Transverse interplanar forces and phonon spectra of strained Si, Ge, and Si/Ge superlattices

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We present a first-principles pseudopotential study of the effects of the (001) biaxial strain on the transverse phonon spectra of Si and Ge along the Δ direction, and of the transverse phonon modes of strained Si/Ge (001) superlattices (SL's). The supercell method is used to calculate the [001] transverse interplanar force constants (IPFC's) of Si and Ge at three strain configurations corresponding to coherent growth on $Si_{1-x}Ge_x$ (001) (with $x=0$, 0.5, and 1) substrates. IPFC's up to the eighth-nearest-neighboring planes were included. It has been found that (i) the strain-induced frequency shift of the transverse optical (TO) branch is in excellent agreement with the available experimental data and has a weak wave vector dependence. (ii) Both the Si- and Ge-like TO confined modes in strained Si/Ge (001) SL's are well described relative to the bulk dispersions by an effective confinement length $d_{\rm eff}=(n+3)a_\perp/4$, where n is the number of monolayers of Si or Ge, and $a_\perp/4$ is the corresponding interplanar distance. (iii) The frequencies of the interface modes are about 400 cm^{-1} and have a strong dependence on the interfaces coupling in short period SL's.

I. INTRODUCTION

Strained Si/Ge superlattices (SL's) have recently attracted much interest because of their promising optical and electronic properties.[1] The vibrational properties of these SL's have been a subject of several experimental[2–10] and theoretical[11–18] investigations. In addition to their fundamental importance, the lattice dynamics of the SL's are essential in the characterization of these man-made materials.

Phonons in strained SL's have renewed interest in the effects of strain on the phonon spectra of the group-IV elemental and the III-V compound semiconductors. Qteish and Molinari[15] and Fasolino, Molinari, and Qteish[16] have studied the effects of the (001) biaxial strain on the longitudinal phonon spectra of Si and Ge along the [001] direction, using a first-principles pseudopotential technique[19] and the interplanar force constant (IPFC) method.[20] They found that the strain-induced frequency shift of the longitudinal-optical branch have a weak wave-vector dependence, and the calculated values are in very good agreement with the available experimental data for both Si and Ge. More recently, de Gironcoli[18] has studied the above effects on the longitudinal and transverse phonon spectra along various high symmetry directions of Si and Ge, using an interatomic force constant approach and a linear response method.[21] The de Gironcoli calculations[18] have shown that the frequency shift of the transverse-acoustical (TA) branch has an opposite sign with respect to that of the transverse optical (TO) one. This behavior is consistent with the signs of the experimental Grüneisen parameters of the TO and TA phonon modes at the Γ and X points,[22,23] but it is in contradiction with the predictions of the Keating model calculations.[13(d),14] Moreover, the latter calculations gave conflicting results for the wave-vector dependence and for the magnitudes of the strain-induced frequency shifts of the TO phonon spectra of Si and Ge propagating along the [001] direction.[13(d),14] Therefore, it is of interest to study the effects of strain on the transverse phonon spectra of these materials using the IPFC method.

In this work we present *consistent* sets of the [001] transverse IPFC's for Si and Ge for three strain configurations, corresponding to pseudomorphic growth on $Si_{1-x}Ge_x$ (001) (with $x=0$, 0.5, and 1) substrates. The transverse IPFC's were calculated using a first-principles pseudopotential technique,[19] the local-density approximation[24] (LDA) for the exchange-correlation potential, and the supercell method. The calculated transverse IPFC's were used to (i) construct the transverse phonon spectra of Si and Ge propagating along the [001] direction, (ii) study the effects of the (001) biaxial strain on these phonon dispersions, and (iii) investigate the general features of the transverse phonon modes in strained Si/Ge (001) SL's.

The rest of the paper is organized as follows. In Sec. II we briefly describe our computational method and give details of the calculations. In Sec. III we report and discuss our results for the [001] transverse IPFC's, the transverse phonon spectra of unstrained bulk Si and Ge, and the effects of strain on these phonon spectra. Section IV is devoted to reporting and discussing our results for the transverse phonon modes in Si/Ge (001) SL's. Finally, in Sec. V we give a summary of our main results and conclusions.

II. METHOD AND COMPUTATIONAL DETAILS

The [001] transverse IPFC's for bulk Si and Ge were calculated using the supercell method for three strain configurations, corresponding to coherent growth on $Si_{1-x}Ge_x$ (001)

TABLE I. Si and Ge, lattice matched to different (001) substrates: $a_{\parallel}$ (in Å) is the in-plane lattice parameter imposed by the substrate and $a_{\perp}$ (in Å) is the lattice parameter in the perpendicular direction calculated using total energy minimization (Refs. 15 and 25); k_i (ii 10^5 dyn/cm) are the [001] transverse IPFC's. For k_0 we show both the calculated value, in parentheses, and the value obtained from the other IPFC's by imposing the acoustic sum rule.

	Si lattice matched to (001) substrates			Ge lattice matched to (001) substrates		
	Si	$Si_{0.5}Ge_{0.5}$	Ge	Si	$Si_{0.5}Ge_{0.5}$	Ge
$a_{\parallel}$	5.39	5.49	5.59	5.39	5.49	5.59
$a_{\perp}/a_{\parallel}$	1.000	0.970	0.938	1.056	1.031	1.000
k_0	(+2.0083)	(+1.9257)	(+1.8327)	(+1.8384)	(+1.7765)	(+1.7061)
k_0	+2.0066	+1.9236	+1.8300	+1.8350	+1.7740	+1.7039
k_{+1}	−1.7746	−1.6797	−1.5748	−1.6554	−1.5832	−1.5047
k_{-1}	−0.2733	−0.2799	−0.2846	−0.2291	−0.2343	−0.2370
$k_{\pm 2}$	+0.0615	+0.0600	+0.0585	+0.0601	+0.0583	+0.0560
k_{+3}	−0.0160	−0.0172	−0.0189	−0.0135	−0.0139	−0.0145
k_{-3}	−0.0847	−0.0856	−0.0881	−0.0803	−0.0819	−0.0831
$k_{\pm 4}$	+0.0169	+0.0172	+0.0173	+0.0181	+0.0183	+0.0186
k_{+5}	−0.0028	−0.0024	−0.0021	−0.0030	−0.0024	−0.0025
k_{-5}	−0.0171	−0.0177	−0.0188	−0.0166	−0.0175	−0.0184
$k_{\pm 6}$	+0.0036	+0.0041	+0.0040	+0.0042	+0.0043	+0.0046
k_{+7}	−0.0015	−0.0018	−0.0016	−0.0018	−0.0019	−0.0021
k_{-7}	−0.0038	−0.0036	−0.0044	−0.0040	−0.0043	−0.0049
$k_{\pm 8}$	+0.0016	+0.0013	+0.0018	+0.0018	+0.0020	+0.0024

(with $x=0$, 0.5, and 1) substrates. Tetragonal supercells of 16 atoms (eight double layers) were used, which enable us to calculate the IPFC's up to the eighth-nearest-neighboring planes. The convergence of the transverse phonon spectra with respect to the highest-order IPFC included in the calculations has been checked by calculating these phonon spectra for unstrained Si and Ge using sets of IPFC's up to the eighth- and sixth-nearest-neighboring planes (the latter were calculated using 12-atom supercells). A very good convergence has been found: for the whole TO branch the frequency difference is less than 1 cm^{-1} for both Si and Ge; for the TA mode at the X point the difference is about 3 and 5 cm^{-1} for Si and Ge, respectively. Therefore, we chose in our present work to use IPFC's up the eighth-nearest-neighboring planes. The structure of the above supercells, for the three strain configurations considered, can be fully determined by two structural parameters, $a_{\perp}$ and $a_{\parallel}$, where $a_{\parallel}$ is the in-plane lattice parameter, taken to be that of the substrate, and $a_{\perp}$ is the lattice parameter along the [001] direction (i.e., $a_{\perp}/4$ is the interplanar distance). The values of $a_{\parallel}$ and $a_{\perp}$ used for Si and Ge are given in Table I, for the above three strain configurations. These values, which were calculated by self-consistent total energy minimization,[15,25] are the same ones used in Refs. 15 and 16. The [001] transverse IPFC's were determined from the calculated Hellmann-Feynman forces obtained by displacing one atom in the supercell by (0.007, 0.007, 0.000) $a_{\parallel}$ (see Ref. 26).

The calculations were performed using a first-principles pseudopotential approach and the Ceperley-Alder form[27] of the LDA as parameterized by Perdew and Zunger.[28] The Kohn-Sham equations were solved by expanding the wave functions in terms of a plane-wave (PW) basis and using the Teter-Payne-Allan conjugate gradient total energy minimization technique.[29] PW's up to 15 Ry in energy were included, which is a very good cutoff for both Si and Ge.[15] The Brillouin-zone integrations were performed by sampling on a regular 4×4×2 Monkhorst-Pack[30] mesh. The pseudopotentials for Si and Ge were generated using the Kerker[31] scheme in the Kleinman-Bylander form.[32] These pseudopotentials were constructed with the use of the valence atomic configurations described in Ref. 33.

III. TRANSVERSE INTERPLANAR FORCE CONSTANTS AND PHONON SPECTRA OF STRAINED Si AND Ge

The [001] transverse IPFC's sets, $\{k_i^{110}\}$, calculated as described in Sec. II for Si and Ge in the three strain configurations considered are given in Table I. Here, the superscript 110 refers to the [110] transverse polarization direction, and i is used as an index for the nearest-neighboring planes. For the [110] polarized transverse phonon spectra, the appropriate sets of IPFC's are related to the previous ones by[34]

$$k_i^{\bar{1}10}=k_{-i}^{110}. \tag{1}$$

The important features to note from Table I are (i) the alternation of sign and the long-range nature of the transverse IPFC's [this feature is characteristic of the covalently bonded materials (Ref. 35)] and (ii) the fulfilling of the acoustic sum rule (the difference between the calculated value of k_0 and that obtained from the acoustic sum rule is less that 0.004×10^5 dyne/cm, which reflects the very good accuracy of our calculations).

In Fig. 1 we show our calculated transverse phonon spectra for unstrained Si and Ge along the Δ direction, using the above IPFC's and the linear chain model,[20] together with the neutron scattering data.[36,37] It should be noted here that in the present geometry the [110] and the [$\bar{1}$10] polarized modes

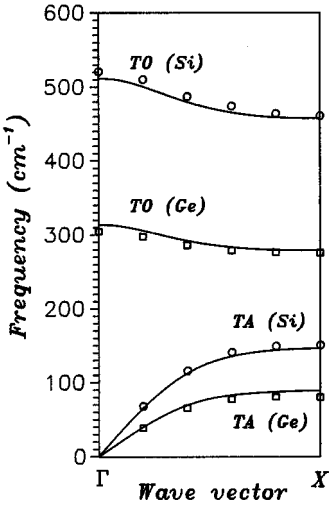

FIG. 1. Calculated transverse phonon dispersions for unstrained bulk Si and Ge along the [001] direction (solid lines). Experimental data from neutron-scattering measurements are shown by circles for Si (from Ref. 37, at $T=300$ K) and squares for Ge (from Ref. 38, at $T=80$ K).

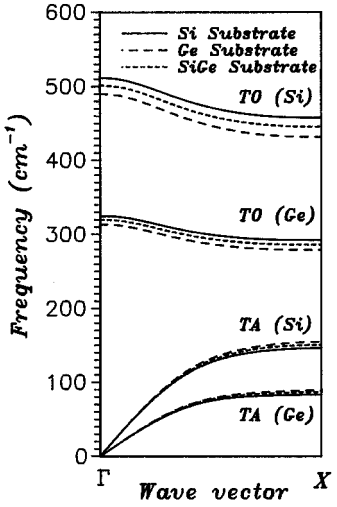

FIG. 2. Calculated transverse phonon dispersions for bulk Si and Ge along the [001] direction at three values of strain, corresponding to lattice matching to a Si substrate (solid lines), a $Si_{0.5}Ge_{0.5}$ substrate (short-dashed lines), and a Ge substrate (long-dashed lines).

are degenerate. Figure 1 shows that our results are in excellent agreement with the experimental data,[36,37] especially for the flatness of the TA branch of Ge. It is well known that the flatness of the TA branch can be reproduced only by including higher-order interactions.[35] The discrepancy between our calculated frequencies and the experimental data for the TO modes ω_{TO} at the Γ and X points are 1.7 and 0.7 %, respectively, for Si and 3.0 and 1.1 %, respectively, for Ge. As for the frequency of the TA mode at the X point, $\omega_{TA}(X)$, the discrepancy is 2.7 and 11.3 %, respectively, for Si and Ge. The large value of the discrepancy in the case of the TA (X) mode of Ge is due to the sensitivity of ω in this mode to the computational ingredients and its rather small value—note that the absolute error in ω of this mode (~ 9 cm^{-1}) is of the same order as that of the TO (Γ) of both Si and Ge (see Fig. 1). It has been found that our results are in better agreement with the experimental data than the transverse spectra for unstrained Si and Ge calculated using the very recently published sets of IPFC's,[38] up to the fifth-nearest-neighboring planes. We believe that the main difference between our results and those of Ref. 38 is mainly because of the Si and Ge pseudopotentials used: the difference between our results calculated using six and eight IPFC's is much smaller than that between our results and those of Ref. 38, and both calculations are well converged with respect to the number of PW's used.

The strain-induced effects on the transverse phonon spectra for Si and Ge were investigated by calculating these spectra at the three strain configurations considered (see Sec. II). The spectra for Si and Ge obtained along the Δ direction are shown in Fig. 2. The important features to note from Fig. 2 are (i) the (001) tensile (compressive) strain in Si (Ge) leads to a downwards (upwards) shift of ω_{TO}, while the ω_{TA} are shifted upwards (downwards). These findings are consistent with the signs of the experimental Grüneisen parameters of these phonon modes[22,23] (negative for the TA modes and positive for the TO modes). (ii) The calculated shift in the ω_{TO} at the Γ point, $\Delta\omega_{TO}(\Gamma)$, is -21.7 and $+11.3$ cm^{-1} for Si lattice matched to a Ge substrate and Ge lattice matched to a Si substrate, respectively. These results are in excellent agreement with the corresponding experimental data,[39,40] -19.7 and $+11.0$ cm^{-1}, respectively. (iii) The $\Delta\omega_{TO}$ along the Δ direction for both Si and Ge show a weak wave-vector dependence, as can be more clearly seen from Fig. 3. The difference between the calculated values of $\Delta\omega_{TO}(\Gamma)$ and $\Delta\omega_{TO}(X)$ is -4.2 cm^{-1} for Si lattice matched to a Ge substrate, and -1.7 cm^{-1} for Ge lattice matched to a Si substrate.

The (001) biaxial strain can be divided into isotropic and uniaxial contributions. Concentrating on the Γ point,[39,40] the

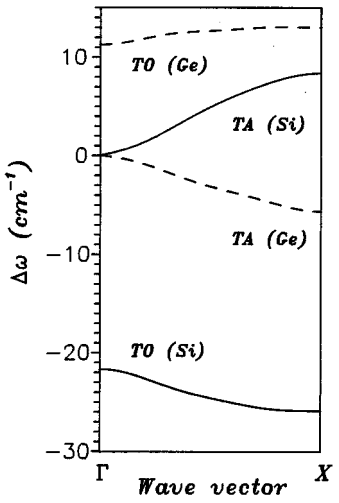

FIG. 3. Strain-induced frequency shift $\Delta\omega$ of the transverse-optical (TO) and transverse-acoustical (TA) modes along the [001] direction for Si (solid lines), in going from a Si to a Ge substrate, and for Ge (dashed lines), in going from a Ge to a Si substrate.

former shifts the averaged frequency of the LO and the two TO modes, $\Delta\overline{\omega}(\Gamma)$, while the latter leads to a splitting between the frequency of the LO (singlet) and the TO (doublet) modes, $\Delta\omega_{\mathrm{LO,TO}}(\Gamma)$. Using the currently calculated values of $\Delta\omega_{\mathrm{TO}}(\Gamma)$ and those of Qteish and Molinari[15] for $\Delta\omega_{\mathrm{LO}}(\Gamma)$ (-30.6 and $+15.2$ cm^{-1} for Si lattice matched to a Ge substrate and Ge lattice matched to a Si substrate, respectively), the calculated $\Delta\overline{\omega}(\Gamma)$ is -24.7 and $+12.6$ cm^{-1} for Si and Ge, respectively, compared with the corresponding experimental results of -23.2 and $+12.5$ cm^{-1}.[39,40] de Gironcoli[18] has found a value of -27 cm^{-1} for $\Delta\overline{\omega}(\Gamma)$ of Si lattice matched to a Ge substrate, which is also in good agreement with our calculations. Moreover, our calculated value of $\Delta\omega_{\mathrm{LO,TO}}(\Gamma)$ is 8.9 and 3.9 cm^{-1} for Si and Ge, respectively, compared with the corresponding experimental values of 10.4 and 4.5 cm^{-1}.[39,40] For Si lattice matched to a Ge substrate, the de Gironcoli calculations[18] gave a value of $\Delta\omega_{\mathrm{LO,TO}}(\Gamma)$ of 3.7 cm^{-1}, which is about three times smaller than the experimental value. He attributed the difference between his calculated result and experiment as a consequence of strong nonlinear effects. We have found that the nonlinear effects are important [$\Delta\omega_{\mathrm{LO,TO}}(\Gamma)$ for Si lattice-matched to a $Si_{0.5}Ge_{0.5}$ substrate is of 7.1 cm^{-1}], but not that strong to explain the de Gironcoli result. The very good agreement between our results for $\Delta\omega_{\mathrm{LO,TO}}(\Gamma)$ and $\Delta\overline{\omega}(\Gamma)$ and the experimentally determined ones, demonstrates the accuracy and the reliability of the present calculations and those of Refs. 15 and 16.

The $\Delta\omega_{\mathrm{TO}}$ and $\Delta\omega_{\mathrm{TA}}$ calculated along the Δ direction for Si and Ge show a linear dependence with respect to strain (see Fig. 2), in the strain range considered. This behavior is consistent with the use of the linear deformation potentials to present the experimental results for these frequency shifts (only available at the Γ point).[39,40]

The linearity of the [001] longitudinal IPFC's for Si and Ge with respect to strain has been demonstrated by Qteish and Molinari.[15] This linearity has very important implications, since it allows us to calculate the phonon spectra of these materials and those of Si/Ge (001) SL's, lattice matched to an arbitrary $Si_{1-x}Ge_x$ (001) substrate.

To investigate the linearity with respect to strain of the transverse IPFC's, the values of the IPFC's for Si and Ge, in the three strain configurations considered (see Table I), were fitted to a straight line equation with respect to the concentration of Ge in the substrate

$$k_i = c_i^0 + c_i^1 x. \tag{2}$$

The resultant values of c_i^0 and c_i^1 are listed in Table II. Although k_0 also shows a linear behavior with respect to x, the fitting of this force constant to a straight line is not necessary because, for any strain configuration, we use the acoustic sum rule to determine the value of k_0 in the actual calculations. The transverse phonon spectra for both Si and Ge in the three strain configurations considered were recalculated using the fitted IPFC's. The maximum deviation between these spectra and the corresponding ones calculated using the original IPFC's is less than 0.5 cm^{-1}. This demonstrates the accuracy of the phonon spectra calculated using the fitted IPFC's for any strain configuration within the above-considered strain range. This finding is consistent with that of the longitudinal IPFC's (see Ref. 15), and it reflects the fact that the strain range considered is small enough that nonlinear effects are negligible.

IV. TRANSVERSE PHONON SPECTRA OF Si/Ge SL's

In this section we will investigate the general features of the transverse phonon modes in strained Si/Ge (001) SL's, pseudomorphically grown on $Si_{1-x}Ge_x$ (001) substrates, using the currently calculated IPFC's (see Table I) and the linear chain model.[20] In this study, ideal superlattices have been assumed (interface roughness and intermixing were neglected; for such effects see, for example, Ref. 41). Moreover, following Refs. 15 and 16, the values of the Si-Ge interplanar distance and the IPFC's across the interfaces are considered to be equal to the mean values of the corresponding ones of the strained materials on the two sides of the interface. The effects of considering for the Si-Ge IPFC's the mean values of the IPFC's of the properly strained Si and Ge have been checked by recalculating the phonon modes of a few superlattices lattice matched to a Si substrate using either Si or strained Ge IPFC's alone for the whole superlattice. It has been found that the difference in the calculated frequency of the interface phonon modes between these two extreme cases is about 4%. Therefore, one can conclude that the effects of the above approximation on the interface phonon modes are quite negligible.

A. General features

The general features of the transverse phonon spectra of the Si/Ge (001) SL's are more diverse than those of the longitudinal ones. True Si- and Ge-like confined modes and interface modes appear in the transverse phonon spectra of the Si/Ge (001) SL's, while only true Si-like confined modes appear in their longitudinal phonon spectra. Moreover, the point-group symmetry of the Si_nGe_m (001) SL's has important consequences on the phonon spectra of these systems: the [110] and [1$\bar{1}$0] polarized transverse 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) symmetry, respectively.[12]

To illustrate the general features of the transverse phonon spectra of the Si/Ge (001) SL's with D_{2h} symmetry, we show in Fig. 4 the calculated curves along the [001] direction for the Si_4Ge_4 (001) SL, lattice matched to a Si substrate. The three modes in the frequency range from 460 to 500 cm^{-1} (492.5, 484.0, and 463.9 cm^{-1}, at the zone center) are true Si-like TO confined modes. The two split phonon modes with frequencies very close to 400 cm^{-1} (403.1 and 396.8 cm^{-1}, at the zone center) are interface-modes, since they lie in the gaps of the transverse phonon continua of bulk Si and Ge. Only interface modes with [1$\bar{1}$0] polarization exist in the present case because all the Si—Ge bonds in the Si/Ge (001) SL's with D_{2h} symmetry lie along the [110] direction. For these symmetric and antisymmetric interface modes, the vibrational amplitudes decay rather rapidly to zero away from the interface, as can be easily seen from the atomic displacements of modes b and c shown in Fig. 4. More discussion about the interface modes will be given below. The modes with frequencies of 295.3, 302.7, and 310.6 cm^{-1} at the zone center are true Ge-like TO confined modes. The four modes in the frequency range from 90 to 140 cm^{-1} are Si-like TA

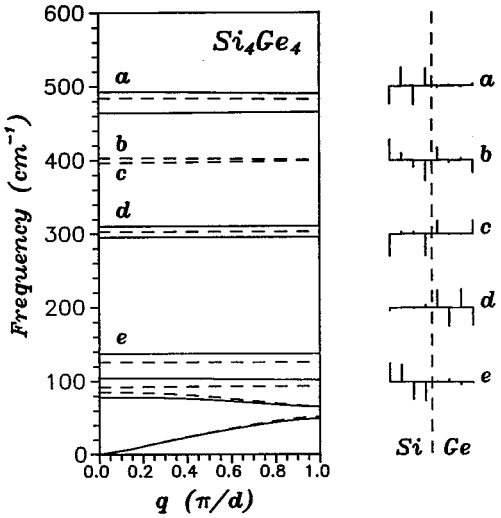

FIG. 4. Transverse phonon dispersions along the [001] direction for the Si_4Ge_4 (001) superlattice grown on a Si substrate, in the SL Brillouin zone (d is the SL period). Solid curves: the [110] polarized modes; dashed curves: the [110] polarized modes. Atomic displacement for selected modes at the zone center are displayed at the right.

confined modes, since they lie above the TA phonon continua of the properly strained bulk Ge. The rest of the modes are TA extended folded modes.

B. Confinement

The aim of this subsection is to investigate the relationship between the TO confined modes in strained Si/Ge (001) SL's and the phonon curves of the constituent strained bulk materials. We plot in Fig. 5 the calculated frequencies of the Si-like TO confined modes ω^j_{TO} (j is the order of the modes starting with the highest-frequency mode) in the $Si_{12}Ge_6$

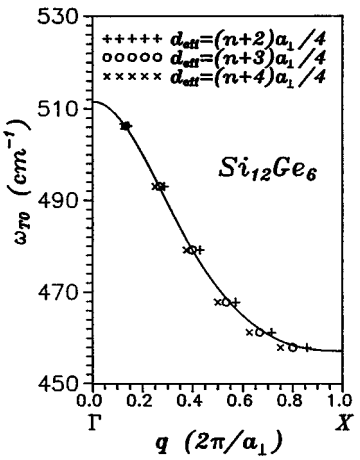

FIG. 5. Frequency of the Si-like TO confined modes w^j_{TO} in the $Si_{12}Ge_6$ (001) superlattice, lattice matched to a Si substrate, plotted onto the TO dispersion of unstrained bulk Si at the effective wave vectors $q_{\mathrm{eff}}=j\pi/d_{\mathrm{eff}}$. Three forms of the effective confinement length d_{eff} are used. Here n is the number of Si monolayers, and $a_\perp/4$ is the corresponding interplanar distance.

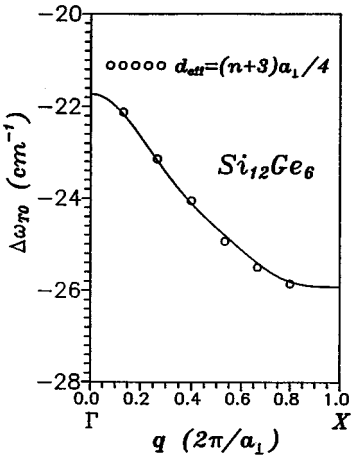

FIG. 6. Frequency shift of the Si-like TO confined modes Δw^j_{TO} for the $Si_{12}Ge_6$ (001) SL, by going from a Si to a Ge substrate, plotted onto the corresponding frequency shift of the TO dispersion of similarly strained bulk Si, at the effective wave vectors $q_{\mathrm{eff}}=j\pi/d_{\mathrm{eff}}$. Here d_{eff} is the effective confinement length (see text).

(001) SL lattice matched to a Si substrate onto the TO phonon curve of unstrained Si at $q_{\mathrm{eff}}=j\pi/d_{\mathrm{eff}}$, where d_{eff} is the effective confinement length. From Fig. 5 it is obvious that the best fit to the bulk dispersion is achieved by considering $d_{\mathrm{eff}}=(n+3)a_\perp/4$, where n is the number of Si monolayers and $a_\perp/4$ is their interplanar distance. Moreover, a similar form for d_{eff} has been found for the Ge-like TO confined modes. The quality of the fitting decreases for the lower-frequency confined modes (higher-order modes). This can be understood, since these modes are less confined to the Si layers than the higher-frequency ones. It should be noted here that the above behavior is not restricted to the $Si_{12}Ge_6$ (001) SL only, but it has been found to be valid for other SL's.

It is worth noting here that in the case of the Si-like LO confined modes, the d_{eff} is given as $(n+1)a_\perp/4$ (Ref. 16). The difference between this d_{eff} and that of the TO confined modes can be understood as a direct consequence of the long-range nature of the transverse IPFC's with respect to the longitudinal ones. To check the validity of this explanation, we have recalculated the best d_{eff} by artificially setting to zero the transverse IPFC's with i larger than 4 and by enforcing the acoustic sum rule. These test calculations gave $d_{\mathrm{eff}}=(n+2)a_\perp/4$, which demonstrates the soundness of our explanation.

In Fig. 6 we plot the frequency shift of the Si-like TO confined modes, $\Delta\omega^j_{\mathrm{TO}}$, in the $Si_{12}Ge_6$ (001) SL, by going from a Si to a Ge substrate onto the shift of the TO phonon curve of bulk Si under the same strain conditions. The almost exact matching between $\Delta\omega^j_{\mathrm{TO}}$ and $\Delta\omega_{\mathrm{TO}}$ of bulk Si at the same values of q_{eff} [with $d_{\mathrm{eff}}=(n+3)a_\perp/4$; see above], shows the transferability of the strain effects on the bulk phonon spectra to the corresponding confined modes in the SL's. Similar conclusions have been reached for the Ge-like TO confined modes, not discussed here, and the Si-like LO confined modes in the Si/Ge (001) SL's.[16] Therefore, from the knowledge of the (001) biaxial strain effects on the pho-

TABLE II. Fitting parameters c_i^0 and c_i^1 used to obtain the transverse IPFC's, $k_i = c_i^0 + c_i^1 x$, for Si and Ge, lattice matched to $Si_{1-x}Ge_x$ substrates with $0 \leq x \leq 1$.

	Si		Ge	
i	c_i^0	c_i^1	c_i^0	c_i^1
+1	−1.7763	+0.1998	−1.6565	+0.1507
−1	−0.2736	−0.0130	−0.2295	−0.0079
±2	+0.0615	−0.0130	+0.0602	−0.0040
+3	−0.0159	−0.0029	−0.0135	−0.0010
−3	−0.0847	−0.0034	−0.0804	−0.0028
±4	+0.0169	+0.0004	+0.0181	+0.0005
+5	−0.0028	+0.0007	−0.0031	+0.0005
−5	−0.0170	−0.0017	−0.0166	−0.0018
±6	+0.0037	−0.0004	+0.0042	+0.0004
+7	−0.0016	−0.0001	−0.0018	−0.0003
−7	−0.0036	−0.0006	−0.0040	−0.0009
±8	+0.0015	+0.0003	+0.0018	+0.0006

non dispersions of bulk Si and Ge, which can be calculated for any biaxial strain configuration using the fitted transverse IPFC's (see Table II) and the longitudinal ones,[15] and the appropriate d_{eff} for the confined modes in SL's, the ω_{TO}^j and ω_{LO}^j in any Si/Ge (001) SL grown on an arbitrary $Si_{1-x}Ge_x$ (001) substrate can be accurately determined.

C. Interface modes

In order to investigate the effects of the interface coupling on the ω of the interface modes in the Si/Ge SL's, we have studied these modes in different Si_nGe_m (001) SL's with D_{2h} symmetry lattice matched to a Si substrate. In these SL's, the interface modes are nondegenerate because of the constraint of symmetry. We have found that the values of ω of the two interface modes in the Si_2Ge_2 (001) SL are 383.4 and 432.3 cm^{-1} at the zone center. The difference in ω between these two modes is found to decrease monotonically by increasing n and/or m. For both n and m larger than 8, the ω of these two interface modes converge to the same value of 400.1 cm^{-1}. The strong dependence of ω of the interface modes on the values of n and m in short-period SL's [note the $\sim$50 cm^{-1} splitting in the frequencies of the interface modes in the Si_2Ge_2 (001) SL] can be easily understood as a result of the long-range nature of the transverse IPFC's, which, in turn, leads to a weakly localized interface mode around the interfaces (see, for example, the atomic displacements of mode b shown in Fig. 4).

V. CONCLUSIONS

The [001] transverse interplanar force constants (IPFC's), up to the eighth-nearest-neighboring planes, for bulk Si and Ge under three strain configurations, which correspond to a pseudomorphic growth on $Si_{1-x}Ge_x$ (001) (with $x=0.0$, 0.5 and 1.0) substrates, have been determined using a first-principles pseudopotential technique. With the use of these IPFC's and the linear chain model, the effects of the (001) biaxial strain on the transverse phonon spectra of Si and Ge have been studied. The transverse phonon modes of the Si/Ge (001) superlattices (SL's) have also been similarly investigated. In the following we summarize our main results and conclusions.

(1) The calculated transverse phonon spectra along the Δ direction of the unstrained Si and Ge, and the variations of these spectra caused by strain, are found to be in very good agreement with the available experimental data.
(2) The strain-induced frequency shift on the transverse-optical (TO) branch along the Δ direction is predicted to have a weak wave-vector dependence for Si and Ge.
(3) The direction of the frequency shift of the transverse-acoustical (TA) spectra caused by the (001) biaxial strain is consistent with the sign of the experimental Grüneisen parameter of the TA mode at the X point for both Si and Ge.
(4) The frequency shifts in the TO and TA phonon spectra are found to be linearly dependent on the strain tensor, at least in the strain range considered.
(5) As expected, true Si- and Ge-like TO confined modes appear in the transverse phonon spectra of the Si/Ge (001) SL's. These modes can best be described with respect to the strained bulk dispersions by an effective confinement length $d_{\text{eff}} = (n+3)a_\perp/4$, where n is the number of Si or Ge monolayers, and $a_\perp/4$ is the corresponding interplanar distance.
(6) The frequencies of the interface modes are about 400 cm^{-1}, and have a strong dependence on the interface coupling in short-period SL's.

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