Interplanar forces and phonon spectra of strained Si and Ge: *Ab initio* calculations and applications to Si/Ge superlattices

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We have studied the effects of biaxial strain in the (001) plane on the interplanar force constants and phonon spectra of bulk Si and Ge for longitudinal propagation along the [001] direction. The results are in good agreement with the available experimental data; moreover, we give predictions for the strain dependence of the bulk dispersions along the Δ line. We provide a practical and accurate way of calculating phonon spectra along [001] for strained [001]-oriented Si/Ge superlattices (SL's), with strain configuration corresponding to growth on arbitrary $Si_{1-x}Ge_x$ substrates. The importance of a correct treatment of strain effects for the understanding of SL phonon physics and for SL characterization is illustrated with results for two prototype superlattices lattice matched to Si and Ge.

I. INTRODUCTION

Recently, there has been increasing interest in the phonon spectra of Si/Ge [001] superlattices both from the experimental[1-6] and from the theoretical[7-9] point of view. Because of the $\sim 4\%$ lattice mismatch between Si and Ge, these superlattices are strained. The proper inclusion of strain effects is important in understanding the properties of such materials and for their characterization. As concerns the determination of structural parameters, for example, investigations of SL phonons by Raman spectroscopy, aimed at determining the strain distribution in the two constituents, started[10,11] very soon after the successful growth of $Si/Si_{1-x}Ge_x$ SL's.

From the lattice-dynamical point of view, the effect of strain is not well known even for bulk Si and Ge: to our knowledge, experimental results are available only at the Γ point,[12,13] and no theoretical calculations exist. Even in the absence of strain, although first-principles studies of phonons in Si and Ge have been performed,[14-17] no *consistent* sets of first-principles force constants for the two materials are available. Sets calculated for both materials within the same scheme and with the same computational ingredients are instead desirable in view of their use for SL calculations.

The purpose of the present paper is to present *ab initio* calculations of the effect of a biaxial strain, corresponding to the epitaxial constraint for pseudomorphic growth along the [001] direction on a lattice-mismatched substrate,[18] on the longitudinal (L) force constants and lattice dynamics of infinite Si and Ge crystals, and to illustrate its relevance for [001] Si/Ge superlattices by studying the phonon spectrum of prototype SL cases. The L interplanar force constants for bulk Si and Ge have been calculated at three values of strain, corresponding to lattice matching to Si, $Si_{0.5}Ge_{0.5}$, and Ge substrates. It has been found that a simple interpolation scheme can be used with high accuracy to obtain the interplanar force constants at values of strain corresponding to arbitrary $Si_{1-x}Ge_x$ substrates. This provides a simple and general way of performing calculations of L phonon spectra for any [001]-oriented Si/Ge superlattice along its growth direction.

In Sec. II, after introducing our method of calculation, we present results for the equilibrium atomic structure of strained bulk Si and Ge and compare them with previous theoretical predictions and with recent experimental data. Section III is devoted to our results for the effect of strain on interplanar force constants and on the resulting phonon dispersions. The implications for the phonons of Si/Ge SL's are briefly discussed in Sec. IV.

II. ATOMIC STRUCTURE OF STRAINED Si AND Ge

Let us consider the Si and Ge infinite crystals in the homogeneous strain configuration corresponding to their lattice matching to a substrate with a different lattice parameter. The geometry is defined by the lattice parameter in the (001) plane ($a_\parallel$), which is dictated by the substrate and determines the strain configuration, and by the lattice constant along the normal direction ($a_\perp$), which is also expected to differ from the unstrained bulk value as a consequence of the $a_\parallel$ variation. For example, Fig. 1 schematically shows the geometry of a free-standing crystal—where the in-plane and the normal lattice parameters are the same ($a_\parallel^0 = a_\perp^0$) and coincide with the equilibrium lattice constant [Fig. 1(a)]—together with the geometry of the same crystal in the presence of biaxial strain [Fig. 1(b)]. The case of Fig. 1(b) corresponds to negative biaxial strain: the in-plane parameter is forced to assume a value larger than the equilibrium one, $a_\parallel > a_\parallel^0$, and the lattice parameter along the [001] direc-

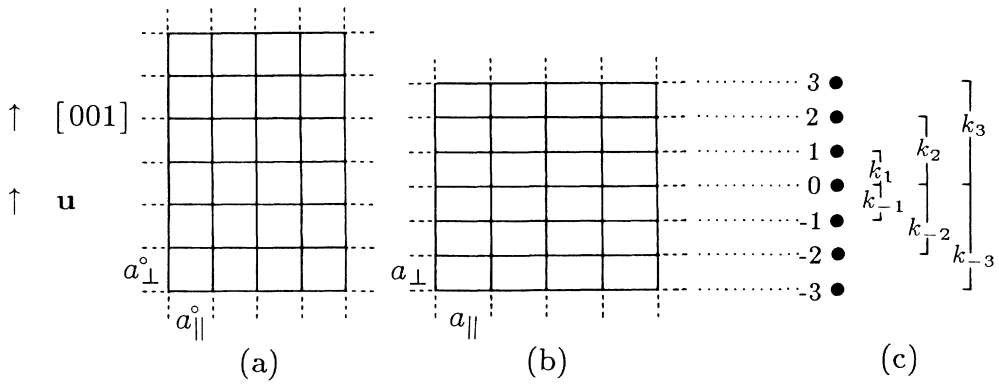

FIG. 1. (a) Sketch of the geometry of a free-standing infinite crystal: in the absence of strain the lattice parameter parallel and perpendicular to the (001) plane is the equilibrium lattice parameter, $a^0_\parallel = a^0_\perp = a^0$. (b) Sketch of the geometry of the same crystal in the presence of biaxial strain in the (001) plane. Here the strain corresponds to lattice matching to a substrate with $a_\parallel > a^0_\parallel$; the lattice parameter along the [001] direction is therefore reduced to a value $a_\perp < a^0_\perp$. This situation qualitatively corresponds to the case of Si lattice matched to a Ge substrate. (c) Mapping of the crystal onto a one-dimensional chain, and definition of the interplanar force constants k_l. For L propagation along [001], $k_l = k_{-l}$, and therefore there is only one atomic plane per unit cell in the linear chain. The values of k_l for unstrained and strained Si and Ge are reported in Table I.

tion therefore assumes a new value $a_\perp < a^0_\perp$, so that $a_\perp/a_\parallel < 1$. Qualitatively, this is the situation occurring when Si is matched to a Ge substrate. In the opposite case (positive biaxial strain, i.e., crystal matched to a substrate with smaller lattice parameter), instead, $a_\perp/a_\parallel > 1$.

In the present work, $a_\parallel$ is taken to be the theoretical equilibrium lattice parameter of Si or Ge or their average, in order to study the three strain configurations mentioned above: lattice-matching to Si, Ge, and $Si_{0.5}Ge_{0.5}$ substrates, respectively. $a_\perp$ is then calculated by total-energy minimization.

The calculations are performed using self-consistent pseudopotential techniques within the density-functional formalism, in the local-density approximation (LDA). $a_\perp/a_\parallel$ is computed using the (distorted) zinc-blende structure; a tetragonal unit cell (eight atoms) is used to compute the force constants. The wave functions are expanded in a plane-wave (PW) basis set, including all waves up to 12 Ry in energy. Nonlocal pseudopotentials are taken from the tabulation of Bachelet *et al.*[19] For the exchange and correlation potentials we use the Ceperley-Alder form[20] as parametrized by Perdew and Zunger.[21] The charge density is integrated over a regular (4×4×2) Monkhorst-Pack (MP) mesh[22] in the first Brillouin zone for the tetragonal cell (giving four different special points in the deformed geometry), and over the (4×4×4) mesh in the zinc-blende cell. The convergence has been tested by increasing the number of special points to the (6×6×2) MP mesh (nine points) and by increasing the PW energy cutoff to 14 Ry. We anticipate that such increase affects the phonon frequencies of Si lattice matched to Si and Ge substrates by less than 1%; the effect on the strain-induced shift is less than 2 cm^{-1}. This shows that our calculations are well converged with respect to both the number of special points and the energy cutoff.

The equilibrium lattice parameters a^0 for unstrained bulk Si and Ge are calculated (also by total-energy minimization) to be $a^0_{Si} = 5.39$ Å and $a^0_{Ge} = 5.59$ Å, respectively.[23] These theoretical equilibrium lattice parameters are used in the following for the free-standing unstrained materials and for the "substrates," i.e., for the values of $a_\parallel$ defining the different strain configurations [see first row of Tables 1(a) and 1(b)]. Note that our equilibrium values for a^0 are underestimated with respect to the experimental values ($a^0_{Si} = 5.430$ Å and $a^0_{Ge} = 5.657$ Å at low temperatures). This is a known problem for Si and Ge, and similar results have been obtained by other groups using LDA with similar pseudopotentials.[16,17,24] It is known, however, that such an underestimate affects elastic constants, bulk modulus, and phonons only marginally, provided that calculations are performed at the theoretical equilibrium value of a^0 (see, e.g., Ref. 16).

The results of our total-energy minimization for $a_\perp/a_\parallel$ are shown in Table I. We find that the interplanar distances $a_\perp$ in the strained materials are closer to the unstrained bulk value $a_\perp/a_\parallel = 1$ than expected if harmonic elasticity theory is applied as in Ref. 25, i.e., using experimental data as input values for a^0_{Si}, a^0_{Ge} and for the elastic constants c_{11} and c_{12} (the results in that case would be $a_\perp/a_\parallel = 1.072$ for Ge lattice matched to Si and $a_\perp/a_\parallel = 0.929$ for Si lattice matched to Ge; the further inclusion of the measured third-order elastic constants would not affect appreciably these values of $a_\perp/a_\parallel$).[26] It is important to notice that the *ab initio* results for $a_\perp/a_\parallel$ are in general affected by the underestimated lattice mismatch between bulk Si and Ge. A correction for this fact would reduce the discrepancy between the *ab initio* results and the above-mentioned results of the elastic model; nevertheless, we estimate that the computed values of $a_\perp/a_\parallel$ would still be slightly closer to 1 than expected from that model.

As concerns comparison with experiments for the structural parameters, the above indication would be consistent with the trend shown in recent x-ray photoelectron diffraction investigations[27] for Si grown pseu-

TABLE I. (a) Si and (b) Ge, lattice matched to different substrates: $a_{\parallel}$ (in Å) is the in-plane lattice parameter imposed by the substrate, $a_{\perp}$ (in Å) is the lattice parameter in the perpendicular direction, calculated by total-energy minimization; v (in 10^2 cm/sec) and k_l (in 10^5 dyn/cm) are the calculated sound velocity and interplanar force constants for longitudinal propagation along the direction of $a_{\perp}$. For k_0, we show both the calculated value (in parentheses) and the value obtained from the other force constants by imposing the acoustical sum rule.

(a)

	Si substrate	Si lattice matched to $Si_{0.5}Ge_{0.5}$ substrate	Ge substrate
$a_{\parallel}$	5.39	5.49	5.59
$a_{\perp}/a_{\parallel}$	1.000	0.970	0.938
v	8507.5	8038.2	7700.3
k_0	2.630 (2.634)	2.442 (2.446)	2.312 (2.308)
k_1	−1.149	−1.076	−1.018
k_2	−0.160	−0.140	−0.127
k_3	−0.008	−0.007	−0.009

(b)

	Si substrate	Ge lattice matched to $Si_{0.5}Ge_{0.5}$ substrate	Ge substrate
$a_{\parallel}$	5.39	5.49	5.59
$a_{\perp}/a_{\parallel}$	1.056	1.031	1.000
v	5457.6	5171.5	4862.8
k_0	2.396 (2.386)	2.263 (2.260)	2.143 (2.142)
k_1	−1.026	−0.981	−0.941
k_2	−0.153	−0.141	−0.130
k_3	−0.014	−0.008	0.000

domorphically on Ge, and it is in good agreement with the 8% reduction of the Poisson ratio of Ge hypothesized in Ref. 28 to explain ion scattering and channeling data. Preliminary indications of a similar possibility are also found[29] in SL samples with the technique described in Ref. 30.

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

In Table I we show the calculated sets of L interplanar force constants for strained bulk Si and Ge in the three different strain configurations. Their definition, following Ref. 14, is schematically illustrated in Fig. 1(c). Notice that, in the present case of *longitudinal* propagation along [001], by symmetry $k_l = k_{-l}$, so that the three-dimensional lattice maps onto a *monatomic* linear chain. The sign of the suffix l is therefore omitted in Table I.

As in Ref. 14, the values of k_l were obtained by displacing one plane of atoms along the [001] direction by 1% of the lattice parameter in a quadrupled cell geometry. The adequacy of such geometry for longitudinal displacements was discussed in Ref. 14. For k_0, we report both the calculated value (in parentheses) and the value obtained by imposing the acoustical sum rule ($k_0 = -\sum_{l \neq 0} k_l$, which follows from translational invariance and ensures vanishing of the acoustical frequency at Γ). This last value is used in all SL phonon calculations. The deviation between these two numbers gives an estimate of our computational errors on the force constants (less than 1%).

Interplanar force constants for unstrained Ge were previously calculated from first principles by Kunc *et al.*,[14] using local pseudopotentials. For unstrained Si, the only *ab initio* set of forces available is the one of Ref. 15, obtained with nonlocal pseudopotentials and a small PW basis. Fleszar and Resta[31] have published sets of interplanar force constants of unstrained Si and Ge obtained by "deconvolution" of interatomic force constants in the bond charge model. In spite of the different approaches, the structure of the calculated sets of interplanar forces k_l, as discussed in detail in Ref. 14, is qualitatively the same. We therefore refer to that paper also for the interpretation of its physical meaning. There are quantitative differences, which affect the phonon frequencies, as will appear from the calculated dispersions shown below.

Our calculated L interplanar force constants of strained bulk Si and Ge under different values of strain, corresponding to lattice matching to $Si_{1-x}Ge_x$ substrates with $x = 0, 0.5, 1$, are found to be linear with x to a good approximation: by performing a least-squares fit of the calculated force constants to a straight line ($k_l = c_l^0 + c_l^1 x$), the difference between the Γ- and X-point phonons obtained from the calculated and fitted force constants is less than 1 cm^{-1}. The fitting parameters, which are useful for studying the case of substrates of intermediate concentrations, are given in Table II.

In Fig. 2 we show our results for the phonon dispersions of unstrained Si and Ge, compared with experimental data from neutron-scattering experiments.[32,33] The agreement is good both for the dispersions and for the ab-

TABLE II. Fitting parameters c_i^0 and c_i^1 used to obtain the interplanar force constants $k_i = c_i^0 + c_i^1 x$ of Si and Ge, lattice matched to $Si_{1-x}Ge_x$ substrates with $0 \le x \le 1$.

	Si		Ge	
i	c_i^0	c_i^1	c_i^0	c_i^1
1	−1.146	0.131	−1.026	0.086
2	−0.159	0.033	−0.153	0.023
3	−0.008	0.002	−0.014	0.014

solute values (notice that the experimental data for Si are taken at room temperature;[32] at low temperature an increase of ~ 5 cm^{-1} is expected[34]).

Figure 3 presents our calculated phonon dispersions for the Si and Ge crystals in the three strain configurations described above. For Si lattice matched to Si, $Si_{0.5}Ge_{0.5}$, and Ge substrates, the Γ-point frequencies are 528.0, 510.8, and 497.4 cm^{-1}, respectively; for Ge matched to the same substrates, they are 311.4, 303.6, and 296.2 cm^{-1}, respectively. The corresponding frequencies at the X point are 421.8, 405.2, and 392.8 cm^{-1} for Si and 250.5, 243.4, and 236.6 cm^{-1} for Ge.

In the strained case, experimental data are available at the Γ point from Raman measurements.[12,13] Using uniaxial strain parameters extracted from such experiments, the strain-induced shifts of ω_{LO}^{Γ} corresponding to Si lattice matched to a Ge substrate and Ge lattice matched to a Si substrate are −31 and +16 cm^{-1}, respectively. Our results are in very good agreement with these data: we obtain −30.6 and +15.2 cm^{-1}, respectively. Moreover, it has been found experimentally[12,13] that the variation of ω_{LO}^{Γ} with strain is linear; this is also reproduced by our calculation, in spite of the almost linear behavior of the force constants (in this range of strain values, the square-root dependence of the frequency on the force constants is well approximated by a linear dependence).

The good agreement both for the dispersion in the unstrained cases and for the strain-induced shifts at Γ

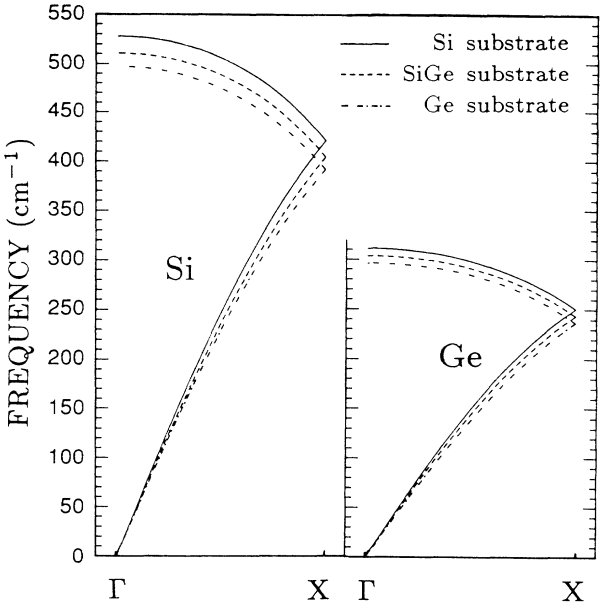

FIG. 3. Calculated longitudinal phonon dispersions for bulk Si and Ge along the [001] direction at three values of strain corresponding to lattice matching to a Si substrate (solid line), $Si_{0.5}Ge_{0.5}$ substrate (dashed line), and Ge substrate (dashed-dotted line). The parameters used in the calculation are shown in Table I.

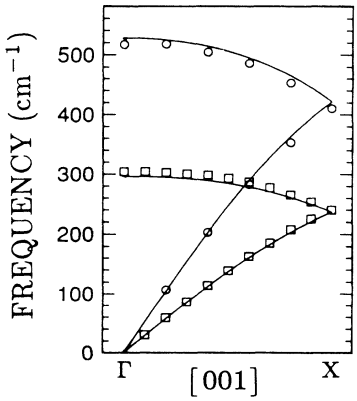

FIG. 2. Calculated longitudinal phonon dispersions for unstrained bulk Si and Ge along the [001] direction (solid lines). Experimental data from neutron-scattering measurements are shown by circles for Si (from Ref. 32, $T = 296$ K) and squares for Ge (from Ref. 33, $T = 80$ K).

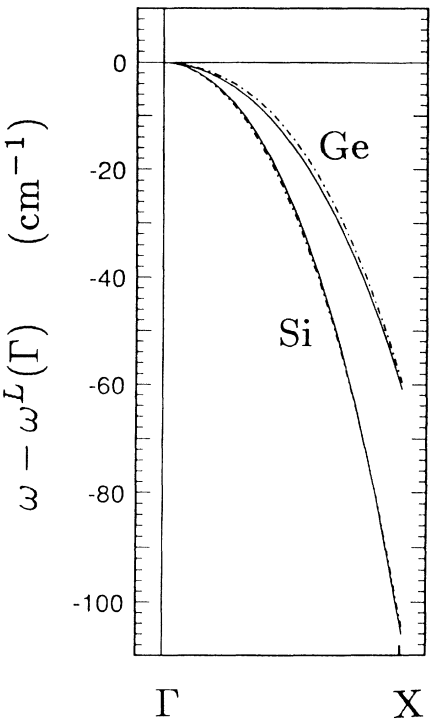

FIG. 4. Enlarged picture of the highest-frequency part of the bulk Γ-X dispersions of Si and Ge, referred to their Γ point frequencies $\omega^L(\Gamma)$. Curves are shown for two values of strain corresponding to lattice matching to Si and Ge substrates (solid and dashed-dotted lines, respectively).

makes us confident in the reliability of the dispersions in the strained configurations, for which no experimental data are available. We predict that the strain dependence of the high-frequency ("optical") part of the dispersions—in particular close to the Γ point—presents relatively small deviations from a rigid shift (see the enlarged plots in Fig. 4); this is particularly true for Si. The implications of this for phonons of Si/Ge superlattices will be discussed below.

IV. RELEVANCE TO THE PHONON SPECTRA OF STRAINED Si/Ge SUPERLATTICES: TWO EXAMPLES

The force constants calculated from first principles can be used to compute phonon dispersions for Si/Ge superlattices grown along the [001] direction, by using a linear chain model.[7] We assume pseudomorphic growth and homogeneous strain distribution within the layers of a given material. Moreover, we assume that both interplanar force constants and interplanar separation at the interface are the average of the corresponding values in the two strained constituents. For the force constants, this assumption is justified due to the small difference in their value for Si and Ge, which is further reduced when the two materials are lattice matched to the same substrate (see Table I). For the interface interplanar separation, the above assumption is consistent with theoretical findings of several groups.[23–25]

In order to illustrate the relevance of the above results to Si/Ge [001]-oriented superlattices, we consider as an example the case of Si_4/Ge_4, lattice matched to Si and Ge substrates (Fig. 5). The general features of the [001] longitudinal spectrum are the same as found in previous theoretical work.[7] In particular, the three topmost modes are confined Si-like modes; a quasiconfined Ge-like mode is found just below the edge of Ge bulk continuum; the rest are folded acoustic modes extending to both Si and Ge; no true interface mode (i.e., exponentially evanescent in both Si and Ge layers) is present for all thicknesses.[7(b)]

We now come to the comparison of the spectra for the two different strain configurations. In this particular case, the nature and the dispersion of modes are very similar in the two configurations (the displacements are indistinguishable on the scale of Fig. 5). Of course, the strain-induced modifications of the bulk dispersions have a direct effect on the SL frequencies; the quasirigid strain-induced shift in the upper part of the Si bulk spectrum leads to a quasirigid shift of the highest Si-like confined modes (the spacing between the first two modes is almost identical in the two cases); on the other hand, the third Si-like confined mode already falls in a frequen-

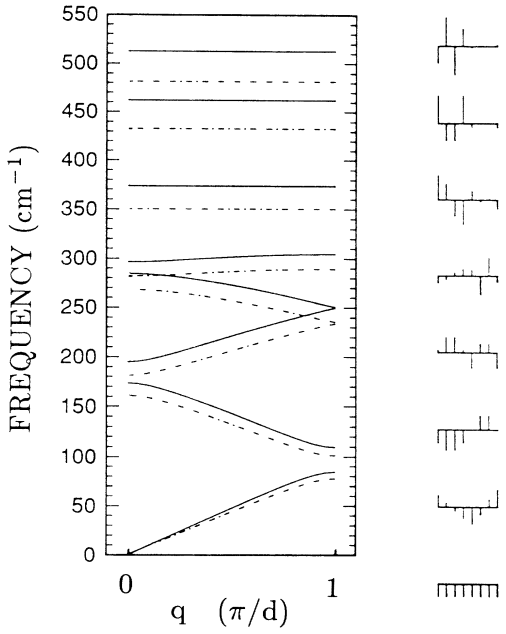

FIG. 5. Longitudinal phonon spectrum of [001]-oriented Si_4Ge_4 superlattices. Left panel: SL dispersion along the [001] direction for two different strain configurations corresponding to lattice matching to Si substrate (solid line) and Ge substrate (dashed-dotted line). Right panel: amplitude of longitudinal Γ-point displacements as a function of the z position of the (001) atomic planes in the unit cell (the sequence of planes in the cell from left to right is Si-Si-Si-Si-Ge-Ge-Ge-Ge). The displacement patterns correspond to modes of decreasing frequency from top to bottom: the three topmost modes are confined Si-like modes; the fourth is a quasiconfined Ge-like mode; the four lowest modes are extended acoustical modes.

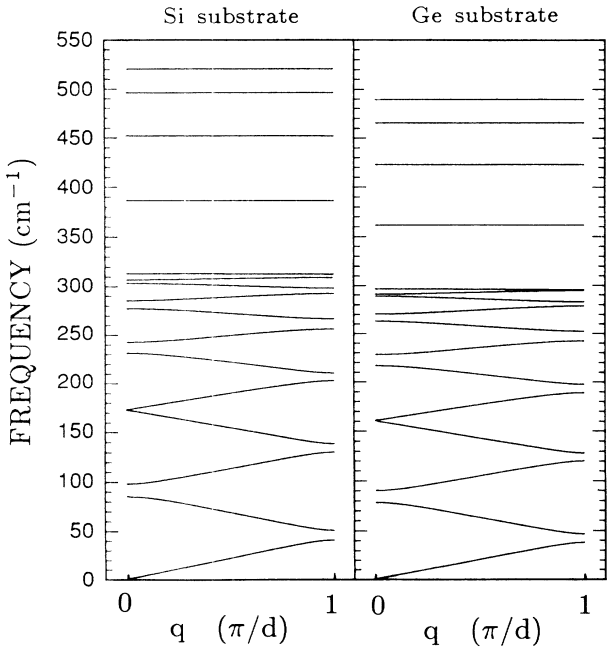

FIG. 6. Longitudinal phonon dispersion along the [001] direction for the [001]-oriented Si_6Ge_{10} superlattice. Left panel: strain configuration corresponding to lattice matching to a Si substrate; right panel: strain configuration corresponding to lattice matching to a Ge substrate.

cy range where the strain-induced shift in the corresponding bulk is no longer rigid, which gives rise to a difference in the frequency spacing between the third and the second confined modes (~ 5 cm^{-1} larger in the case of a Si substrate than for a Ge substrate). This implies that the comparison between the confined Si-like superlattice frequencies and the corresponding bulk dispersion (by "unfolding"[35]) in general is only meaningful when the appropriate *strained* bulk dispersion is used. On the other hand, our finding that the shift induced by strain is practically rigid in the highest part of the spectrum provides a justification for the procedure—which is commonly used—of measuring the strain in the Si layer by measuring the shift of the first confined mode with respect to the unstrained Γ-point mode.

Concerning Ge-like quasiconfined modes,[7(c)] we find—on the contrary—that a naive extension of such a procedure for strain characterization is not justified, due to the fact that their dispersion is not negligible and may change significantly with strain. As an example, in Fig. 6 we show the spectrum of Si_6Ge_{10}: the modes lying just below the edge of the allowed bulk Ge frequencies not only experience a shift due to lattice matching to different substrates, but are also affected in their dispersion and displacement patterns. A straightforward extension of the "unfolding" procedure[35] to Ge-like modes is not appropriate, because of their finite dispersion. The relation between SL quasiconfined modes[7(c)] and the corresponding bulk frequencies will be discussed elsewhere.[36] Finally, we mention that the variations in the bulk Si and Ge sound velocities with strain (see Table I and Ref. 37) have to be taken into account in the study of folded acoustic modes, and may yield appreciable differences in position and size of doublet splittings at the zone center or zone edge. A more extensive study of strained Si/Ge SL's will be presented elsewhere.[36]

V. CONCLUSIONS

We have performed a first-principles calculation of the structure and the longitudinal interplanar force constants of bulk Si and Ge, at three values of strain corresponding to lattice matching to Si, SiGe, and Ge substrates, along the [001] direction. Using these force constants, the bulk phonon spectra along the Δ line have been obtained. Our results are in good agreement with the available experimental data, which exist only for the unstrained dispersions and the strain-induced shifts at Γ, and provide the first predictions for the strain dependence of the dispersions. By considering prototype superlattice cases, we have shown that the detailed knowledge of the effects of strain on the bulk spectra may have important implications in the study of phonon spectra of Si/Ge superlattices. We have provided a simple and accurate way of calculating [001] dispersions of Si/Ge [001] superlattices grown on any $Si_{1-x}Ge_x$ substrate by presenting the appropriate interplanar force constants.

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[35]For a discussion on the relation between confined SL modes and bulk dispersions, particularly in GaAs/AlAs systems, see, e.g., the following recent reviews: B. Jusserand and M. Cardona, in *Light Scattering in Solids V: Superlattices and Other Microstructures,* edited by M. Cardona and G. Güntherodt (Springer, Berlin, 1989), p. 49; J. Menéndez, J. Lumin. **44**, 285 (1989), and references therein. In analogy with GaAs/AlAs, an accurate theoretical determination of the form of such a relation for Si/Ge superlattices is of great interest: assuming well-known layer thicknesses and small disorder effects, it would allow us to obtain information about the unknown strained bulk dispersions from experimental data on SL confined modes; conversely, it would allow structural characterization of SL samples (disorder effects or thickness parameters) once the strain effects on the bulk dispersion are known. See also Ref. 9(a).

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