# Linear-chain-model interpretation of resonant Raman scattering in $Ge_nSi_m$ microstructures

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We use a linear-chain model with bond polarizabilities to simulate the Raman spectrum of a $Ge_5Si_5$ microstructure which presents interface roughness both in the atomic scale and in the form of terraces of lateral dimensions equal or superior to $10^2$ Å. The model is not very successful in reproducing the effects of the short range roughness, but simulates effectively the consequences of terracing on the Raman spectrum of our sample. A detailed line shape analysis of one of these Raman lines leads to insights into the electronic states which are responsible for the resonant effects in the Raman cross section. [S0163-1829(96)02220-5]

## I. INTRODUCTION

Raman scattering is a useful technique for characterizing short period superlattices since lattice vibrations have a strong dependence on their structural characteristics.[1] This technique has been successfully applied to $Ge_nSi_m$ ($n$ and $m$ of the order of a few monolayers) multiple quantum wells and superlattices by comparing experimental results with theoretical model calculations.[2–8] The acoustic part of the spectrum is very sensitive to the large scale structure of the sample, such as overall periodicity, capping and buffer layers, number of repetitions, etc.[2,3] On the other hand, the optical modes are sensitive to characteristics of the $Ge_nSi_m$ unit, such as layer thickness and interface roughness.[4–9] Also, the dependence of the Raman cross section of optical modes on the photon energy of the incoming laser light (resonant Raman scattering) gives useful information about electronic transitions, yielding their transition energy as well as determining whether these transitions take place between extended or confined electronic states. In particular, for $n$ and $m$ of the order of 5 monolayers (ML), a resonant transition at $\hbar\omega_L \sim 2.4$ eV confined within the Ge layers has been reported. The precise nature of this transition and its connection to bulk Ge states is still unclear, being attributed to either $\mathbf{E}_0$-like or $\mathbf{E}_1$-like transitions.[10–15] A recent study of the Raman spectrum of $(Ge_5Si_5)_N$ structures ($N \simeq 1-5$) has shown that not only the intensity but also the line shape of some Raman lines depend strongly on the incident photon energy.[9] This dependence was attributed to large scale lateral terracing ($d \gtrsim 100$ Å), which would produce exciton confinement in wells of different well widths (different $n$) within a given Ge layer in the $(Ge_nSi_m)_N$ structure. For this to be true one assumption is made: that the quasiconfined Ge-Ge optical mode has a monotonic increase in its frequency as $n$ increases, just as a truly confined optical mode would. This assumption was made[9] using purely phenomenological arguments and indications given by calculations performed for materials similar to those actually studied.[4–8]

In the present work we use a linear-chain model (LCM) with bond polarizabilities[2,3] to simulate the Raman spectra of one of the samples studied in Refs. 9, 12, and 13. Its structure is composed of several repetitions of a $(Ge_5Si_5)_5Ge_5$ sequence separated by thick ($\sim$ 300 Å) Si spacer layers. In a previous work,[3] we used this model to analyze in detail the spectra of similar structures, both in the acoustic ($\omega \leqslant 100$ cm$^{-1}$) and optic ($\omega \geqslant 250$ cm$^{-1}$) frequency shift range. There, we showed that the latter depends only on the $Ge_nSi_m$ unit within the sample. Therefore the spectrum of our more complicated sample, in this frequency-shift region, is indistinguishable from that of an infinite $Ge_nSi_m$ superlattice. Here we explore the advantages, as well as intrinsic limitations, of the model and apply it to the quantitative study of the Raman spectrum of a sample containing both short and long range interface roughness. We concentrate on the properties of the Raman line originating in the Ge-Ge vibration and explain its line shape for a given photon energy of the incoming laser ($\hbar\omega_L$) as a superposition of lines produced from Ge layers of different thicknesses (different $n$). In this way we simulate the existence of terraces within a given Ge layer. By fitting the experimental line shapes for various $\hbar\omega_L$'s in this manner, we obtain resonances for the cross sections of modes confined within terraces of different widths. This allows us to estimate the confinement energies of the electronic states as a function of layer width which, in turn, yields information about the nature of the electronic transition involved in this resonance.

## II. EXPERIMENT

The sample was grown by molecular beam epitaxy at low temperature on a Si(100) substrate.[16] It consists of six quantum wells (QW's) of approximately 5 ML of Ge separated by 5 ML of Si. Those $(Ge_5Si_5)_5Ge_5$ units are repeated ten times and are separated from one another by thick ($\sim$ 300 Å) spacer layers of Si.

Raman scattering measurements were performed at room temperature in the backscattering configuration using several lines of Ar-ion and Kr-ion lasers. Normalized intensities were obtained by dividing the intensity of the Raman feature of the $Ge_5Si_5$ structure by that of the Si optical phonon peak originating in the bulk Si parts of the sample. Since the purpose of our discussion is to compare the resonant cross sec-

 

tion of a given phonon line originating in different lateral sections of the same Ge layer, more elaborate absorption corrections[10] are not necessary. Unpolarized scattered radiation was analyzed by a SPEX 1401 double monochromator with standard photon-counting detection.

## III. RESULTS AND DISCUSSION

The experimental data are compared to the simulated spectra produced by a LCM with bond polarizabilities for the calculation of Raman intensities. The model is very well known,[1–3] and its applications to the type of Ge/Si microstructures used in our experiments are described in detail in Ref. 3. In this model, whole planes of atoms are represented by a single point of mass given by that of the atom composing the plane. Force constants between these point masses are chosen so as to reproduce the bulk dispersion relation of the constituent bulk materials. In particular, for longitudinal phonons in Si-Ge systems two force constants (first and second neighbors) are sufficient to give a good reproduction of the dispersion relations of both Si and Ge.[2,3] To a certain extent, interface smudging can be introduced in this one-dimensional chain by substituting the pure Si or Ge atoms on both sides of the interface by mixed atoms with masses

$$m_{\mathrm{Ge}}(x)=(1-x)m_{\mathrm{Ge}}+xm_{\mathrm{Si}}, \tag{1}$$

$$m_{\mathrm{Si}}(x)=(1-x)m_{\mathrm{Si}}+xm_{\mathrm{Ge}}, \tag{2}$$

with $0\leqslant x\leqslant 0.5$. Similar averages for the force constants between mass points in the linear chain complete a simple approach to simulate short range interface roughness due to atomic interdiffusion of Si and Ge across the interface planes. The simplicity of the model makes it useful to experimentalists as a tool for interpreting actual spectra. However, this simplicity can introduce artifacts which must be spotted in order to use it correctly in the interpretation of experimental results. In a recent work[3] we discussed the application of the model to the interpretation of spectra from structures of the type $[(\mathrm{Ge}_n\mathrm{Si}_m)_{N-1}\mathrm{Ge}_n\mathrm{Si}_M]_p$, of which the one discussed here is a particular case ($n=m=5$, $N=6$, $M=221$, and $p=10$). There we found out that for frequency shifts $\omega\geqslant 250\ \mathrm{cm}^{-1}$, the spectra from these complex structures were indistinguishable from those of infinite $\mathrm{Ge}_n\mathrm{Si}_m$ superlattices. Hence, in order to save computing time, we use infinite $\mathrm{Ge}_n\mathrm{Si}_m$ periodic structures for our calculations.

The question we would like to pursue is that of large scale roughness, or terracing, raised in Ref. 9. In this earlier work we proposed the existence of lateral structures of length scale of the order of or larger than 100 Å in order to explain the broad asymmetric shape of the Ge-Ge Raman peak and its dependence on the photon energy of the exciting laser ($\hbar\omega_L$). The basic premise in Ref. 9 was that this vibration was confined within the Ge layers and thus its frequency increased monotonically as layer thickness increased. When working close to resonance with electronic transitions between states also localized in the Ge layers, $\hbar\omega_L$ can resonate with terraces of a given size (provided the lateral dimensions of the terrace are of the order of coherence length of the electronic states). Under this condition, the contribution to the Raman line shape from vibrations localized in this terrace will be enhanced over those of the vibrations localized at different terraces. This would provoke the observed variations in line shape and apparent peak position of the Ge-Ge Raman line as $\hbar\omega_L$ is swept around the resonant region.[9] Thus the crucial points to be tested theoretically are that of the confinement of these vibrations and that of the dependence of their frequencies on the thickness of the Ge layers. Once this is done, the actual line shape could be reproduced as a superposition of contributions from different $n$'s in $\mathrm{Ge}_n\mathrm{Si}_m$ structures. In this way we try to simulate the terracing, which implies the existence of wells of different widths within a given Ge layer. Finally, the dependence of each relative contribution on $\hbar\omega_L$ can be obtained. This we shall pursue in steps. First we examine the strong and weak points of the model by comparing its predictions with those of more sophisticated supercell models.[4–7] Next we study the issue of confinement of the Ge-Ge vibration by examining the calculated results for fictitious structures of the type $\mathrm{Ge}_5\mathrm{Si}_m$ with $m=5$–60 (from superlattices to isolated MQW's). In so doing we separate the predictions which apply to a real structure from eventual artifacts introduced by the simplification of reducing the actual three-dimensional (3D) problem to a one-dimensional chain. Finally we apply these results to the spectra of our sample.

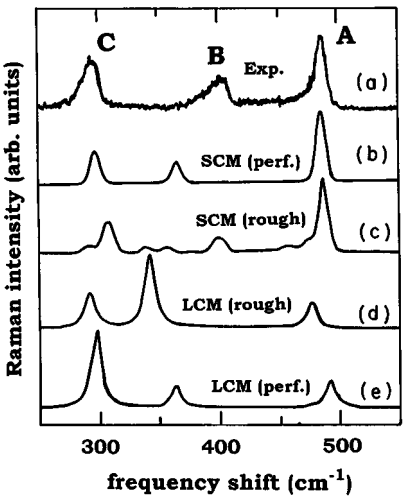


FIG. 1. Raman spectra of a $\mathrm{Ge}_4\mathrm{Si}_4$ strain-symmetrized superlattice. (a) Experimental results; SCM calculation for (b) perfect and (c) rough interfaces (all from Ref. 5); our LCM calculation for (d) perfect and (e) rough interfaces.

### A. Comparison of the LC and SC models

Alonso *et al.*[4] used a supercell model (SCM) to simulate the spectrum of a $\mathrm{Ge}_4\mathrm{Si}_4$ superlattice. The upper curve of Fig. 1 shows the experimental spectrum of such a sample, in the optical-phonon region. Peaks $A$, $B$, and $C$ in this spectrum are normally called the Si-Si, Si-Ge, and Ge-Ge peaks. Such peaks appear in $\mathrm{Ge}_n\mathrm{Si}_m$ structures for a wide variety of values of $n$ and $m$ (from $n,m\sim 2$ up to $n,m\sim 20$).[4,6] Supercell calculations[4–7] reproduce three peaks. Figure 1(b) reproduces the spectra calculated in Ref. 4 assuming perfect interfaces. The eigenmodes show that the vibrations producing peak $A$ are entirely confined in the Si layers, while those producing peak $C$ are nearly confined in the Ge layers, with

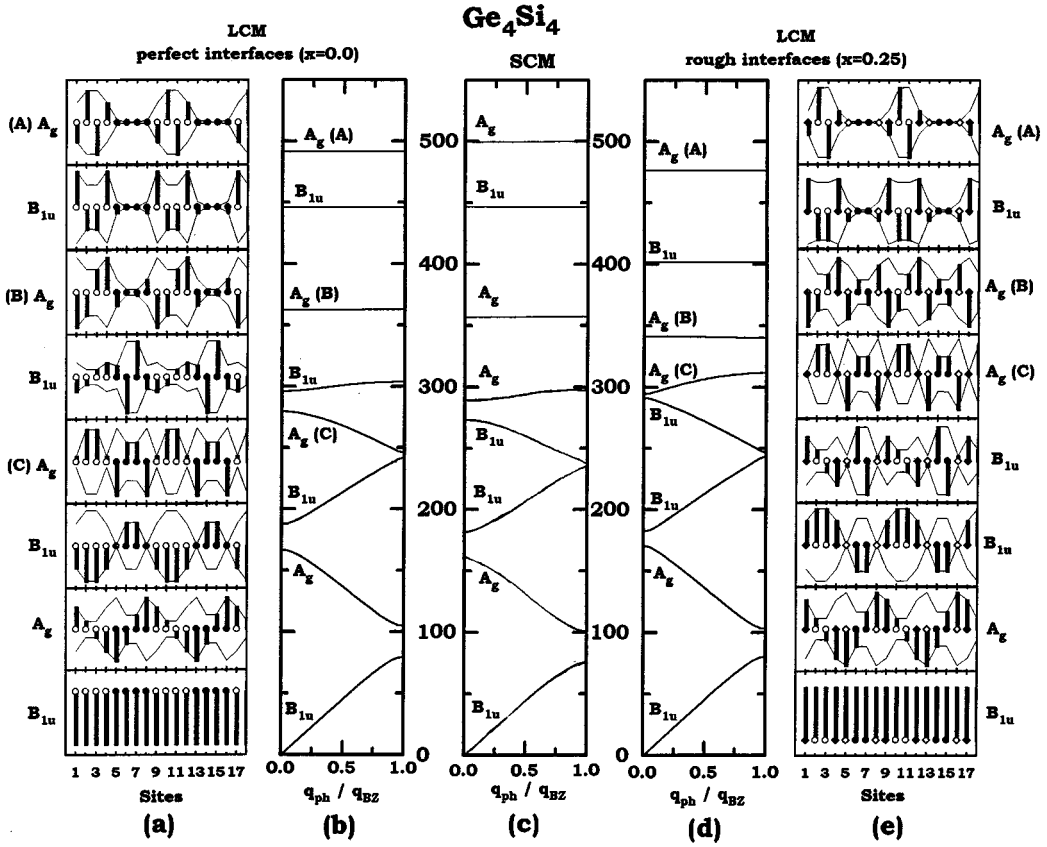


FIG. 2. Atomic displacements calculated with the LCM for a $Ge_4Si_4$ superlattice with (a) perfect and (e) rough interfaces. Dispersion relations calculated for this sample for perfect interfaces with (b) LCM and (c) SCM; (d) LCM with rough interfaces.

a small ''leakage'' into the Si layers where they propagate as an acoustical mode.[3,4] The interpretation of peak *B* is more delicate. The eigenmodes of the supercell calculation for perfect interfaces and those of our linear-chain model [shown in Fig. 2(a)] are identical, and so are the dispersion relations for the different phonons obtained by both models [Figs. 2(b) and 2(c)]. So both models agree in their predictions for structures with perfect interfaces. Introducing short range interface roughness into the LCM does not greatly affect either the normal modes or the dispersion relations [Figs. 2(d) and 2(e)]. This is also true for the SCM, except where peak *B* is concerned. For this particular vibration, the Si and Ge atoms on either side of a perfect interface vibrate out of phase, which led Alonso *et al.*[4] to dub this mode a Si-Ge mode. On the other hand, the atomic motions[17] portrayed in Fig. 2(a) bear a closer resemblance to those of the first overtone of the Si-confined optical mode, which spills over into the first Ge layer. This property led Dharma-wardana *et al.*[2] to name it the $l=2$ Si-Si mode. The real difference between these two ways of thinking becomes evident when we take into consideration the effects of short range interface roughness. The first striking difference between Fig. 1(a) and Fig. 1(b) is that in the experimental spectra this peak (peak *B*) is broad and asymmetric, in contrast with the calculated one [Fig. 1(b)]. Also, the position of the calculated peak for perfect interfaces is considerably different from that of the similar line in the experimental spectrum. Theoretical and experimental line shapes can be brought into coincidence (in both position and shape) by introducing disordered $Ge_xSi_{1-x}$ planes on both sides of the interface [Fig. 1(c) and Fig. 3 of Ref. 4)]. The more recent, and very thorough, calculation of this type by de Gironcoli *et al.*[7] shows that this line originates in longitudinal vibrations in these two alloy planes, which are confined within them. Thus they are interface modes because they are confined in these planes on both sides of the interface, and also they are the Si-Ge vibration of a disordered

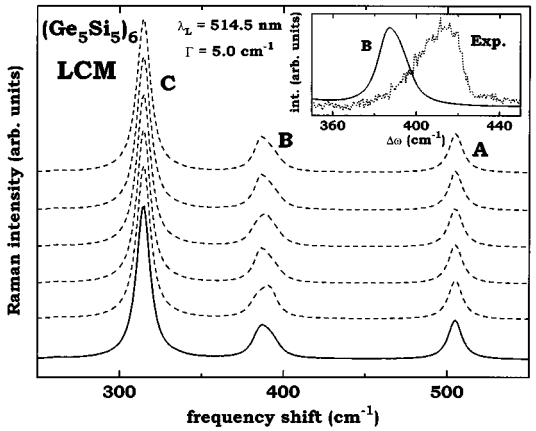


FIG. 3. Simulations of the spectrum for a $(Ge_5Si_5)_6$ structure using the LCM with randomly chosen rough interfaces (see text). The dashed curves each represent a given random configuration while the bottom curve is the average of those. The inset shows the comparison between the calculated and experimental spectrum for peak *B*.

$Ge_xSi_{1-x}$ alloy. This view is reinforced by the experimental fact that this line appears with the same shape and position in all types of $Ge_nSi_m$ superlattices[7,8] as well as in Ge single quantum wells,[9] where the concept of an ''overtone'' of a Si mode is meaningless. In sharp contrast to this, introducing roughness in the LCM, in the manner described above, does not alter the nature of the vibrations originating peak *B* in the Raman spectrum. This mode remains better described as an overtone of the Si-Si vibration [see Fig. 2(e)]. The failure of the LCM to give a realistic description of this Raman peak results from the inability of the 1D representation (which has exact symmetries, even when interface roughness is included) to reproduce the effects of disorder, successfully simulated in the SCM. In order to see if this deficiency could be overcome, we tried to introduce randomness into the 1D LCM. For this type of calculation we chose a $Ge_5Si_5$ structure, the eigenmodes of which represent those of the sample used in our experiments. Disorder is introduced by constructing a six-period $(Ge_5Si_5)_5$ sequence which we then repeat infinitely. We introduced roughness in all 12 Ge/Si interfaces in the manner of Eq. (1) , but the value of $x$ for each interface was chosen randomly among $x=0.15$, $x=0.20$, $x=0.25$, with equal probability for each value of $x$. Various randomly generated configurations were calculated. The results are displayed in Fig. 3, where the bottom curve is the superposition of the five configurations of the upper curves. The inset shows a detail of the *B* peak which is now asymmetric, but still does not reproduce the experimental peak position. Also the eigenvectors (not shown) are *not* those of vibrations localized around the interface region. This randomization procedure does not affect the positions and line shapes of peaks *A* and *C*. It is clear, then, that the effects of microroughness are not very well reproduced by the LCM and, in particular, the results obtained for peak *B* with this model cannot be used to interpret experimental spectra. On the other hand, the model can still be used to simulate the effects of terracing on peaks *A* and *C*. The first originates in vibrations entirely confined within the Si layers (Fig. 2). In this case the model predicts, for $Ge_nSi_m$ structures, symmetric peaks which do not depend on the value of $n$ and are well described by the conventional treatment of cutting the bulk-Si dispersion relation at points in $\vec{q}$ space given by[1,10]

$$\omega_A=\omega(q_l), \tag{3}$$

$$q_l=\frac{4\pi l}{a(m+\delta)}, \tag{4}$$

where $l$ represents the $l$th confined mode, $a$ is the bulk lattice parameter, and $\delta$ accounts for penetration of the envelope function of the displacements into adjacent layers. A comparison of the results of the LCM model for $n=5$ and various values of $m$ with the predictions of Eq. (3) for the first $(l=1)$ Si confined mode is shown in the upper part of Fig. 4(a). Excellent agreement is obtained with $\delta = 0.65$, which coincides with the conventional wisdom for confined optical modes.[6] The treatment of peak *C*, normally called Ge-Ge vibration, is more delicate and deserves a separate discussion, which we do next.

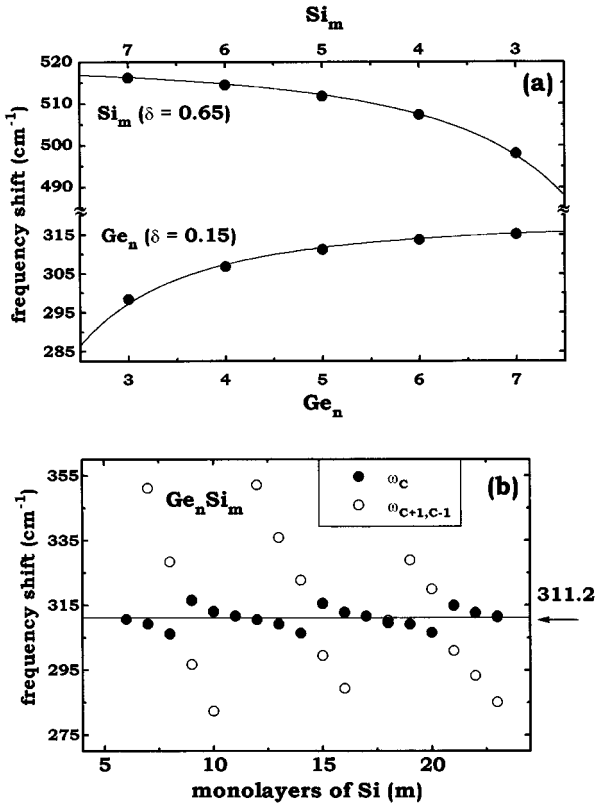


FIG. 4. (a) Frequencies of the modes originating lines *A* (upper trace) and *C* (lower trace) for different thicknesses of the Si or Ge layers. The values calculated with the LCM are displayed as closed circles while those predicted by Eqs. (3) and (4) are represented by solid lines. (b) Frequencies of peaks *C* (closed circles) and $C\pm1$ (open circles) calculated with the LCM for a $Ge_5Si_5$ structure with variable $m$.

### B. Confinement of the Ge-Ge vibration

The crucial point now is to see how the LCM describes the confinement effects in the Ge-Ge vibration (peak *C* of the Raman spectrum). As previously discussed, this peak is mostly confined within the Ge layer with a small leakage into the Si layer, where it propagates as an acoustic mode (Fig. 2). In a perfect crystal, this leakage will produce interference effects in a periodic $Ge_nSi_m$ structure, which cause strong oscillations of $\omega_C$ as a function of $n$ or $m$. The one-dimensional LCM reproduces this eccentric behavior, as reported in Ref. 2. This oscillation has a periodicity for both $n$ and $m$, which depends on the mass ratio of the constituent atoms.[2] Such behavior is exemplified in Fig. 4(b) where $\omega_C$ is plotted vs $m$ for various $Ge_5Si_m$ structures. In a real situation, however, we expect that these interferences [and their accompanying variations in $\omega_C(m)$] should be destroyed by the presence of the $Ge_xSi_{1-x}$ planes at the interfaces. In this case $\omega_C(m)$ should be approximately independent of $m$. Thus, the oscillations in $\omega_C(m)$ calculated by the model would not be observed and can be treated as an artifact.[18] In order to eliminate this artifact from the calculated values of $\omega_C$, we have to examine the nature and periodicity of these oscillations in more detail. In Fig. 4(b) we see that the pattern of oscillations repeats itself with a period $\Delta m=6$. An examination of the normal modes of the vibrations originating peak *C* and those of the two neighboring

branches (the ones immediately above and below in energy) reveals that for most values of $m$ there are two Raman-active modes (either $C$ and $C+1$ or $C$ and $C-1$), which are denoted in Fig. 4(b) by full (open) circles for the $C(C\pm1)$ mode. These frequencies oscillate in a periodic pattern symmetrically around its mean value ($\omega_C = 311.2\ \mathrm{cm}^{-1}$). In each period, a single value of $m$ exists for which the $C\pm1$ lines are not Raman active. In these cases $\omega_C$ falls exactly on the horizontal line ($\omega_C = 311.2\ \mathrm{cm}^{-1}$) which defines the mean value of these oscillations. After each of these values, the pattern repeats itself in a way similar to energy level anticrossings, with the $C$ and $C\pm1$ Raman-active lines ''pushing'' one another away from the line defining the mean value. After $\Delta m = 6$, again, there is only one Raman-active line ($C$) whose frequency is exactly $\omega_C = 311.2\ \mathrm{cm}^{-1}$. This goes on repeating itself indefinitely (we tested the interval from $m = 5$ to 50) in exactly the same fashion. The points with only one Raman line ($m=5,11,17,23,\ \ldots$) all have $\omega_C = 311.2\ \mathrm{cm}^{-1}$ and this is the mean value of the oscillation in $\omega_C(m)$ for each period. These ''anticrossings'' are the results of the exact symmetry that microroughness destroys in the real 3D case. Hence the recipe for eliminating this artifact[18] is to find this mean value of $\omega_C$ for each value of $n$. This can be done by reproducing a plot such as that of Fig. 4(b) for each choice of Ge layer thickness, or by calculating $\omega_C(n,m)$ for the value of $m$ in which the neighbors of peak $C$ ($C\pm1$) are not Raman active. The considerations of Dharma-wardana *et al.*[2] suggest that each Ge atom, being almost three times as heavy as a Si atom, is equivalent to three Si atoms within a given linear chain. By this rule, once $\omega_C(n_0) = \omega_C(n_0,m_0)$ has been isolated as one of those points lying on the mean line of $\omega_C(n_0,m)$, the equivalent points for other values of $n$ will be $\omega_C(n_0\pm1, m_0\mp3)$, $\omega_C(n_0\pm2, m_0\mp6)$, etc. This recipe actually works, and the values of $\omega_C(n)$ found in this way for $3\leqslant n\leqslant 7$ are on the lower part of Fig. 4(a) (circles). The solid line in this figure represents the ''folded'' frequencies from the bulk dispersion, in a manner analogous to that of Eqs. (3) and (4) for the Si-confined mode. We see that also for this mode the hypothesis of confinement works very well. In fact the value of $\delta = 0.15$ which gives the best fit suggests that this mode has an even greater degree of confinement than the Si-Si mode.

### C. Resonant cross section of the Ge-Ge mode

The above discussion shows that, after circumventing intrinsic artifacts of the LCM, this model can be used to describe the results of terracing in the Raman spectrum of $Ge_nSi_m$ superlattices. In a sample containing several such terraces the actual Raman intensity should be obtained as a superposition of peaks localized within each terrace. Thus it could be written as

$$I_C(\omega_L,\omega)=\sum_n n\,\alpha_n(\omega_L)\mathrm{L}[\omega,\omega_C(n),\Gamma_n], \qquad (5)$$

where the factor $n$ occurs because each terrace contributes to the intensity in direct proportion to its width, $\omega_L$ is the laser frequency, $\alpha_n(\omega_L)$ contains the resonant part of the cross section for the exciton confined within this terrace, and L is a standard Lorentzian line shape:

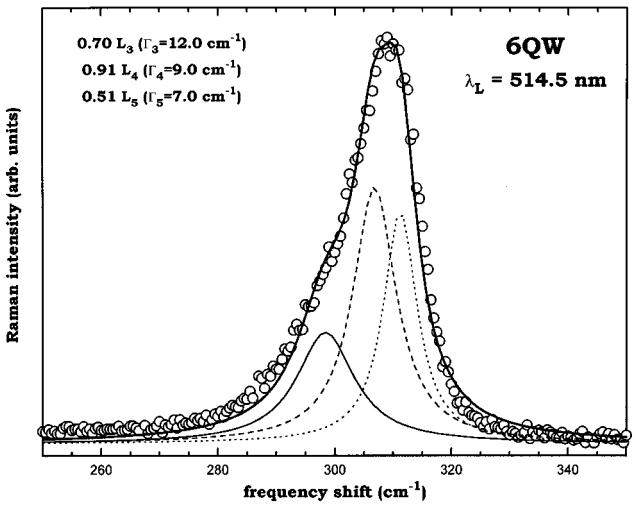


FIG. 5. Line $C$ in the Raman spectrum (circles) fitted with a superposition of lines calculated for different Ge layer thicknesses (solid line). Each line composing the fit is shown below.

$$\mathrm{L}[\omega,\omega_C(n),\Gamma_n]=\frac{\Gamma_n}{[\omega-\omega_C(n)]^2+\Gamma_n^2}. \qquad (6)$$

In Eq. (5) $\omega$ is the Raman shift, $\omega_C(n)$ is the frequency of the confined Ge-Ge phonon, and $\Gamma_n$ is its homogeneous line broadening. We assume that this line broadening is dominated by the short range roughness at the Ge/Si interface which makes $\Gamma_n$ larger for smaller $n$, since the fraction of the Ge layer taken over by this roughness is larger as $n$ gets smaller. Such a fit for a representative spectrum is shown in Fig. 5. Here we used only three terraces $n = 3$, 4, and 5 and $\Gamma_3{:}\Gamma_4{:}\Gamma_5$ in the approximate ratio of 5:4:3, with the values of $\omega_C(n)$ from Fig. 4. The observed fit is excellent and similar fits were obtained for the spectra of the same sample for several laser frequencies in the range $1.92\ \mathrm{eV}\leqslant\hbar\omega_L\leqslant 2.7$ eV.

The values of $\alpha_n(\omega_L)$ obtained from these fits are plotted in Fig. 6 for each terrace size. The lines are least-square fits to Lorentzians, the center frequencies (width) of which would represent the energy (lifetime broadening) of the exciton confined within each terrace.[19] The results of Fig. 6 are consistent with the hypothesis of selective resonance by excitons confined in different terraces. This consistency is shown because both $E_{\mathrm{exc}}(n)$ and $\Gamma_{\mathrm{exc}}(n)$ increase as $n$ decreases. The first is a consequence of the greater confinement for smaller $n$'s and the second reflects the larger percentual influence of the small scale roughness in narrower terraces, which reduces the exciton lifetime.

Finally, the data of Fig. 6 can be compared to a simple envelope-function calculation for the confinement of an $E_0$-like electronic transition within the Ge layers of the $Ge_nSi_m$ structure. This simple calculation was found useful in describing those parts of the modulated reflectivity spectra attributed to these types of transition.[14] This comparison is shown in the inset of Fig. 6, where the points are the value of $E_{\mathrm{exc}}$ from our fit (with error bars given by $\pm\ 0.2\Gamma_n$) and the solid line is the result of the envelope-function calculation. The observed increase in the transition energy as $n$ decreases

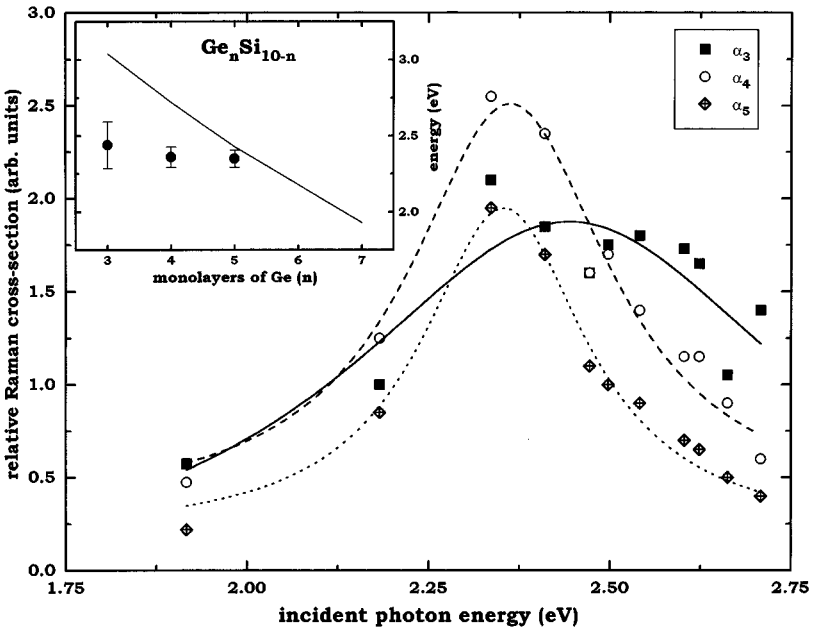


FIG. 6. Values of $\alpha_n(\omega_L)$ from Eq. (5) vs $\omega_L$ obtained as explained in the text (circles, diamonds, and squares) fitted to Lorentzian line shapes. The inset shows the center energies of these three Lorentzian curves (circles) compared to an envelope-function calculation (solid line) for $\mathbf{E}_0$-like states.

is much slower than that predicted for an $\mathbf{E}_0$-type transition. The results are, therefore, more in consonance with the hypothesis that the resonance in the Raman cross section originates in $\mathbf{E}_1$-like transitions of bulk Ge states, modified by folding and confinement as proposed in Ref. 13.

## IV. SUMMARY AND CONCLUSIONS

Simulation of Raman spectra by a simple linear-chain model permits us to obtain insight into the origin of the vibrations which originate both the Ge-Ge and Si-Si peaks of the Raman spectrum of all samples, although it fails to describe the Si-Ge peak. Judicious use of the model permits a quantitative study of the variations in line shape and position of the Ge-Ge line as the laser-line frequency changes. This study confirms the existence of terraces, first proposed in Ref. 9, and favors the interpretation of the resonance appearing in the Raman cross section as originating in $\mathbf{E}_1$-like transitions of bulk Ge modified by the effects of confinement and zone folding, proposed in Ref. 13.

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[17] In this figure atomic displacements are shown perpendicularly to the linear chain for the sake of display clarity. These displacements, however, are really along the chain and this should be taken into account when checking the symmetry ($u$ or $g$) of a given mode.

[18] The term ''artifact'' is used to describe a prediction of the model which is not observed experimentally. This prediction, however, would be observed if a structure with *absolutely* perfect interfaces could be grown. In this case, the model would even describe correctly peak $B$ in the Raman spectrum.

[19] This is a naive way of representing the resonant Raman cross section for a localized exciton. The real situation could be much more complex and should be treated with a detailed understanding of the Raman mechanism. The present approach intends only to give rough estimates of the dependence of confinement energy on well width for the electronic transition responsible for this resonance.