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Author(s)	Tamura, S.; 田村, 信一郎; Wolfe, J. P.
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Acoustic phonons in multiconstituent superlattices

S. Tamura

*Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
and Department of Engineering Science, Hokkaido University, Sapporo 060, Japan**

J. P. Wolfe

Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

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Acoustic phonons propagating parallel to the growth direction of a periodic superlattice composed of more than two different constituent layers are studied theoretically. We give general formulas for the phonon dispersion relation and the width $\Delta\nu$ of frequency gaps existing at the center and boundary of the folded Brillouin zone. We also calculate the structure factor for phonons and find that δ -function peaks corresponding to Bragg reflection have prefactors proportional to $\Delta\nu$. This relation can be used to explain the relative magnitude of transmission dips found at frequencies satisfying the Bragg condition.

I. INTRODUCTION

Acoustic-phonon propagation in periodic and quasi-periodic (Fibonacci) superlattices has been studied extensively both experimentally¹⁻⁵ and theoretically.⁶⁻¹⁰ Though superlattices consist typically of a periodic array of alternating layers, there has been a growing interest in those having more than two layers in a unit cell. Such multiconsistent superlattices have been proposed¹¹ and fabricated.¹²

Phonons in an ideal, periodic superlattice are Bragg reflected when their wave number q parallel to the growth direction satisfies $q = q_m = m\pi/D$, where m is an integer and D is the period of the superlattice. These wave numbers correspond to the center and boundary of the folded-Brillouin zone defined by $-\pi/D \leq q \leq \pi/D$. At $q = q_m$ frequency gaps (phonon stop bands) in the dispersion relation are produced.¹³ In a real superlattice with a finite number of periods, phonons in these frequency gaps have a finite transmission probability through the superlattice but large dips in transmission are predicted in general.¹⁰ This phonon filtering effect of a superlattice has been observed experimentally both by phonon spectroscopy^{1,2,4} and by phonon imaging.^{3,5,10}

It is well known that the condition for Bragg reflection is determined by the relative magnitudes between the phonon wavelength and the length of a period. However, related effects on phonons due to Bragg reflection, such as the width of frequency gaps and magnitude of transmission dips, depend sensitively on the structure of the layers comprising the unit cell of a superlattice.

In the present work we shall study theoretically the acoustic phonons in superlattices with N layers ($N \geq 2$) per period. This study was motivated by the transmission rate shown in Fig. 1, which is calculated for transverse acoustic (TA) phonons propagating normal to interfaces of a (001)-GaAs/AlAs superlattice.⁹ The superlattice assumed is a periodic array $ABAB\dots$ consisting of seven A [$= (42\text{-}\text{\AA} \text{ GaAs}) (17\text{-}\text{\AA} \text{ AlAs})$] and seven B

[$= (20\text{-}\text{\AA} \text{ GaAs}) (17\text{-}\text{\AA} \text{ AlAs})$] blocks, which is a periodic version of the Fibonacci superlattice fabricated by Merlin *et al.*,¹⁴ i.e., $ABAABABA\dots$. A simple question is why some of transmission dips (especially that corresponding to the fourth-order Bragg reflection) are small and some are large. In order to answer this kind of question we shall calculate the phonon dispersion relation and the structure factor for phonons in the general multilayer superlattice depicted in Fig. 2, where the unit cell composed of N layers repeats periodically. (Note that in the above example, $N = 4$ and $D = 96 \text{ \AA}$.)

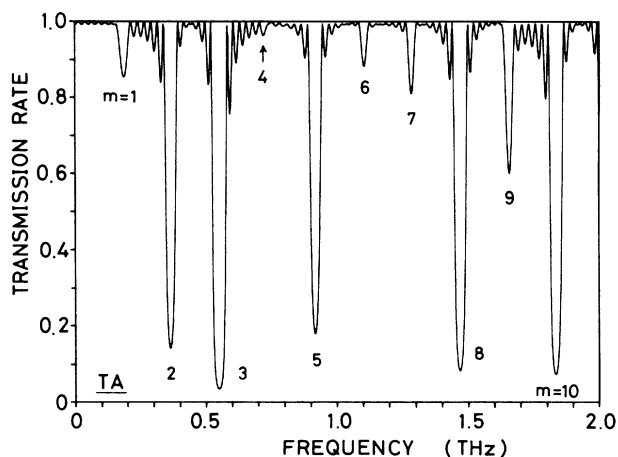


FIG. 1. Frequency dependence of TA phonon transmission rate propagating normal to the (001) interface of four-layer superlattice 42- \AA GaAs-17- \AA AlAs-20- \AA GaAs-17- \AA AlAs. The number of periods assumed for this calculation is seven. Dips in transmission are indexed according to the order of Bragg reflection in the ideal superlattice with infinite repetition of the unit cell.

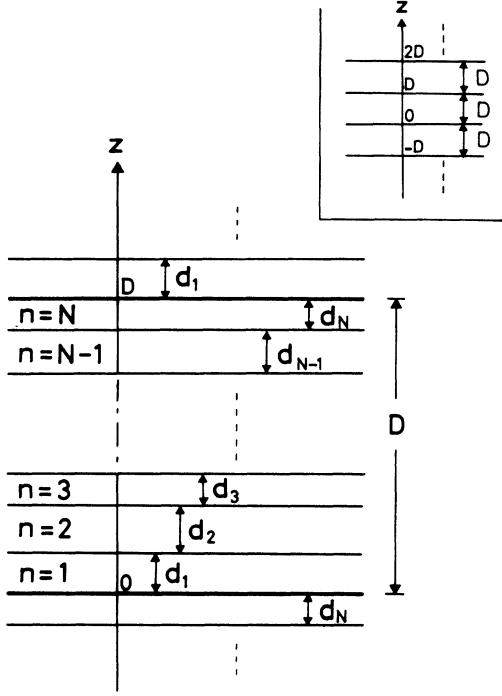


FIG. 2. Schematic of a periodic superlattice consisting of N layers in a unit cell. Thickness of the n th layer is d_n and the length of a period is D .

II. DISPERSION RELATION

We consider phonons with wave vectors perpendicular to interfaces. By assuming the decoupling among different phonon modes, we denote by U_n and S_n the nonvanishing components of phonon displacement and

stress in n th layer with thickness d_n ($1 \leq n \leq N$). Explicitly, they are written as

$$U_n(z) = A_n \exp(ik_n z) + B_n \exp(-ik_n z), \quad (1)$$

$$S_n(z) = i\omega Z_n [A_n \exp(ik_n z) - B_n \exp(-ik_n z)],$$

where A_n and B_n are amplitudes, k_n is the wave number, ω is the angular frequency, and the acoustic impedance in the n th layer $Z_n = \rho_n v_n$, with ρ_n the mass density and v_n the phonon phase velocity. U_n and S_n should satisfy (a) the continuity condition at each interface and (b) an appropriate periodicity condition. Specifically, these conditions are given by

$$(a) \quad W_n \left[\sum_{l=1}^n d_l \right] = W_{n+1} \left[\sum_{l=1}^n d_l \right] \quad (1 \leq n \leq N-1), \quad (2)$$

$$(b) \quad W_N(D) = e^{iqD} W_1(0), \quad (3)$$

where we have defined $W_n(z) \equiv (U_n(z), S_n(z))$, $D = \sum_{n=1}^N d_n$ is the period, and q is the superlattice wave number of phonons. These conditions provide $2N$ equations with respect to $A_1 - A_N$ and $B_1 - B_N$. In order that they have a nontrivial solution, the determinant of $2N \times 2N$ matrix consisting of the coefficients of A_n and B_n ($1 \leq n \leq N$) should vanish. The phonon dispersion relation ω versus q is obtained directly from this condition. The calculation is somewhat tedious but straightforward. The result can be written explicitly by introducing operators $Q^{(0)}, Q_n^{(1)}, Q_{m,n}^{(2)}, \dots$, which operate on an arbitrary function $g(\eta_1, \eta_2, \dots, \eta_N)$ of $\eta_1, \eta_2, \dots, \eta_N$, where $Q^{(0)}$ assigns $\eta_j = 1$ ($1 \leq j \leq N$), $Q_n^{(1)}$ assigns $\eta_n = -1$ and $\eta_j = 1$ ($j \neq n$), $Q_{m,n}^{(2)}$ assigns $\eta_m = \eta_n = -1$ and $\eta_j = 1$ ($j \neq m, n$), and so on. With the use of these operators, the dispersion relation is¹⁵

$$2^N \left[\prod_{n=1}^N Z_n \right] \cos(qD) = \left[Q^{(0)} - \sum_{i=1}^N Q_i^{(1)} + \sum_{\substack{i=1, j=1 \\ (i < j)}}^N \sum_{i=1}^N Q_{i,j}^{(2)} - \dots + (-1)^{[N/2]} \gamma \sum_{\substack{i=1, j=1 \\ (i < j < \dots < p)}}^N \sum_{p=1}^N \dots \sum_{i,j,\dots,p}^{(N/2)} Q_{i,j,\dots,p}^{([N/2])} \right] \\ \times \prod_{n=1}^N (\eta_n Z_n + \eta_{n+1} Z_{n+1}) \cos \left[\sum_{l=1}^N \eta_l \Omega_l \right], \quad (4)$$

where $Z_{N+n} \equiv Z_n$, $\Omega_n = k_n d_n = \omega d_n / v_n$, $\gamma = 1$ ($\frac{1}{2}$) if N is odd (even), and $[n]$ means the maximum integer which does not exceed n . For $N=2$, Eq. (4) is reduced to the well-known form of the dispersion relation given by Rytov.¹⁶ For $N=3$ Eq. (4) is reduced to that given by Nakayama *et al.*,¹² or by Santos and Ley.¹⁷ However, Eq. (4) is the nontrivial extension of these previous works.

For the four-layer GaAs/AlAs superlattice discussed above, Eq. (4) becomes (by putting $n=1=3=\text{GaAs}$ and $n=2=4=\text{AlAs}$)

$$\cos(qD) = \cos(\Omega_1 + \Omega_2 + \Omega_3 + \Omega_4)$$

$$- \frac{(Z_1 - Z_2)^2}{2Z_1 Z_2} \sin(\Omega_1 + \Omega_3) \sin(\Omega_2 + \Omega_4) \\ + \frac{1}{2} \left[\frac{Z_1^2 - Z_2^2}{Z_1 Z_2} \right]^2 \sin \Omega_1 \sin \Omega_2 \sin \Omega_3 \sin \Omega_4. \quad (5)$$

In Fig. 3 the dispersion curves given by Eq. (5) are plot-

ted for the TA mode.¹⁸ Frequency gaps are created at $qD = m\pi$ because for $Z_1 \neq Z_2$ the modulus of the right-hand side of Eq. (5) exceeds unity, whereas $|\cos(qD)| \leq 1$. It is important to note that the central frequency and frequency width of the gaps are well correlated with the central frequency and depth of transmission dips of Fig. 1, respectively.

III. WIDTH OF FREQUENCY GAPS

Provided that all layers in a unit cell have acoustic impedances of the same order of magnitude, we can also

derive a formula for the width of frequency gap by a perturbation calculation. By keeping terms up to second order in the difference of acoustic impedance we have from Eq. (4)

$$2^N \left[\prod_{n=1}^N Z_n \right] \cos(qD) = \left[\prod_{n=1}^N (Z_n + Z_{n+1}) \right] \cos \left[\sum_{l=1}^N \Omega_l \right] + \left[\sum_{n=1}^N P_n^{(N)} \right] \cos \left[\sum_{l=1}^N \eta_l \Omega_l \right], \quad (6)$$

where

$$P_n^{(N)} = (Z_n - Z_{n+1}) [(Z_{n+1} - Z_{n+2}) Q_{n+1}^{(1)} + (Z_{n+2} - Z_{n+3}) Q_{n,n+1}^{(2)} + \cdots + \gamma (Z_{n+[N/2]} - Z_{n+1+[N/2]}) Q_{n+1, n+2, \dots, n+[N/2]}^{(N/2)}]. \quad (7)$$

Now we assume that $\omega = \omega_m + \delta\omega_m$ at $q = q_m$, where ω_m is the zeroth order in $\epsilon_{ij} = (Z_i - Z_j)/\bar{Z}$ ($\bar{Z} \equiv \sum_{n=1}^N Z_n/N$) and given by

$$\omega_m = \frac{m\pi}{\sum_{n=1}^N (d_n/v_n)}. \quad (8)$$

This is the phonon frequency at the center of the m th band gap. Next, we assume that the magnitude of $(\delta\omega_m/\omega_m)^2$ is the same order as ϵ_{ij}^2 . Equating terms of the order of ϵ_{ij}^2 in Eq. (6), we have

$$\left[\frac{\delta\omega_m}{\omega_m} \right]^2 = \frac{1}{(2m\pi\bar{Z})^2} \sum_{n=1}^N \left[(Z_n - Z_{n+1})^2 + 2(-1)^m P_n^{(N)} \cos \left[\omega_m \sum_{l=1}^N \frac{\eta_l d_l}{v_l} \right] \right]. \quad (9)$$

Applying this formula again to the four-layer GaAs/AlAs superlattice exemplified above, we obtain

$$\left[\frac{\delta\omega_m}{\omega_m} \right]^2 = (-1)^m \left[\frac{\epsilon_{12}}{m\pi} \right]^2 \left\{ -\sin \left[\omega_m \left[\frac{d_1 + d_3}{v_1} \right] \right] \sin \left[\omega_m \left[\frac{d_2 + d_4}{v_2} \right] \right] + 4 \sin \left[\omega_m \frac{d_1}{v_1} \right] \sin \left[\omega_m \frac{d_2}{v_2} \right] \sin \left[\omega_m \frac{d_3}{v_1} \right] \sin \left[\omega_m \frac{d_4}{v_2} \right] \right\}. \quad (10)$$

The width of the m th frequency gap is $\Delta v_m = \delta\omega_m/\pi$. In Table I we have tabulated up to $m=10$ the gap width $\Delta v_m^{\text{exact}}$ given exactly from the dispersion relation (5) and Δv_m obtained by the above formula (10). The agreement of Δv_m with $\Delta v_m^{\text{exact}}$ is excellent, validating the approximation we have employed. Incidentally, we note $\epsilon_{12}^2 = 0.033$ for TA mode in GaAs/AlAs heterostructures.¹⁸

IV. STRUCTURE FACTOR

The effects on Bragg reflection of a multilayer structure in a unit cell are also understood by examining the structure factor of superlattices for phonons. For phonons with superlattice wave number q propagating normal to interfaces spaced by D , the interference of reflected phonons is described by the structure factor

$$S(q) = \sum_n e^{2inqD} = \frac{\pi}{D} \sum_m \delta(q - q_m). \quad (11)$$

The δ -function peaks of $S(q)$ mean that Bragg reflection

occurs for phonons with $q = q_m$. Here, we note that q is the wave number of a modulated plane wave propagating in a whole superlattice, independent of the detailed structure in a unit cell. The existence of multilayers in the unit cell causes extra reflections at their boundaries and gives additional phases to the structure factor. This amounts to the modification $S(q) \rightarrow S_N(q) = f_N(q)S(q)$, where

$$f_N(q) = \sum_{n=1}^N r_{n,n+1} \exp \left[2i \sum_{l=1}^n \Omega_l \right], \quad (12)$$

and $r_{n,n+1}$ is the amplitude-reflection coefficient at the interface between n th and $(n+1)$ th layers (for phonons impinging on the interface from the n th layer). Explicit expression for $r_{n,n+1}$ is derived from Eqs. (1) and (2) as

$$r_{n,n+1} = \frac{Z_n - Z_{n+1}}{Z_n + Z_{n+1}}. \quad (13)$$

Here, we remark that Eq. (12) is derived by neglecting multiple phonon reflections [which add terms of the or-

TABLE I. Frequency ν and gap width $\Delta\nu$ associated with Bragg reflection of TA phonons in 42-Å GaAs–17-Å AlAs–20-Å GaAs–17-Å AlAs superlattice.

m	ν_m (GHz)	$\Delta\nu_m^{\text{exact}}$ (GHz)	$\Delta\nu_m$ (GHz)
1	184	7.5	7.5
2	367	25.7	25.6
3	551	38.4	38.4
4	735	1.8	1.7
5	919	24.7	24.6
6	1102	4.7	4.6
7	1286	6.2	6.2
8	1470	31.1	31.0
9	1645	11.8	11.8
10	1837	32.1	32.1

der of $r_{n,n+1}^3$ to Eq. (12)] and assuming perfect phonon transmission at interfaces except at the one from which phonons are reflected. This approximation is valid for most superlattices because $|r_{n,n+1}r_{n+1,n}| = |r_{n,n+1}|^2 \ll 1$ and $t_{n,n+1}t_{n+1,n} = 1 - |r_{n,n+1}|^2 \simeq 1$, where $t_{n,n+1} = 1 + r_{n,n+1}$ is the amplitude transmission coefficient. For example, at a (001)-GaAs/AlAs interface $|r_{\text{GaAs,AlAs}}|^2 = 0.0082$ for the TA mode and 0.0074 for the longitudinal acoustic (LA) mode.¹⁸ Thus the layered structure in a unit cell affects the relative strength of Bragg reflection but not the basic Bragg condition.

Now, we calculate f_N at $q = q_m$ for which the structure factor is nonvanishing. In the lowest order in the difference of acoustic impedance we can put $r_{n,n+1} = \epsilon_{n,n+1}/2$ and $\omega = \omega_m$. Hence, after a bit of algebra as described in the Appendix we derive a simple equation

$$S_N(q) = \frac{\pi}{D} \sum_m f_N(q_m) \delta(q - q_m), \quad (14)$$

where f_N is related to $\delta\omega$ defined by Eq. (9) as

$$|f_N(q_m)|^2 = [m\pi(\delta\omega_m/\omega_m)]^2. \quad (15)$$

Thus, the modulation factor $f_N(q_m)$ which determines the intensity of the m th Bragg reflection is proportional to the width of the corresponding gap in phonon dispersion relation. This establishes the close correlation between the magnitude of transmission dips in Fig. 1 and the width of frequency gaps shown in Fig. 3, which was previously noted.

V. CONCLUSION

To conclude, we have derived a formula for the dispersion relation of acoustic phonons propagating normal to the interfaces of multiconstituent superlattices. The formulation is exact in the context of continuum elasticity theory. The formula for the width of the frequency gap $\Delta\nu$ in the dispersion relation is also derived from a perturbation calculation, and gives very accurate numerical values for the majority of superlattices. Our calculations also establish a close relationship between $\Delta\nu$ and the interference effects of phonons reflected at different interfaces of constituent layers. We believe that these general results will be useful for comparison to future experi-

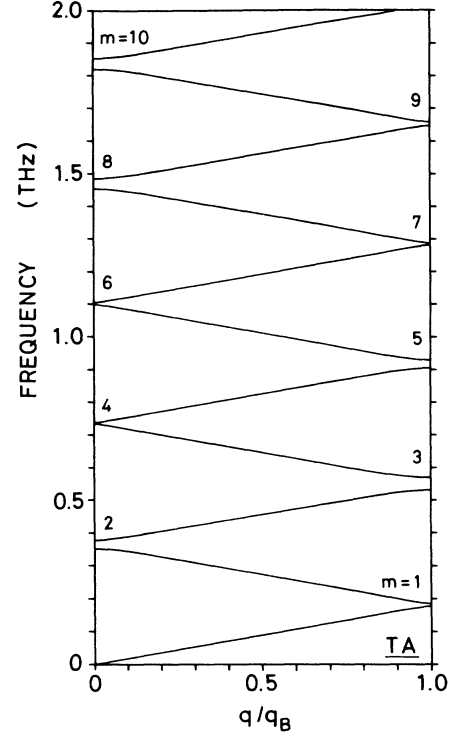


FIG. 3. Dispersion relation of TA phonons propagating normal to the interface of four-layer superlattice identical to the one in Fig. 1. The period (D) is 96 Å and $q_B = q_1 = \pi/D = 3.27 \times 10^6 \text{ cm}^{-1}$ is the magnitude of the wave number at the folded-zone boundary. Zone-center and zone-boundary gaps are indexed according to the order of Bragg reflection.

ments because in most spectroscopic experiments phonons propagating normal to the interfaces of a superlattice are detected.

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APPENDIX

In this appendix we shall derive Eq. (15). Multiplying $r_{n',n'+1} \exp(-2i \sum_{l=1}^{n'} \Omega_l)$ by Eq. (12) and summing over n' , we obtain

$$|f_N(q)|^2 = \sum_{n=1}^N r_{n,n+1}^2 + 2 \sum_{j=1}^{N-1} \sum_{n=1}^{N-1-j} r_{n,n+1} r_{n+j,n+j+1} \times \cos \left[2 \sum_{l=n+1}^{n+j} \Omega_l \right], \quad (A1)$$

where $r_{N,N+1} \equiv r_{N,1}$. At $q = q_m$, $\Omega_n = \omega_m d_n / v_n \equiv \Omega_n^{(m)}$ and $\sum_{n=1}^N \Omega_n = m\pi$ hold in the zeroth order of ϵ_{ij} . Hence, from (A1) we can derive

$$|f_N(q_m)|^2 = \sum_{n=1}^N r_{n,n+1}^2 + 2(-1)^m \sum_{j=1}^{[N/2]} \sum_{n=1}^N \gamma_j r_{n,n+1} r_{n+j,n+j+1} Q_{n+1,n+2,\dots,n+j}^{(j)} \cos \left[\sum_{l=1}^N \eta_l \Omega_l^{(m)} \right], \quad (\text{A2})$$

where $\gamma_j = 1$ ($1 \leq j \leq [N/2] - 1$) and $\gamma_{[N/2]} = \gamma$. Using Eq. (13) and keeping the terms up to ϵ_{ij}^2 , (A2) is reduced to

$$|f_N(q_m)|^2 = \frac{1}{4\bar{Z}^2} \sum_{n=1}^N (Z_n - Z_{n+1})^2 + \frac{(-1)^m}{2\bar{Z}^2} \sum_{j=1}^{[N/2]} \sum_{n=1}^N \gamma_j (Z_n - Z_{n+1})(Z_{n+j} - Z_{n+j+1}) Q_{n+1,n+2,\dots,n+j}^{(j)} \times \cos \left[\sum_{l=1}^N \eta_l \Omega_l^{(m)} \right], \quad (\text{A3})$$

where $Z_{n+N} \equiv Z_n$ ($1 \leq n \leq N - 1$). Comparing (A3) with Eqs. (7) and (9), we establish Eq. (15), i.e.,

$$|f_N(q_m)|^2 = (m\pi)^2 (\delta\omega_m / \omega_m)^2.$$

*Present address.

¹V. Narayanamurti, H. J. Störmer, M. A. Chin, A. C. Gossard, and W. Wiegmann, Phys. Rev. Lett. **43**, 2012 (1979).

²O. Koblinger, J. Mebert, E. Dittrich, S. Döttinger, W. Eisenmenger, P. V. Santos, and L. Ley, Phys. Rev. B **35**, 9372 (1987).

³D. C. Hurley, S. Tamura, J. P. Wolfe, and H. Morkoc, Phys. Rev. Lett. **58**, 2446 (1987).

⁴P. V. Santos, J. Mebert, O. Koblinger, and L. Ley, Phys. Rev. B **36**, 1306 (1987).

⁵D. C. Hurley, S. Tamura, J. P. Wolfe, K. Ploog, and J. Nagle, Phys. Rev. B **37**, 8829 (1988).

⁶R. E. Camley, B. Djafari-Rouhani, L. Dobryzynski, and A. A. Maradudin, Phys. Rev. B **27**, 7318 (1983).

⁷M. J. Kelly, J. Phys. C **18**, 5963 (1985).

⁸S. Tamura and J. P. Wolfe, Phys. Rev. B **35**, 2528 (1987).

⁹S. Tamura and J. P. Wolfe, Phys. Rev. B **36**, 3491 (1987).

¹⁰S. Tamura, D. C. Hurley, and J. P. Wolfe, Phys. Rev. B **38**, 1427 (1988).

¹¹L. Esaki, L. L. Chang, and E. E. Mendez, Jpn. J. Appl. Phys. **24**, L529 (1981).

¹²N. Nakayama, K. Kubota, S. Chika, H. Kato, and N. Sano,

Solid State Commun. **58**, 475 (1986).

¹³A. S. Barker, Jr., J. L. Merz, and A. C. Gossard, Phys. Rev. B **17**, 3181 (1978).

¹⁴R. Merlin, K. Bajema, R. Clarke, F. Y. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. **55**, 1768 (1985).

¹⁵The equivalent but apparently different expression for the dispersion relation can also be derived by using the formula $\cos(qD) = \text{Tr}(T_N)/2$, where T_N is a unimodular 2×2 transfer matrix defined by $T_N = t_N t_{N-1} \cdots t_2 t_1$, with

$$t_n = \begin{pmatrix} \cos(k_n d_n) & (i\omega Z_n)^{-1} \sin(k_n d_n) \\ -i\omega Z_n \sin(k_n d_n) & \cos(k_n d_n) \end{pmatrix}.$$

¹⁶S. M. Rytov, Akust. Zh. **2**, 71 (1956) [Sov. Phys.—Acoust. **2**, 68 (1956)].

¹⁷P. V. Santos and L. Ley, Phys. Rev. B **36**, 3325 (1987).

¹⁸In numerical calculations, the following values were used: for AlAs $\rho = 3.76 \text{ g/cm}^3$, $C_{11} = 120.2$, and $C_{44} = 58.9$ (in units of 10^{10} dyn/cm^2); for GaAs $\rho = 5.36 \text{ g/cm}^3$, $C_{11} = 118.8$, and $C_{44} = 59.4$ (in units of 10^{10} dyn/cm^2). [See S. Adachi, J. Appl. Phys. **58**, R3 (1985).]