Ab initio pseudopotential calculations of the transverse and longitudinal phonon spectra of Ge, α-Sn, and α-Sn/Ge superlattices

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A combination of a first-principles pseudopotential plane wave and the interplanar force constants (IPFC's) methods is used to calculate the transverse (T) and longitudinal (L) phonon spectra along [001] of Ge and biaxially strained α-Sn, which correspond to a coherent growth on α-Sn, α-$Sn_{0.5}Ge_{0.5}$, and Ge(001) substrates. The calculated sets of IPFC's are also used to investigate the phonon spectra of α-Sn/Ge superlattices (SL's) pseudomorphically grown on a Ge substrate. Our results for both the T and L phonon spectra of unstrained α-Sn are in good agreement with the experimental data, and their variations with respect to the (001)-biaxial strain are predicted. Despite the large lattice mismatch between Ge and α-Sn, the calculated phonon spectra of α-Sn show a linear variation with respect to the strain state. The T and L confined and interface phonon modes in the α-Sn/Ge SL's are discussed, in comparison with the corresponding phonon spectra of bulk Ge and properly strained α-Sn. In particular, the Ge-like L- and T-optical confined modes in α-Sn_m/Ge_n SL's are well described relative to the bulk dispersions of Ge by effective confinement lengths equal to $(n+1)a_0$(Ge)/4 and $(n+3)a_0$(Ge)/4, respectively. [S0163-1829(99)00926-1]

I. INTRODUCTION

The recent progress in the growth techniques, such as the molecular-beam epitaxy (MBE), has allowed for the growth of high-quality superlattices (SL's) with very large lattice mismatch between their constituent materials. Of particular interest here is the α-Sn/Ge SL's that have been grown by low-temperature MBE by Wegscheider and co-workers,[1,2] on a Ge(001) substrate. The lattice mismatch between Ge and α-Sn is of 14.6%. The growth of such man-made materials has opened the way for further band-gap engineering among the group-IV semiconductors.[3–5] It has been found that α-Sn/Ge SL's with direct narrow band gaps can be obtained, under certain conditions.[4] The main aim of this work is two-fold: (i) to provide accurate predictions for the effects of the biaxial strain on the phonon spectra of α-Sn, (ii) to investigate the phonon modes in ideal α-Sn/Ge SL's, grown on a Ge(001) substrate.

Phonons in semiconductor SL's have been the subject of a large number of experimental and theoretical investigations.[6] In addition to their fundamental importance, phonons in SL's are essential in the characterization of these very interesting materials. New features have been observed in the phonon spectra of the semiconductor SL's, such as the confined optical, interface, and folded acoustical modes. Moreover, phonons in strained SL's have renewed the interest in the effects of the biaxial strain on the phonon spectra of bulk semiconductors. The effects of the (001) biaxial strain on the longitudinal (L) (Ref. 7) and transverse (T) (Ref. 8) phonon spectra of Si and Ge have been thoroughly investigated, using a first-principles pseudopotential plane-wave (PP-PW) technique[9] combined with the interplanar force constants (IPFC's) method.[10] This approach is found to give results in excellent agreement with the available experimental data for both the L and T phonon spectra of Si and Ge, and the induced shifts of these phonon spectra due to the biaxial (001) strain.[7,8] Furthermore, the obtained sets of IPFC's were used to investigate the phonon spectra of Si/Ge SL's. It has been found that the confined phonon modes can be described relative to the bulk dispersions by effective confinement lengths $d_{\text{eff}}=(n+1)a_\perp/4$ for the Si-like L-optical (LO) modes, and $d_{\text{eff}}=(n+3)a_\perp/4$ for the Si-like and Ge-like T-optical (TO) modes.[7,8] Here, n is the number of Si or Ge atomic layers in the SL unit cell, and $a_\perp/4$ is the corresponding interplanar distance.

As for α-Sn, no information, to the best of our knowledge, is available in the literature about the effects of the biaxial strain on its phonon spectra. Moreover, the phonon modes in α-Sn/Ge SL's have only been studied by using a phenomenological approach based on the Keating model,[11] and very briefly by assuming a mass approximation.[7(b)] The former approach is proved to be inappropriate for studying the biaxial strain-induced effects on the phonon spectra of Si and Ge, see Ref. 8, whereas the second approach is found to overestimate, by 30 cm^{-1}, the frequency of the LO mode at the zone center of α-Sn. Therefore, an accurate study of the biaxial strain effects on the phonon spectra of α-Sn and the phonon modes in α-Sn/Ge SL's is in order.

In this work we used the method of Refs. 7 and 8 to calculate the L and T phonon spectra along [001] of unstrained bulk α-Sn, and the effects of the (001) biaxial strain on these phonon spectra. Moreover, the calculated sets of IPFC's are used to investigate the phonon modes along [001] in some α-Sn/Ge SL's, lattice matched to a Ge(001) sub-

strate. Since only one phonon propagation direction is considered in this work, the direction of the IPFC's; substrate, and biaxial strain will, hereafter, be suppressed. In Sec. II, we briefly describe our computational method and give the details of the calculations. In Sec. III, we report and discuss our results for the *T*- and *L*-IPFC's, phonon spectra of unstrained Ge and α-Sn, and the strain-induced effects on the phonon spectra of α-Sn. In Sec. IV, we report and discuss the calculated *T* and *L* phonon modes in α-Sn/Ge SL's. Finally, we give in Sec. V a summary of our main results and conclusions.

II. METHOD AND COMPUTATIONAL DETAILS

The *T*-and *L*-IPFC's of unstrained bulk Ge and biaxially strained α-Sn were calculated by using the supercell method. Three strain configurations have been considered for α-Sn, which correspond to a coherent growth on α-$Sn_{1-x}Ge_x$ substrates, with $x=0$, 0.5, and 1. Tetragonal supercells of eight (twelve) atoms were used to calculate the *L*-(*T*-) IPFC's. This enables us to determine the IPFC's up to the fourth (sixth) nearest-neighboring planes for the *L* (*T*) polarization. The convergence of the phonon spectra with respect to the highest-order IPFC included in the calculations has been checked previously for Si and Ge,[7,8] and the above choice is found to be an excellent one. A similar check has been performed for unstrained bulk α-Sn. For example, by increasing to eight the highest-order *T*-IPFC included, the maximum change in the calculated frequency of the TO and *T*-acoustical (TA) phonon modes is of 1 cm^{-1}, as it is the case for Si and Ge.[8]

The structure of the above supercells can be fully determined by two structural parameters: an in-plane lattice parameter ($a_{\parallel}$) that is assumed to be equal to that of the substrate, and a perpendicular lattice parameter ($a_{\perp}$). In our present work we have used the experimental data for the equilibrium lattice parameters (a_0^{Expt}) of bulk Ge and α-Sn, which are of 5.65 Å (Ref. 12) and 6.49 Å (Ref. 13), respectively. It is worth noting here that this choice is different from the one adopted in Refs. 7 and 8, where we have used the calculated values of a_0 (a_0^{Theo}). This is mainly because we found that this choice gives a better quantitative agreement between the calculated phonon spectra of α-Sn and the corresponding experimental data, see below. For this reason, we have also recalculated the *L*- and *T*-IPFC's of unstrained Ge and its phonon spectra, at a_0^{Expt}.

The values of $a_{\perp}$ of α-Sn with the above three strain configurations were determined by using the macroscopic elasticity theory.[14] The used values of the elastic constants c_{11} and c_{12} are of 0.690 and 0.293 Mbar,[15] respectively. It has been found that the elasticity theory result for the Sn-Sn interplanar distance in the α-Sn/Ge SL's, grown on a Ge substrate, is in very good agreement with the observed value.[1] Here we have also checked this choice by calculating the $a_{\perp}/a_{\parallel}$ ratio of bulk α-Sn lattice matched to a Ge substrate, using the PP-PW method.[9] The so-calculated value is of 1.25, which is in excellent agreement with the elasticity theory result of 1.27. Furthermore, we have checked the effects of such small discrepancy in the Sn-Sn interplanar distance on the calculated phonon spectra of bulk α-Sn, which are found to be very small [less that 2 cm^{-1} for the whole LO and *L*-acoustical (LA) branches].

TABLE I. Calculated *L*-IPFC's (in 10^5 dyn/cm), $\{k_i\}$, for unstrained bulk Ge and biaxially strained α-Sn, lattice matched to three different substrates. For k_0, we show both the calculated value, in parentheses, and the value obtained from the other IPFC's by using the acoustic sum rule. The used values of $a_{\parallel}$ and $a_{\perp}$ are also shown.

	Ge	α-Sn		
	Ge sub.	Ge sub.	α-$Sn_{0.5}Ga_{0.5}$ sub.	α-Sn sub.
$a_{\parallel}$ (Å)	5.65	5.65	6.07	6.49
$a_{\perp}$ (Å)	5.65	7.20	6.85	6.49
k_0	(+2.0470)	(+1.9870)	(+1.7061)	(+1.4165)
k_0	+2.0448	+1.9834	+1.7022	+1.4142
$k_{\pm 1}$	−0.9084	−0.9371	−0.7860	−0.6456
$k_{\pm 2}$	−0.1221	−0.0662	−0.0741	−0.0666
$k_{\pm 3}$	+0.0072	+0.0171	+0.0116	+0.0039
$k_{\pm 4}$	+0.0009	−0.0055	−0.0026	+0.0011

The *L*- and *T*-IPFC's were determined from the calculated Hellmann-Feynman forces after displacing one atom in the supercell by $(0.000,0.000,0.007)a_{\perp}$ and $(0.007,0.007,0.000)a_{\parallel}$, respectively. The calculations were performed by using a PP-PW approach and the Ceperley-Alder data for the exchange-correlation energy[16] as parametrized by Perdew and Zunger.[17] The Kohn-Sham equations were solved by using the Teter-Payne-Allan conjugate gradient total-energy minimization technique.[18] PW's up to 15 and 18 Ry in energy were used to expand the wave functions of Ge and α-Sn, respectively. The energy cutoff of Ge is the one we used in Ref. 8. The energy cutoff of α-Sn has been checked and found to give a very good convergence. For example, by increasing this cutoff energy to 22 Ry, it has been found that the change in the frequency of the LO and LA modes of unstrained bulk α-Sn is less than 1 cm^{-1}. The Brillouin-zone integrations were performed by sampling on a regular $4\times4\times2$ Monkhorst-Pack[19] mesh. The used Ge pseudopotential is the one we have used in our previous work.[8] For Sn we used a scalar relativistic pseudopotential generated by using the Kerker scheme,[20] in the Kleinmann-Bylander form.[21] In the generation of this pseudopotential we have used the atomic configuration $5s^2 5p^2$ for the *s* and *p* components and the ionic configuration $5s^1 5p^{1.75} 5d^{0.25}$ for the *d* component. The used core radii are of 1.9, 2.2, and 3.0 atomic units (a.u.) for the *s*, *p*, and *d* components, respectively. The nonlinear exchange-correlation core corrections are not included in this work.

III. IPFC's AND PHONON SPECTRA FOR UNSTRAINED Ge AND STRAINED α-Sn

The calculated sets of *L*- and *T*-IPFC's, $\{k_i\}$, as described in Sec. II, of unstrained bulk Ge and biaxially strained α-Sn (with three strain configurations) are listed in Tables I and II. In the case of the *T*-IPFC's, the given values are for the [110] polarization direction. Those of the $[1\bar{1}0]$ polarization are related to the listed values by

$$k_i^{1\bar{1}0} = k_{-i}^{110}. \tag{1}$$

TABLE II. As in Table I, but for the *T*-IPFC's.

Force constant	Ge	α-Sn		
	Ge sub.	Ge sub.	α-$Sn_{0.5}Ge_{0.5}$ sub.	α-Sn sub.
k_0	(+1.5740)	(+1.4018)	(+1.2667)	(+1.1346)
k_0	+1.5717	+1.3987	+1.2641	+1.1322
k_{+1}	−1.3729	−1.3301	−1.1819	−1.0245
k_{-1}	−0.2514	−0.1163	−0.1261	−0.1408
$k_{\pm 2}$	+0.0595	+0.0454	+0.0406	+0.0361
k_{+3}	−0.0163	−0.0069	−0.0071	−0.0072
k_{-3}	−0.0814	−0.0463	−0.0457	−0.0493
$k_{\pm 4}$	+0.0200	+0.0091	+0.01031	+0.0115
k_{+5}	−0.0070	−0.0038	−0.0036	−0.0042
k_{-5}	−0.0187	−0.0079	−0.0091	−0.0112
$k_{\pm 6}$	+0.0085	+0.0032	+0.0038	+0.0049

The IPFC's of α-Sn show the same general features as the corresponding ones of Si and Ge,[7,8] namely, the very good convergence with respect to the size of the used supercells to calculate them; the alternation of sign in the case of the *T*-IPFC's, and the very good fulfilment of the acoustic sum rule (which reflects the very good accuracy of our calculations). Because of the use of a_0^{Expt} in this work, the present IPFC's for unstrained bulk Ge are smaller than the corresponding ones reported in Refs. 7 and 8. For example, the present value of k_0 of the *T* polarization is smaller than that of Ref. 8 (1.7061×10^5 dyn/cm) by about 7%.

Figure 1 depicts the calculated *L* and *T* phonon curves along the Δ direction of unstrained Ge and α-Sn, using the calculated IPFC's (at both a_0^{Expt} and a_0^{Theo}) and the linear-chain model,[9] together with the neutron-scattering data.[22,23] The main features to note from this figure are as follows: (i) The phonon modes calculated at a_0^{Expt} are softer than the corresponding ones calculated at a_0^{Theo}. This is most noticeable in the TO modes of Ge, and both the TO and LO modes of α-Sn, where the difference in their calculated frequencies is between 10 and 15 cm^{-1}. (ii) The overall very good agreement between our calculated results at a_0^{Expt} and the experimental data can be easily inferred, for both Ge and α-Sn. In the case of α-Sn, the error in the calculated frequency of the TO mode at the Γ point, $\omega_{\mathrm{TO}}(\Gamma)$, is 2% and 7.5% in the case of using a_0^{Expt} and a_0^{Theo}, respectively. This is the reason behind our choice of using a_0^{Expt} in this work. (iii) For cubic elemental semiconductors, the TO and LO phonon modes at the zone center are degenerate. This is not the case in our calculations, because of the different computational ingredients used to calculate the *L*- and *T*-IPFC's. This is mainly due to the different **k**-points sampling resulting from the different lengths of the supercells used, and the atomic displacements that may lead to some enharmonic effects (neglected in the present work). However, the splitting of the TO and LO modes at the Γ point is about 2% of $\omega_{\mathrm{TO}}(\Gamma)$, which is of the same order as the discrepancy between our calculated results and the experimental data. Therefore, this discrepancy can be used as an estimate of the uncertainty in our results.

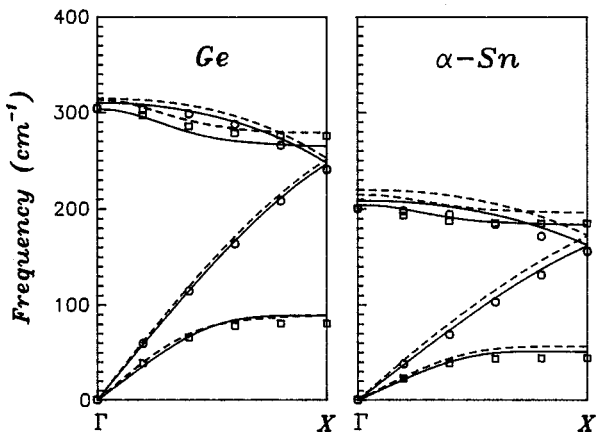

FIG. 1. Calculated phonon dispersion relations along [001] of unstrained bulk Ge and α-Sn, at a_0^{Expt} (solid lines) and a_0^{Theo} (dashed lines). Experimental data from neutron-scattering measurements are shown by circles and squares for *L* and *T* polarizations, respectively. The experimental results are taken from Ref. 22 for Ge (at $T=80$ K) and from Ref. 23 for α-Sn (at $T=90$ K).

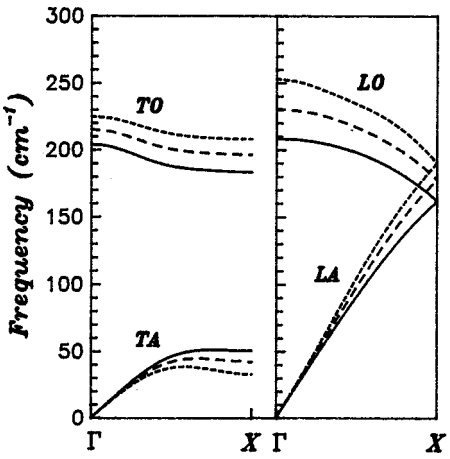

FIG. 2. Calculated *L* and *T* phonon dispersions along [001] of bulk α-Sn with three biaxial strain configurations, corresponding to lattice matching to α-Sn (solid lines), α-$Sn_{0.5}Ge_{0.5}$ (long-dashed lines), and Ge (short-dashed lines) substrates.

The biaxial strain induced effects on the *L* and *T* phonon spectra of α-Sn were investigated by calculating these spectra at the above three strain configurations. The results are shown in Fig. 2. The important features to note from this figure are as follows. (i) The compressive biaxial strain leads to an upward shift in the frequency of the TO, LO, and LA phonon modes, while it leads to a downward shift of that of the TA modes. This behavior is consistent with that of the phonon spectra of Ge,[7,8] lattice matched to $Si_{1-x}Ge_x$ substrates, which, in turn, is consistent with the sign of the experimental values of the Grüneisen parameters[24] of these phonon modes (positive for the TO, LO, and LA, and negative for the TA). (ii) The calculated shifts in the *L* and *T* phonon spectra show almost a linear variation with respect to the strain state, despite the large strain range considered. (iii) The strain-induced shift in the frequency of the TO and LO phonon modes over the Δ direction show a weak and a quite strong wave-vector dependence, respectively. By going from α-Sn to Ge substrates, the difference in the shift of the calculated values of ω_{LO}, $\Delta\omega_{\mathrm{LO}}$, at the Γ and *X* points is 15.9 cm^{-1}, while it is only 4.1 cm^{-1} in the case of $\Delta\omega_{\mathrm{TO}}$. (iv) For α-Sn lattice matched to a Ge substrate, the calculated values of $\Delta\omega_{\mathrm{LO}}(\Gamma)$ and $\Delta\omega_{\mathrm{TO}}(\Gamma)$ are 44.5 and 22.1 cm^{-1}, respec-

tively. Experimental data for the strain-induced effects on the phonon spectra of α-Sn are unavailable, and, so, the above results serve as predictions.

The (001) biaxial strain can be divided into isotropic and uniaxial contributions. Concentrating on the optical-phonon modes at the Γ point, the former contribution shifts the averaged frequency of the LO and the two TO modes, $\Delta\overline{\omega}(\Gamma)$, while the latter yields a splitting between the frequency of the LO (singlet) and the TO (doublet) modes, $\Delta\omega_{\mathrm{LO\,TO}}(\Gamma)$. For α-Sn lattice matched to a α-$Sn_{0.5}Ge_{0.5}$ substrate, the calculated values of $\Delta\overline{\omega}(\Gamma)$ and $\Delta\omega_{\mathrm{LO\,TO}}(\Gamma)$ are 14.8 and 11 cm^{-1}, respectively. Whereas, in the case of the lattice matching to a Ge substrate, they are 29.6 and 22.4 cm^{-1}, respectively. This reflects more clearly the linearity of the biaxial strain induced frequency shifts.

IV. PHONON SPECTRA OF α-Sn/Ge SL's

In this section we will use the above calculated IPFC's to investigate the general features of the *L* and *T* phonon modes in strained α-Sn/Ge SL's lattice matched to a Ge substrate. In this study, ideal superlattices have been assumed (interface roughness and intermixing were neglected). Moreover, both the Sn-Ge interplanar distance and the IPFC's across the interface are assumed to be equal to the mean values of the corresponding ones in Ge and properly strained α-Sn. The effects of using this approximation for the Sn-Ge IPFC's have been checked by calculating the phonon spectra of several α-Sn/Ge SL's (lattice matched to a Ge substrate) by using the IPFC's of either Ge or strained α-Sn alone for the whole SL. For example, it has been found that the difference in the calculated frequencies of the interface phonon modes between these two extreme cases is about 2.5% of their values (about 250 cm^{-1}, see below), which justifies the use of the above approximation.

The present approach is inappropriate for investigating the effects of the intermixing on the phonon spectra of SL's. These effects have been studied in the case of the α-Sn/Ge and Si/Ge SL's, using the Keating model.[11] This work has shown that there are two main effects of the intermixing that can be summarized as follows. (i) In the presence of intermixing the interface region looks like an alloy of the constituent materials. Thus, additional peaks appear in the Raman spectra of these SL's that originate from the alloyed interface layers. (ii) The presence of alloyed interface layers reduces the effective thickness of the pure atomic layers, which leads to a downward shift in the frequency of the confined modes. As noted above, such effects are neglected in this work.

A. General features

In Fig. 3, we show the *T* and *L* phonon dispersions of bulk α-Sn lattice matched to a Ge substrate, together with those of unstrained Ge. From this figure, the expected main features for the phonon spectra of the α-Sn/Ge SL's are as follows: (i) the existence of true LO confined modes in the Ge layers, (ii) the existence of only quasiconfined LO modes in the α-Sn layers, since the LO phonon branch of strained α-Sn lies in the LA continuum of Ge, (iii) the lack of *L* interface modes, because of the absence of gaps in the *L* phonon continuum of Ge and strained α-Sn, (iv) the existence of true

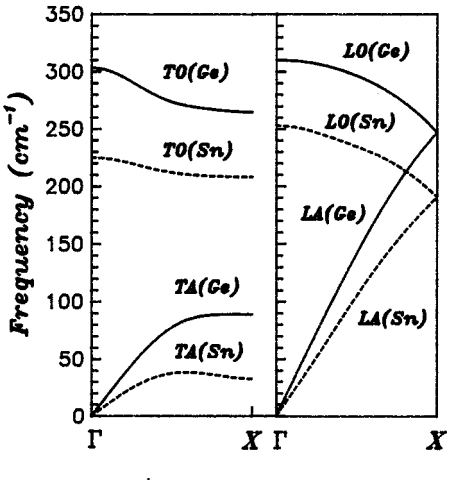

FIG. 3. Superposition of the calculated *L* and *T* phonon dispersions along [001] for unstrained bulk Ge and for biaxially strained bulk α-Sn, lattice matched to a Ge substrate.

Ge-like and α-Sn–like TO confined modes, (v) the occurrence of *T* interface modes, because frequency gaps do exist in the superposition of the *T* phonon spectra of Ge and strained α-Sn.

To illustrate the general features of the *L* phonon spectra of the α-Sn/Ge SL's, we show in Fig. 4 those of the α-Sn_4/Ge_4 SL. The two top-most modes, with frequencies 302.9 and 276.5 cm^{-1} at the zone center, are true Ge-like LO confined modes. The next three modes just below (with frequencies 244.9, 217.7, and 204.5 cm^{-1} at the Γ point) are α-Sn–like quasiconfined LO phonon modes. This can be seen from the corresponding displacement patterns, where the amplitude of the displacements of the Ge layers are sig-

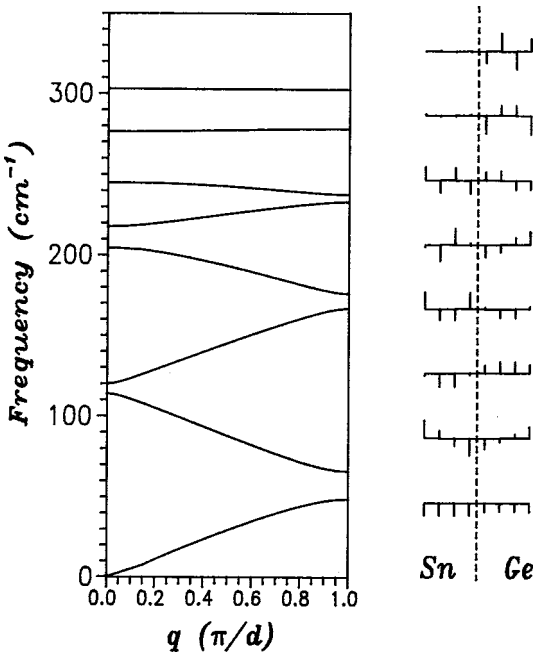

FIG. 4. The *L* phonon dispersions along [001], in the SL Brillouin zone, for the α-Sn_4/Ge_4 SL, lattice matched a Ge substrate. *d* is the SL period. Atomic displacements of the selected modes at the zone center are also displayed.

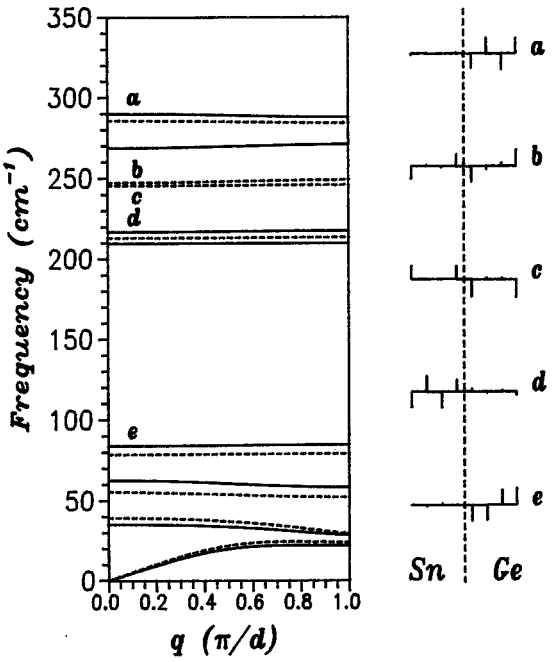

FIG. 5. As in Fig. 4, but for the T phonon dispersions. Solid curves: the [110] polarized modes. Dashed curves: the $[1\bar{1}0]$ polarized modes.

nificant but they are clearly smaller than those of the Sn layers. The rest are LA extended folded modes. As expected, no L interface modes have been found in this and other studied α-Sn/Ge SL's.

The symmetry of the α-$Sn_m/Ge_n(001)$ SL's has important consequences on their T phonon spectra. The [110] and $[1\bar{1}0]$ polarized T phonon modes are degenerate and nondegenerate in the (001) SL's with D_{2d} (odd n and m) and D_{2h} (even n and m) point groups, respectively.[25]

To illustrate the general features of the T phonon spectra of the α-Sn/Ge SL's with D_{2h} symmetry, we show in Fig. 5 those of the α-Sn_4/Ge_4 SL. The three modes in the frequency range between 260 and 300 cm^{-1} (with frequencies 289.8, 285.7, and 268.7 cm^{-1}, at the Γ point) are true Ge-like TO confined modes. The two phonon modes with frequencies very close to 250 cm^{-1} (245.5 and 247.4 cm^{-1}, at the zone center) are interface modes, since they lie in a frequency gap of the T phonon continua of bulk Ge and the properly strained bulk α-Sn (see Fig. 3). These values are in good agreement with the value obtained by Raman spectroscopy of about 260 cm^{-1} (Ref. 26). Only $[1\bar{1}0]$ polarized interface modes exist in the present case because all the Sn-Ge bonds in the α-Sn/Ge SL's with D_{2h} symmetry lie along $[1\bar{1}0]$. For these interface modes, the displacement amplitudes decay rather rapidly to zero away from the interface, as can be easily seen from the atomic displacement patterns of modes b and c, also shown in Fig. 5. The three modes in the frequency range between 200 and 220 cm^{-1} (with frequencies 216.8, 213.1, and 209.7 cm^{-1}, at the zone center) are true α-Sn–like TO confined modes. The four modes in the frequency range from 50 to 90 cm^{-1}, are Ge-like TA confined modes, since they lie above the TA phonon continua of the properly strained bulk α-Sn. The rest are TA extended folded modes.

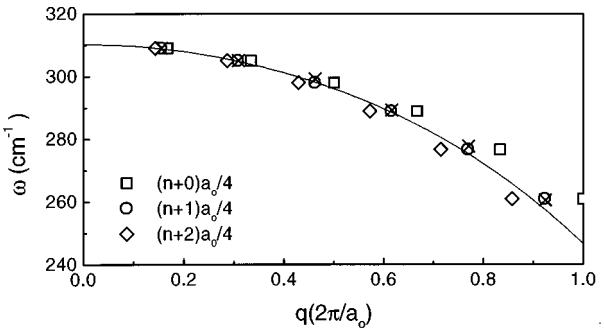

FIG. 6. Frequency of the Ge-like LO confined modes (see text) in the α-Sn_4/Ge_{12} SL, lattice matched to a Ge substrate, plotted onto the LO dispersion of unstrained bulk Ge. Three forms of d_{eff} are used. The frequency of the Ge-like LO confined modes in the α-Sn_2/Ge_{12} SL, by using $d_{\text{eff}}=(n+1)a_0/4$, are also plotted (crosses).

B. Confinement

In this subsection, we will investigate the relationship between the true Ge-like LO and TO confined modes in α-Sn/Ge SL's, lattice matched to a Ge substrate, and the corresponding phonon curves of bulk Ge. In Fig. 6 we plot the calculated frequencies of Ge-like LO confined phonon modes, ω^j_{LO} (j is the order of the modes starting with the highest-frequency one), in the α-Sn_4/Ge_{12} SL onto the LO phonon curve of bulk Ge at $q_{\text{eff}}=j\pi/d_{\text{eff}}$, where d_{eff} is the effective confinement length. This figure shows that the best fit to the LO bulk dispersions is achieved by $d_{\text{eff}}=(n+1)a_0/4$. Here, n is the number of monolayers of unstrained Ge and $a_0/4$ is the interplanar distance between them. This result is consistent with the d_{eff} of the Si-like LO confined modes in Si/Ge SL's (Ref. 7).

The situation of Ge-like TO confined modes is more complicated. This is because of the existence of two T polarization directions ([110] and $[1\bar{1}0]$), and of the effects of the symmetry of the SL's on these phonon modes. We plot in Fig. 7 the calculated frequencies of the Ge-like TO confined modes, ω^j_{TO}, in the α-Sn_4/Ge_{12}, α-Sn_5/Ge_{11}, and α-Sn_4/Ge_4 SL's onto the TO phonon curve of bulk Ge at $q_{\text{eff}}=j\pi/d_{\text{eff}}$. Three forms of d_{eff} have been considered. From this figure, it is evident that a very good description of these modes, with both [110] and $[1\bar{1}0]$ polarizations, relative to the TO curve of bulk Ge can be obtained by $d_{\text{eff}}=(n+3)a_0/4$. The quality of the fitting decreases for the two or three low-frequency TO confined modes (higher-order modes). This can be understood, since these modes are less confined to Ge layers than the ones with higher frequencies. This result is in accord with that of Ref. 8, for the Si-like and Ge-like TO confined modes in Si/Ge SL's. One may argue, according to Fig. 7(c), that the ω^j_{TO}, of the $[1\bar{1}0]$ polarized confined modes in the α-Sn_4/Ge_{12} SL are better fitted by $d_{\text{eff}}=(n+2)a_0/4$. This is true. However, the first two of these modes ($j=1$ or 2) are also very well described by $d_{\text{eff}}=(n+3)a_0/4$. Furthermore, $d_{\text{eff}}=(n+3)a_0/4$ is almost the average of the [110] and $[1\bar{1}0]$ polarized Ge-like TO confined modes in α-Sn_4/Ge_4 SL. Therefore, $d_{\text{eff}}=(n+3)a_0/4$ can be used, to a very good approximation, as d_{eff} of all the Ge-like TO confined modes in the α-Sn/Ge SL's. The difference in the

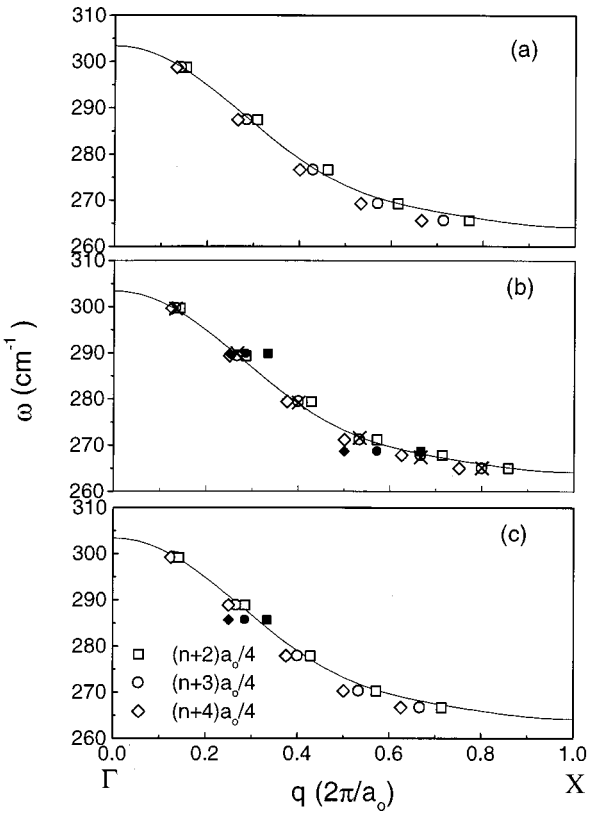

FIG. 7. As in Fig. 6, but for the Ge-like TO confined modes in α-Sn_5/Ge_{11} SL (a) and in α-Sn_4/Ge_{12} SL, with both [110] (b) and $[1\bar{1}0]$ (c) polarizations. The frequency of the Ge-like TO confined modes with [110] polarization in the α-Sn_2/Ge_{12} SL, by using $d_{\text{eff}}=(n+3)a_0/4$, are also plotted (crosses). Those of the α-Sn_4/Ge_4 SL are also shown (solid symbols, for the same three forms of d_{eff}).

forms of d_{eff}, of the LO and TO confined modes has been explained as a direct consequence of the fact that the *T*-IPFC's are of longer range than the *L* ones (for more details, see Ref. 8).

Because of the very large lattice mismatch between Ge and α-Sn, the grown α-Sn_m/Ge_n SL's, on a Ge substrate, have only one or two Sn monolayers.[1,2] It would be of interest to study the effects of having such very small numbers of Sn monolayers in the above SL's on the confinement of their Ge-like TO and LO phonon modes. For this reason, we have studied the confinement of these modes in the α-Sn_2/Ge_{12} and α-Sn_1/Ge_{13} SL's. It has been found that the confinement of the Ge-like phonon modes is very slightly affected by such a decrease in the number of Sn monolayers. For example, the frequency width of the Ge like LO confined modes in the α-Sn_2/Ge_{12} and α-Sn_4/Ge_{12} SL's is of 0.3 and 0.5 cm^{-1}, respectively, whereas, that of the Ge-like TO confined modes is of 0.5 and 2.5 cm^{-1}, respectively. In Figs. 6 and 7 we also plot the centers of these narrow frequency bands of the Ge-like LO and [110] polarized TO confined modes in the α-Sn_2/Ge_{12} SL, respectively, onto the corresponding curves of bulk Ge. Here, only one form of d_{eff} has been used in each case [$(n+1)a_0/4$ and $(n+3)a_0/4$, respectively]. The obtained results lie almost on top of the corresponding ones of the α-Sn_4/Ge_{12} SL. Therefore, one can conclude that the above forms of d_{eff} are still valid even for such a very small number of Sn monolayers in the SL unit cell.

C. Interface modes

As noted above, only *T* interface phonon modes exist in the α-Sn_m/Ge_n SL's. These modes are degenerate and nondegenerate in the α-Sn/Ge SL's with D_{2d} and D_{2h} symmetries, respectively. For Si_n/Ge_m SL's with D_{2h} symmetry, we have found that the frequency of the two interface modes converge to the same value when both *n* and *m* are greater than eight.[8] Otherwise, a splitting occurs because of the interface-interface interaction. The same behavior has been for the interface modes in α-Sn/Ge SL's with D_{2h} symmetry. For example, their frequencies in the α-Sn_4/Ge_4 SL are of 245.5 and 247.4 cm^{-1}, see above. This can be easily understood, since the long-range nature of the *T*-IPFC's of α-Sn is similar to that of Ge and Si. Therefore, a splitting in the frequency of the interface modes is expected in all the experimentally grown α-Sn/Ge SL's with D_{2h} symmetry, on a Ge substrate (at least). To show this, we have studied the interface phonon modes in α-Sn_2/Ge_n SL's with $n=2,4,...,12$. We have found that the frequencies of the two interface modes at the Γ point change monotonically by increasing *n*, for *n* less than or equal to eight, between the values of 237.7 and 263.1 cm^{-1} (in the α-Sn_2/Ge_2 SL) and 240.0 and 248.85 cm^{-1} (in the α-Sn_2/Ge_8 SL). For *n* larger than eight, the frequencies of these interface modes stay almost unchanged, with a split of about 8 cm^{-1}.

V. CONCLUSIONS

The longitudinal and transverse phonon spectra along [001] for bulk Ge and (001) biaxially strained α-Sn were studied, using first-principles pseudopotential and interplanar force constants methods. The general features of the *T* and *L* phonon spectra of α-Sn/Ge superlattices, lattice matched to a Ge(001) substrate, have also been similarly investigated. In the following we summarize our main results and conclusions.

(1) The calculated *L* and *T* phonon spectra for unstrained Ge and α-Sn are found to be in very good agreement with experiment.

(2) An almost rigid shift is predicted for the TO phonon branch of α-Sn due to the (001) biaxial strain, while that of the LO branch shows a quite strong wave-vector dependence.

(3) The Ge-like LO and TO confined phonon modes in α-Sn_m/Ge_n SL's are well described with respect to the corresponding curves of bulk Ge by effective confinement lengths equal to $(n+1)a_0(\text{Ge})/4$ and $(n+3)a_0(\text{Ge})/4$, respectively.

(4) In α-Sn/Ge SL's, quasiconfined LO and truly confined TO Sn-like phonon modes have been found.

(5) Only *T* interface phonon modes in α-Sn/Ge SL's have been found, with a frequency of about 250 cm^{-1}.

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