Contribution of strain-induced modulation to the sound velocity in lattice-mismatched quasiperiodic superlattices

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The propagation of longitudinal-acoustic waves through a quasiperiodic superlattice composed of layers belonging to the cubic symmetry group is explored in terms of the interfacial strain effects. The results show features that seem unique to the lattice-mismatched superlattices. We find that the strain-induced modification of the propagation velocity in this type of superlattice is more pronounced and may be positive or negative, depending only on the velocity difference in the respective media. We also obtain universal formulas for the effective elastic coefficient and average and effective sound velocities, as well as the relevant modulation amplitude, which depends on the quasiperiodic index p. These expressions are applied to analyze the folded acoustic-phonon spectra of semiconductor Si-Ge_xSi_{1-x} and GaAs/$Ga_{1-x}Al_xAs$ quasiperiodic Fibonacci superlattices. Our predictions for peak positions of the Raman spectra are in reasonable agreement with the experimental data.

I. INTRODUCTION

The one-dimensional (1D) quasiperiodic superlattice (QPSL) is neither a periodic lattice nor a fully disordered one, many sharp doublet peaks with unequal intervals can still be observed by Raman scattering.[1-6] This means that acoustic waves in such a QPSL are Bragg reflected; and their frequency shift satisfies a linear dispersion relation so that the quasiperiodicity originating in the Fibonacci sequence causes so-called zone-folding effects on the acoustic phonon modes. Although there is now a well-established understanding of 1D quasiperiodic superlattices, the influence of the imperfections in the structure on various physical properties of such systems, however is not known. For example, if the interfacial mismatch strain is not negligible, how are the acoustical and optical properties affected by it in the observed phonon spectrum? For 1D periodic superlattices a lot of experiments and theories have already been done which answered such questions successfully.[7-9] However, in a quasiperiodic superlattice there is a dense distribution of scattering peaks throughout the total low-frequency regime (≤ 100 cm^{-1} for LA modes or ≤ 50 cm^{-1} for TA modes). In addition, the positions of the main Raman peaks not only depend on the stage number of the Fibonacci sequence but also on the strain-induced modification. In fact a few experiments have confirmed these,[4-6] especially in the strained-layer Si-Ge_xSi_{1-x} quasiperiodic Fibonacci superlattice (QPFSL).

Wahlström and Chao[10] first calculated the Raman spectra of GaAs/AlAs QPFSL's either with an ideal interface or with some imperfections. But the effects from interfacial strain-induced modulation on phonon spectra were not included in their model. According to the work of Jusserand *et al.*[11] on periodic GaAs/AlAs Fibonacci superlattices, while the interfacial acoustic impedance modulation nearly vanishes, the displacement field can be expressed as a plane wave with an effective sound velocity. In this case the superlattice behaves somewhat like an effective homogeneous medium, and the wave suffers no reflection at any interface. However, in a lattice-mismatched QPFSL, this is not the case in reality. For this type of superlattice, the lattice-constant mismatch is accommodated by interfacial strains rather than by the formation of the misfit dislocations. The existence of such internal strains should substantially modify the phonon spectra and lead to a large correction on propagation velocity of the acoustic waves. Modulation of this kind may cause the predicted Raman spectra deviate from experimental data. Thus, in order to incorporate the strain-induced modification in the phonon spectrum, a more general theory for the acoustic-wave propagation becomes necessary.

In this paper we present a theoretical analysis of the low-frequency Raman spectra for Si-Ge_xSi_{1-x} and GaAs/$Ga_{1-x}Al_xAs$ QPFSL's in terms of strain effects. These two systems appear to be good candidates for ascertaining the contributions of the strain-induced modification. The results show features which seem unique to the lattice-mismatched superlattices. In Sec. II we will discuss the propagation problem of the acoustic waves for [001]-oriented QPFSL. In the limit of long-wavelength we derive an analytical expression for the effective sound velocity, including the effects of the strain-induced modification. Results from these calculations and comparisons and comparisons with available experimental observations are presented in Sec. III. Section IV is used for a brief summary and conclusions.

II. ACOUSTIC-WAVE PROPAGATION IN QPFSL'S

A. Effective elastic coefficient

The acoustic vibrations in a QPFSL are able to be described by elastic waves propagating in a structured continuum. To the advantage of both experimental study and theoretical analysis, Si-Ge_xSi_{1-x} and GaAs/$Ge_{1-x}Al_xAs$ superlattices are usually grown along the [001] axis. In rectangular Cartesian coordinates we consider an infinite superlattice with its growth direction along the z axis, x and y lying in the plane of the layers. Each layer is assumed to have cubic symmetry, and is characterized by its elastic constant and density. It follows that the acoustic displacement field, at a given frequency, fulfills the wave equation

$$w^2\rho(z)u(z)=-\frac{\partial}{\partial z}\left[C(z)\frac{\partial u(z)}{\partial z}\right], \quad (1)$$

where $u(z)$ can be obtained by solving the above equation in each layer and then applying boundary conditions at each interface. The conditions that assume the continuity of the displacement and the stress at the interfaces restrict the phonon frequencies and wave vectors, in the low-frequency case, to those values satisfying the simple dispersion relation[1-6]

$$w=w^{\pm}_{n,m}\equiv|q\pm k_{n,m}|v_{\text{eff}}, \quad (2)$$

where $q=|\mathbf{k}_i-\mathbf{k}_s|$ depends on the scattering configuration and excited wavelength, $k_{n,m}=2\pi(n\tau+m)/d$ where n and m are arbitrary integers, and v_{eff} the effective sound velocity of the elastic waves along z. In the absence of gaps Eqs. (2) represents simply the folding of the normal linear relationship between frequency and wave vector with slop v_{eff}.

Since the scattering processes of such elastic waves are primarily due to the photoelastic mechanism, when the sound velocities differ far less than the photoelastic coefficients, one can approximately replace the effective sound velocity of a quasiperiodic superlattice by following calculations. First let $C^A_{\alpha\beta},\sigma^a_{\alpha\beta},\epsilon^A_{\alpha\beta}$ and $C^B_{\alpha\beta},\sigma^B_{\alpha\beta},\epsilon^B_{\alpha\beta}$ represent the components of the elastic, stress, and strain tensors, respectively. Superscripts A and B refer to the two basic elements, respectively, and $C_{\alpha\beta},\sigma_{\alpha\beta},\epsilon_{\alpha\beta}$ refer to the effective properties of the quasiperiodic superlattices. The detailed prescriptions for forming a Fibonacci lattice from two structural units A and B can be found in the Ref. 12. To formulate the wave propagation in quasiperiodic structures we utilize the concepts outlined in Ref. 4 and invoke a two-dimensional (2D) periodic lattice, the whole set of reciprocal vertices labeled (n,m) in reciprocal space is projected onto an 1D axis whose direction is not crystallographic; we therefore yield a quasiperiodic 1D sequence with the structure factor[4-6]

$$S(k)=\frac{\tau^2}{d}\sum_{n,m}\frac{\delta_{k,k_{n,m}}}{iX_{n,m}}[\exp(iX_{n,m}\tau^{-2})-\exp(-iX_{n,m}\tau^{-1})], \quad (3)$$

and the substructure factors of the two basic elements

$$S_A(k)=\frac{\tau^2}{d}\sum_{n,m}\frac{\delta_{k,k_{n,m}}}{iX_{n,m}}[\exp(iX_{n,m}\tau^{-2})-\exp(-iX_{n,m}\tau^{-3})], \quad (4)$$

$$S_B(k)=\frac{\tau^2}{d}\sum_{n,m}\frac{\delta_{k,k_{n,m}}}{iX_{n,m}}\exp(-ikd_A)\times[\exp(iX_{n,m}\tau^{-4})-\exp(-iX_{n,m}\tau^{-3})]. \quad (5)$$

Here $X_{n,m}=2\pi\tau^2(md_A-nd_B)/d$ in dependent on the indices (n,m) and the contents of the basic elements. Corresponding to Fourier-transform form of an arbitrary function in a periodic lattice

$$\Phi(k)=S_p(k)\phi(k),$$

where $S_p=L^{-1}\sum_n\delta(k,k_n)$ is the structural factor, we can give an analogous transform of Φ in a quasiperiodic lattice

$$\Phi(k)=S_A(k)\Phi_A(k)+S_B(k)\Phi_B(k).$$

With this definition we need only to consider longitudinal vibration of the elastic waves along z. From the symmetry of the problem, the continuum model expression for the compressional strain field in reciprocal 1D space is therefore described by the strain component

$$\epsilon_{33}(k)=S_A(k)\epsilon^A_{33}(k)+S_B(k)\epsilon^B_{33}(k)=\bar{\epsilon}_{33}\delta(k)+(\epsilon^A_{33}-\epsilon^B_{33})\sum_{n,m}\delta(k,k_{n,m})S(k), \quad (6)$$

where $\bar{\epsilon}_{33}=(\epsilon^A_{33}\tau d_A+\epsilon^B_{33}d_B)/d$ is the spatial average of the effective strain in the structure. On the other hand, the Fourier transform of the mass density can be carried out in the same procedures. Since the density difference $|\rho_A-\rho_B|$ is much smaller than average density of the two constituent layers, we may keep the zeroth-order term

$$\rho=(\tau d_A\rho_A+d_B\rho_B)/d, \quad (7)$$

as the effective density of quasiperiodic superlattice.

For a superlattice composed of cubic layers such as GaAs/AlAs, the point-group symmetry is reduced to D_{2d} from T_d, exhibited by the host materials. As a result, the elastic constant C_{33} in the superlattice is different from C_{11} due to anisotropy. Therefore, for respective basic element layers, the Hooke's law gives the relation of stress-strain to be linearly related to elastic constants by

$$\sigma^j_{33}=C^j_{11}\epsilon^j_{33}+C^j_{12}(\epsilon^j_{11}+\epsilon^j_{22}) \quad \text{for } j=A \text{ and } B. \quad (8)$$

The stress component in superlattice, due to tetragonal symmetry, should be

$$\sigma_{33}=C_{33}\epsilon_{33}+C_{13}(\epsilon_{11}+\epsilon_{22}). \quad (9)$$

We note that we are dealing with a quasiperiodic ideal multilayer in which the acoustic wave propagate. In the present case, the strain field is still a modulated plane wave but does not satisfy Bloch theorem. Now, we only consider the propagation of the strain field normal to the surface. This restriction excludes the possibility of coupling between the different polarization waves. Let us look for a solution of this kind strain field in the plane-wave approximation. Then the strain component of a z-propagating compressional wave is

$$\epsilon_{33} \simeq \bar{\epsilon}_{33}(z) = \epsilon(z)\exp[i(wt - kz)] \quad (10)$$

and

$$\epsilon^{j}_{33}(z) = \epsilon^{j}(z)\exp[i(wt - kz)] \quad \text{for } j = A \text{ and } B \ . \quad (11)$$

Matching the expression for the stress in the various regions through the use of the boundary conditions of $\sigma_{33} = \sigma^{A}_{33} = \sigma^{B}_{33}$. Substituting of Eqs. (8)–(11) into Eq. (6), we have the following effective elastic coefficient involving corresponding quantities in the respective media for the longitudinal acoustic waves:

$$\frac{d}{C_{33}} = \left[\frac{\tau d_A}{C^{A}_{11}} + \frac{d_B}{C^{B}_{11}} \right] \delta(k) + \left[\frac{d}{C^{A}_{11}} - \frac{d}{C^{B}_{11}} \right] \sum_{n,m} \delta(k, k_{n,m}) S(k) \ , \quad (12)$$

where $S(k, k_{n,m})$ is the structure factor and d is set as $d = \tau d_A + d_B$, the average lattice parameter.

B. Average sound velocity

The second terms in Eq. (12) are generally smaller than the first one, and can often be considered as a perturbation. We may keep the first term only when $|C^{B}_{11} - C^{A}_{11}| \ll C^{A}_{11} C^{B}_{11} / C_{11}$, or as zeroth-order approximation. Such simplifications help to emphasize the physical meanings involved. First, let us discuss the solution of this approximation. Substitution Eq.(7) into (12) we may find

$$\sqrt{C_{33}/\rho} = d \left\{ \frac{(\tau d_A)^2}{C^{A}_{11}/\rho_A} + \frac{d_B^2}{C^{B}_{11}/\rho_B} + \left[\frac{d}{C^{A}_{11}} - \frac{d}{C^{B}_{11}} \right] \sum_{n,m} \delta(k, k_{n,m}) S(k) \ , \right. \quad (13)$$

where

$$R = \rho_A \sqrt{C^{A}_{11}/\rho_A} / \rho_B \sqrt{C^{B}_{11}/\rho_B}$$

is the ratio of the acoustic impedances. For cubic symmetry, there are three independent elastic constants, labeled C_{11}, C_{12}, and C_{44}, and the velocity of the bulk longitudinal waves along a crystal axis is $v_l = \sqrt{C_{11}/\rho}$. Thus, we can define $\bar{v}_l = \sqrt{C_{33}/\rho}$, $v_l{}^A = \sqrt{C^{A}_{11}/\rho A}$, and $v^{B}_{l} = \sqrt{C^{B}_{11}/\rho_B}$, respectively; an equivalent expression of Eq. (13), i.e., an average sound velocity in QPFSL's, is

$$\bar{v}_l = d \left[\left[\frac{\tau d_A}{v_l{}^A} \right]^2 + \frac{d_B}{v_l^B} \right]^2 + \frac{\tau d_A d_B}{v_l{}^A v_l^B} \left[\frac{\rho_A v_l{}^A}{\rho_B v_l^B} + \frac{\rho_B v_l^B}{\rho_A v_l{}^A} \right] \Bigg]^{-1/2} \ . \quad (14)$$

The expression of Eq. (14) in appearance is rather similar to Eq. (16) of Ref. 13, when $d_1 = \tau d_A$ and $d_2 = d_B$. It implies that the dispersion relation of the acoustic phonons in quasiperiodic superlattices is no remarkable changes comparing with that or periodic superlattices only when neglecting the structural and strain-induced modulation. In general, we may take $\bar{v}_l$ to replace v_{eff} in Eq. (2) as a good approximation. Here, we should be borne in mind that in the process of deriving v_{eff} the high-order terms of the Fourier transform have been ignored. However, for a lattice-mismatched superlattice, the strain-induced changes for v_{eff} can be considered as follows.

C. Effective sound velocity

According to our previous work,[14] in discussing the phonon spectrum excited by surface acoustic modes , one must take into account the presence of the acoustic impedance, for which its effects not only modify phonon line intensities but lead to the asymmetry of some observable doublets.[11] In the case of an infinite quasiperiodic superlattice, the Fourier transform of the acoustic modulation exhibits a dense distribution. The correction of the sound velocity may be derived from a simple perturbation calculation based on the Fourier transforms of the Eq. (6). Consequently, the sound velocity of the longitudinal elastic waves is approximately given by

$$v_{\text{eff}} = \bar{v}_l \left[1 - \frac{(v_B^2 - v_A^2)\bar{v}^2}{2 v_A^2 v_B^2} \sum_{n,m} S(k_{n,m}) + \frac{3\bar{v}^4 (v_B^2 - v_A^2)^2}{8 v_A^4 v_B^4} \sum_{n,m} \sum_{i,j} S(k_{n,m}) S(k_{i,j}) - \cdots \right] , \quad (15)$$

where v_A and v_B are, respectively, the sound velocities of the bulk elastic waves in the basic elements A and B. If assuming that the contents of the basic element A are completely different from those of B, then we have

$$|S(k_{n,m})|^2 = \left| \frac{4\tau^2 \sin(k_{n,m} d_A/2) \sin(X_{n,m}/2\tau)}{k_{n,m} X_{n,m} d} \right|^2 . \quad (16)$$

In general the effects of higher-order terms are quite small and can be ignored; if we keep only the linear terms, the contribution of the strain-induced modification to the effective sound velocity at order p is found to be

$$\Delta_p = \left| \frac{(v_A^2 - v_B^2)\bar{v}^2}{2 v_A^2 v_B^2} \right| \frac{d}{\pi^2 d_A} \left| \sin \left[\frac{\tau d_A \tau^p}{d} \right] \sin \left[\frac{\tau d_A \tau^{1-p}}{d} \right] \right| , \quad (17)$$

here we have selected $d_A = \tau d_B$ for a 2D square lattice and transformed the quasiperiodic indices (n,m) into index p, because the second term in Eq. (15) becomes small as either $k_{n,m}$ or $X_{n,m}$ gets large and achieves its maximum values when n and m are neighboring Fibonacci numbers, defined iteratively by $F_p = F_{p-1} + F_{p-2}$ for $p \geq 2$, with $F_0 = 0$ and $F_1 = 1$. Therefore, the strain-induced modulation on the sound velocity of the QPFSL's is mostly from several largest Fourier components. Nevertheless, the sum of high-order terms in

Eq. (15) is not negligible, and may accurately determine the positions of the folded acoustic modes in a low-frequency Raman spectrum. This conclusion can be checked with available experimental data of the Si-Ge_xSi_{1-x} and GaAs/$Ga_{1-x}Al_xAs$ Fibonacci-modulated superlattices.

III. DISCUSSION OF RESULTS

A. Si-Ge_xSi_{1-x} QPFSL's

For Si-Ge_xSi_{1-x} strained-layer QPFSL's, Dharma-wardana *et al.*[4] estimated the effective sound velocity of the longitudinal-acoustic waves as 8.0 km/s based on the bulk sound velocities of Si and Ge and the measured x (0.48) value of the Ge_xSi_{1-x} alloy. Comparison of their calculated and observed Raman peak frequencies shows that although all measured doublet Raman peaks can be approximately predicted, the calculated peak positions are slightly lower than the corresponding measured ones. According to our work in Sec. II, the numerical calculations have been completed. Here, we let $\bar{v}_l = 8.0$ km/s, the average sound velocity in the Si-Ge_xSi_{1-x} Fibonacci superlattices; and the other parameters used are as follows:

$$d_A = 54\ \text{Å},\quad \rho(\text{Si}) = 2330\ \text{kg/m}^3,\quad v_A = 8.4\ \text{km/s}\ ,$$

$$d_B = 42\ \text{Å},\quad \rho(\text{Ge}) = 5323\ \text{kg/m}^3,\quad v_B = 7.3\text{km/s}\ .$$

The strain-induced modulation on the effective sound velocity can be expressed as a function of quasiperiodic indices (n,m) or index p; such a modulation is shown in Fig. 1(a). An important feature can be seen clearly in this figure that the maximum modulation essentially occurs at $|p| \le 10$, whereas for large $|p|$ the strain does not contribute to the modification of sound velocity in the QPFSL's. On the other hand, in the limit of $\epsilon_{33}^A - \epsilon_{33}^B \approx 0$, Eq. (15) reduces to Eq. (14), corresponding to the case of vanishingly small strain-induced modulation. Note that the sound-velocity difference $v_l^A - v_l^B$ in this superlattice is greater than zero so that $v_{\text{eff}} \ge \bar{v}_l$. Calculations from Eq. (15) for Si-$Ge_{1-x}Si_x$ QPFSL's indicate that the perturbation correction of the effective sound velocity amounts to 0.317 km/s, which means that the actual sound velocity in this superlattice is nearly 8.32 km/s. Using Eq. (2) we further calculate the Raman peak positions according to the results of Dharma-wardana *et al.*[4] Table I displays corresponding experimental and calculated Raman data both from Ref. 4 and our present work. In accordance with Ref. 4 we have used the Brillouin shift of $w_B = (5.3 \pm 0.3)$ cm^{-1}. Comparison of the two kinds of approaches demonstrates that the effective sound velocity of the quasiperiodic superlattices is dependent on strain-induced modulation existing in the systems, and our results coincide with experimental observations.

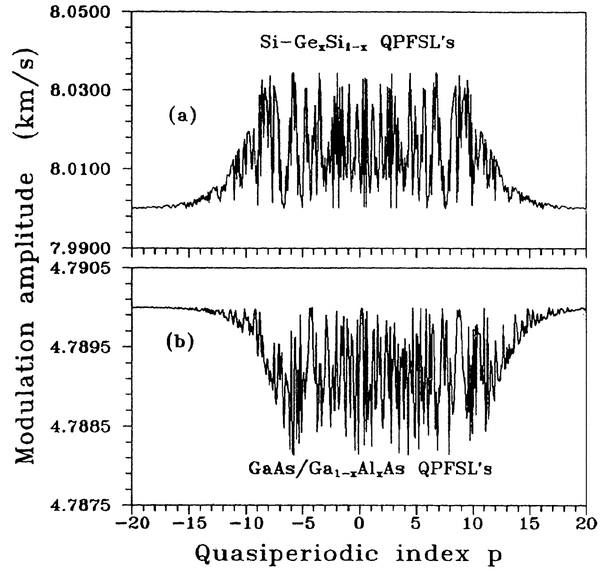

FIG. 1. A plot of modulation amplitude Δ_p vs quasiperiodic index p for (a) Si-Ge_xSi_{1-x} quasiperiodic Fibonacci superlattice and (b) GaAs/$Ga_{0.75}Al_{0.25}As$ quasiperiodic Fibonacci superlattice.

B. GaAs/$Ga_{1-x}Al_xAs$ QPFSL's

Although the effects of the strain-induced modification on phonon spectra of the Si-Ge_xSi_{1-x} QPFSL'S have been verified, whether our present model is valid for the other system remains unclear. Therefore, in Fig. 1(b) we also give the relationship of modulation amplitude versus quasiperiodic index p for GaAs/$Ga_{1-x}Al_xAs$ ($x = 0.25$) QPFSL's,[5] where the lattice mismatch is much smaller than that of Si-Ge_xSi_{1-x} systems. As we saw in the preceding subsection, the modification from the largest

TABLE I. The main spectral lines in the quasiperiodic Si-Ge_xSi_{1-x} ($x \simeq 0.48$) Fibonacci superlattice. Corresponding the larget Fourier compnents, the phonon frequency has been expressed as $w_{n,m}^{\pm} = w_p^{\pm} \equiv |2\pi\tau^p v_{\text{eff}} d^{-1} \pm w_B|$, p being an integer. Note that the Raman spectra usually contain an error about a half of a wave number.

	Phonon frequency (cm^{-1})[a]									
$w_p^{\pm}$	w_{-2}^-	w_{-2}^+	w_{-1}^-	w_{-1}^+	w_0^-	w_0^+	w_1^-	w_1^+	w_2^-	w_2^+
Theory[b]	2.6	13.2	7.5	18.1	15.4	26.0	28.2	38.8	48.9	59.5
Expt.[b]		13.5		18.5	15.7	26.9	29.2	39.9	51.0	60.9
This work	2.9	13.5	8.0	18.6	16.3	26.9	29.6	40.2	51.1	61.7

[a] Brillouin shift $w_B = 5.3 \pm 0.3$ cm^{-1}.

[b] See Ref. 4.

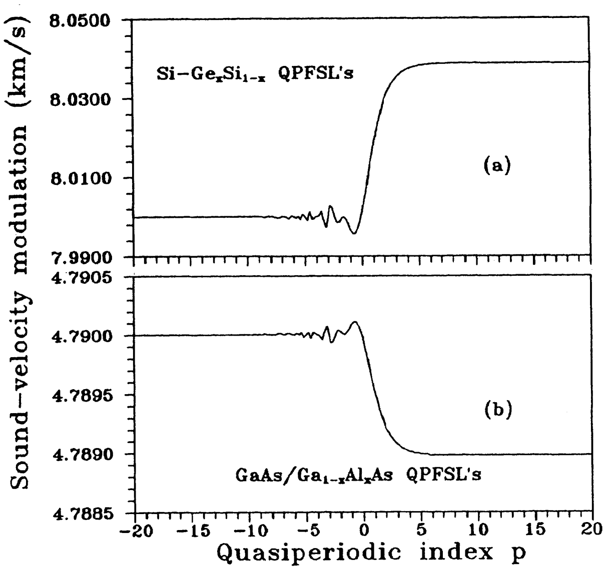

FIG. 2. Effects of the strain-induced modulation on sound velocity (a) for Si-Ge$_x$Si$_{1-x}$ and (b) GaAs/Ga$_{0.75}$Al$_{0.25}$As QPFSL's. For simplicity, we have transformed quasiperiodic indices (n,m) into index p through the relation of $(m+n\tau)=\tau^p$, where m and n span all the integers.

Fourier components is universal, as expected. The modulation features of the sound velocity for these two superlattices are identical in their qualitative appearance (see Fig. 1), however, the modulation amplitudes are radically different, because of nearly vanishing lattice mismatch in GaAs/Ga$_{1-x}$Al$_x$As. This amplitude in Si-Ge$_x$Si$_{1-x}$ is much greater than that of GaAs/Ga$_{1-x}$Al$_x$As.

The numerical procedures to obtain the dependence of modulation amplitude on quasiperiodic indices (n,m) for GaAs/Ga$_{1-x}$Al $_x$As QPFSL's are given as follows. First, based on Refs. 2 and 5, the parameters used for present calculation are

$$d_1^A=50.8\ \text{Å}\ ,\quad d_1^B=22.6\ \text{Å},\quad d_2=22.6\ \text{Å},$$
$$v(\text{GaAs})=4.72\ \text{km/s}\ ,\quad v(\text{AlAs})=5.12\ \text{km/s}\ ,$$
$$\rho(\text{GaAs})=5315\ \text{kg/m}^2\ ,\quad \rho(\text{AlAs})=3745\text{kg/m}^3\ .$$

The mass density of ρ(Ga$_{0.75}$Al$_{0.25}$As) is obtained by linear interpolation between GaAs and AlAs. As to the sound velocity of it, we have determined v(Ga$_{0.75}$Al$_{0.25}$As)=4.94 km/s by an arithmetical average of the corresponding bulk values. With all these specifications, we can yield the values of v_A and v_B by

$$v_A=[d_1^A v(\text{GaAs})+d_2 v(\text{Ga}_{0.75}\text{As}_{0.25}\text{As})]/d_A$$
$$=4.79\ \text{km/s}\ , \tag{18}$$

and

$$v_B=[d_1^B v(\text{GaAs})+d_2 v(\text{Ga}_{0.75}\text{As}_{0.25}\text{As})]/d_B$$
$$=4.83\ \text{km/s}\ . \tag{19}$$

Finally, the effective sound velocity is determined easily by evaluating Eqs. (14) and (15), and the numerical computation gives $v_{\text{eff}}=4.66$ km/s, nearly 3% less than its rms spatial average ($\bar{v}=4.79$ km/s).[5] We should point out that the contribution of the strain-induced modulation to the effective sound velocity, in this superlattice, is negative due to $v_A-v_B<0$. If one does not take into account the effect of the strain modification as underlined above, the resulting theoretical values are slightly higher than the measured ones we would expect. Based on such an analysis, in Table II we have listed the theoretical and experimental data of GaAs/Ga$_{0.75}$Al$_{0.25}$As superlattices, both from Ref. 5 and our present work. Each double peak is labeled by two superscripts, plus and minus signs. Here we only select the Raman data from 4579- and 6471-Å excitations, and the corresponding Brillouin shifts are 3.25 and 1.85 cm^{-1}, respectively.

From Tables I and II one can see that the two data determined from experiments and our theoretical work, comparatively speaking, are more closer than the predictions from Refs. 4 and 5. However, the small differences between these results remain and can be attributed to the experimental error, because the frequency shift w in Raman spectrum commonly has an absolute instrument width of ±0.5 cm^{-1}.

In order to understand the effect of the strain-induced modulation on effective sound velocity, we have calculat-

TABLE II. Comparison between the main peak positions in the Raman spectra of quasiperiodic GaAs/Ga$_{1-x}$Al$_x$As ($x\simeq0.25$) Fibonacci superlattice and the predictions of the calcuation.

	Raman frequency shift (cm^{-1})									
$w_p^\pm$	w_{-1}^-	w_{-1}^+	w_0^-	w_0^+	w_1^-	w_1^+	w_2^-	w_2^+	w_3^-	w_3^+
	457.9-nm excitation ($w_B=3.25$ cm^{-1})									
Theory[a]	2.8	9.3	6.5	13.0	12.5	19.0	22.2	28.7	38.0	44.5
Expt.[a]	2.9	9.8		12.3	12.3	18.7	21.7	28.2	37.6	43.6
This work	2.6	9.1	6.2	12.7	12.1	18.6	21.6	28.1	36.9	43.4
	647.1-nm excitation ($w_B=1.85$ cm^{-1})									
Theory[a]	4.2	7.9	7.9	11.6	14.0	17.7	23.9	27.6	39.5	43.2
Expt.[a]		7.5	7.5		13.8	17.2	23.5	27.3	39.0	42.5
This work	4.0	7.7	7.6	11.3	13.5	17.2	23.0	26.7	38.3	42.0

[a] See Ref. 5.

ed v_{eff} for some fixed indices (n,m) according to Eqs. (14) and (15). The numerical results are shown in Fig. 2(a) for Si-Ge_xSi_{1-x} QPFSL's. For the sake of comparison, we have also shown the GaAs/$Ga_{1-x}Al_xAs$ QPFSL's case in Fig. 2(b). Here we have transformed indices (n,m) into index p for simplicity. Obviously the modulation from the Fourier components $p < -3$ can be ignored, and the contributions of the strain-induced modulation mainly arise from the Fourier components corresponding to $p \geq 0$. Moreover, such contributions are positive for Si-Ge_xSi_{1-x} and negative for GaAs/$Ga_{1-x}Al_xAs$ QPFSL'S.

IV. SUMMARY AND CONCLUSION

In summary, we have investigated the explicit contributions of strain-induced modulation to the effective sound velocity based on an ideal interfacial model, ignoring interfacial disorder induced by lattice mismatch between the constituent layers. This model involves only the wave velocities v_A and v_B in the respective media, the thicknesses of two basic elements as well as the detailed structure of the QPFSL's, but can give a good prediction for peak positions of the folded acoustic-phonon modes. It suffices for our principal purpose of understanding the essential features of the internal strains due to lattice mismatch. Meanwhile, this simple approximation may be valid for the case of periodic strained-layer superlattices.

Strictly speaking, the phonon spectra in an actual superlattice are subjected to additional modifications by the introduction of various imperfections such as independent disorder and correlated disorder.[10] They will give rise to a slight increase of the linewidth and the decrease of the scattering intensity for phonon spectra. In addition, the disorder will lead to the asymmetry of some doublet peaks. In our present work, the obtained expression of the average sound velocity is universal and valid for arbitrary QPFSL's; in particular, it includes the influence of the acoustic impedances. If this influence can be neglected, Eq. (14) will be equal to adding the transit time in each constituent layer.[11] On the other hand, the excellent agreement between our predictions and experimental observations suggests that this model is reasonable, and is a possible explanation for the deviations of the corresponding results in Refs. 4 and 5.

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