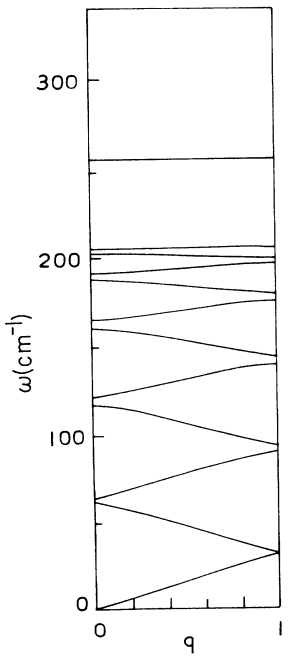

FIG. 8. Calculated longitudinal-phonon-dispersion curves along the [001] direction for an $(\alpha\text{-Sn})_{10}/(\text{Ge})_2$ SL grown pseudomorphically on an α-Sn(001) substrate.

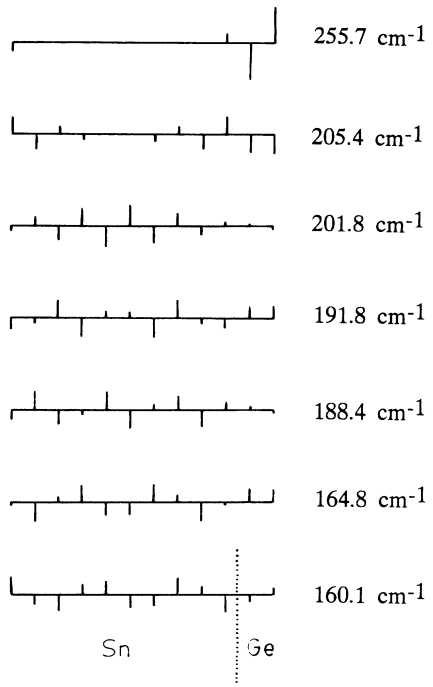

FIG. 9. Displacement patterns of some selected modes in Fig. 8.

with D_{2h} point-group symmetry, the two interface modes are split. For a SL belonging to D_{2d}, no splitting is expected due to the constraint of symmetry. The displacement patterns of interface modes in $(\alpha\text{-Sn})_4/(\text{Ge})_4$ and $(\alpha\text{-Sn})_2/(\text{Ge})_6$ SL's on Ge(001) are given in Fig. 10 for showing how interface modes are localized at the interface. If the D_{2h} symmetry exists, frequencies of the two interface modes remain nearly unchanged with changes in thickness of either Ge or Sn layers. For instance, the frequencies of two interface modes in an $(\alpha\text{-Sn})_4/(\text{Ge})_4$

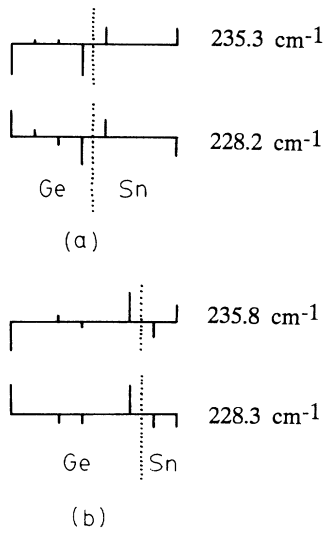

FIG. 10. Displacement patterns of $[1\bar{1}0]$-polarized interface modes for (a) $(\alpha\text{-Sn})_4/(\text{Ge})_4$ and (b) $(\alpha\text{-Sn})_2/(\text{Ge})_6$ SL's.

SL are 235.3 and 228.2 cm^{-1}; in an $(\alpha\text{-Sn})_2/(Ge)_6$ SL they are 235.8 and 228.3 cm^{-1}. Even in an $(\alpha\text{-Sn})_2/(Ge)_{20}$ SL, the frequencies are virtually unchanged, at 234.7 and 229.4 cm^{-1}.

IV. CONCLUSIONS

In summary, geometrical structures of α-Sn/Ge SL's are studied by a generalized Keating model through elastic-strain-energy minimization. For α-Sn/Ge SL's, proper substrates are suggested in order to obtain a symmetrically strained SL with as large a thickness as possible. In addition, phonon spectra are also studied. The general features of the phonon spectra are found to have close similarity with those of Si/Ge systems. It is found that for a SL grown on a Ge(001) substrate, the Ge-like confined modes can be well described by the bulk dispersion with the effective confinement length taken as $d_{\text{eff}}=(n+1)a/4$, where n is the number of Ge monolayers. The Sn-like confined modes, on the contrary, are quite complex. The odd-order Sn-like modes are found to be more confined than the even-order modes. No interface modes are found in the longitudinal polarization, but such modes do appear in the transverse polarization around 232 cm^{-1}.

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