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Author(s)	Mizuno, Seiji
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Eigenfrequency and decay factor of the localized phonon in a superlattice with a defect layer

Seiji Mizuno
Department of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan
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We theoretically study the localized vibrational modes in a superlattice with a defect layer. In particular, we derive simple formulas for the eigenfrequency of this localized mode and the corresponding decay factor. Our formulas show explicitly how these quantities depend on the constituent layers of the superlattice and also the width of the defect layer. These formulas are useful for systematic understanding of the localized acoustic phonons in superlattice.

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In the last two decades, extensive studies[1,2] have been devoted to understand quantum transport properties related to the electron tunneling through the potential barriers. Essentially, the tunneling occurs as a result of the wave nature of electrons. Thus, it should also occur for classical waves, such as light and sound waves, and their quanta, i.e., photons and phonons. To see the tunneling effect in the phonon system, we should prepare the opaque barrier for phonons. An example is the superlattice (SL) structure. The key idea is to utilize the fact that in a periodic SL Bragg reflection occurs for phonons with the frequency inside the frequency gap induced by a periodicity much longer than the lattice spacing. The amplitude of these phonons decays exponentially inside the SL; i.e., the wave vectors of these phonons have an imaginary part. Thus, we can regard the SL as a barrier for phonons. Furthermore, a double-barrier system for phonons can be realized by connecting SL's in series. The propagation of the acoustic phonons in this system was studied in our previous work.[3] In this paper, the transmission rate was calculated and the existence of the resonant peaks inside the frequency gap was shown theoretically. When the frequency of the incident phonon coincides with a resonant frequency, the phonon can go through the whole system without attenuation. This resonant frequency is equivalent to the eigenfrequency of the vibrational mode confined in the bulk part sandwiched between the SL's. Figure 1 illustrates the similarity between the SL-bulk-SL structure and the double-barrier quantum-well structure for electrons. The above confined mode can be also regarded as a vibrational mode localized at a ''defect layer'' (i.e., the sandwiched bulk part breaking the periodicity of the SL). Very recently, Chen *et al.*[4] numerically studied the property of the localized acoustic phonons in SL's with defect layers using a transfer matrix method. They discussed how the eigenfrequency and decay factor of localized mode change with the constituent layers of SL's and also the widths of the defect layer (i.e., the distance between two SL's). Here, it should be noted that the results they calculated are reproducible with the use of the general equation obtained in Ref. 3. Since this equation has a complicated and no explicit form, the eigenfrequencies were graphically (and numerically) examined in previous paper (Fig. 7 in Ref. 3). The simple expression for the eigenfrequency is useful not only for systematic understanding of the localized acoustic phonons in SL's with a defect layer but also for the design of the phonon tunneling device (the double-barrier system for phonons) to be used for the detection or generation of quasimonochromatic acoustic phonons.[5] In the present paper, we derive an explicit expression for the eigenfrequency of this localized mode. The expression for the corresponding decay parameter (or localization degree) is also derived. Furthermore, the periodicity of the resonant frequency and the decay factor as a function of the width of the defect layer is discussed. Though this periodicity was pointed out in Ref. 6, no physical explanation was given.

A schematic picture of the system we consider is illustrated in Fig. 2, where the defect layer is artificially embedded in the infinite SL. Throughout the paper, we consider the case where the wave vector of phonons is perpendicular to the interfaces of the layer. In this case, three phonon modes are decoupled from each other if the interfaces are a mirror-symmetry plane. That is, we can treat only one mode, e.g., the longitudinal mode. Also, the continuum model which should be valid for sub-THz phonons is assumed for each constituent layer. In the continuum model, the lattice displacement $U_i(z)$ and stress $S_i(z)$ for the acoustic mode are expressed in terms of linear combinations of the transmitted and reflected waves:

$$U_i(z)=c_i^t e^{ik_i z}+c_i^r e^{-ik_i z}, \tag{1}$$

$$S_i(z)=i\omega Z_i(c_i^t e^{ik_i z}-c_i^r e^{-ik_i z}). \tag{2}$$

Here, i is an index specifying constituent layers, c_i^t and c_i^r are the amplitudes of the transmitted and reflected waves, respectively, k_i is the wave number, $Z_i=\rho_i v_i$ is the acoustic impedance given by the product of the mass density ρ_i and the sound velocity v_i, and $\omega=k_i v_i$ is the frequency. The lattice displacement and stress should be continuous at the interfaces of adjacent layers. From this condition, we can obtain the equation governing the lattice displacement:[3]

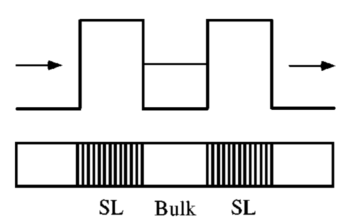

FIG. 1. Double-barrier system for phonons.

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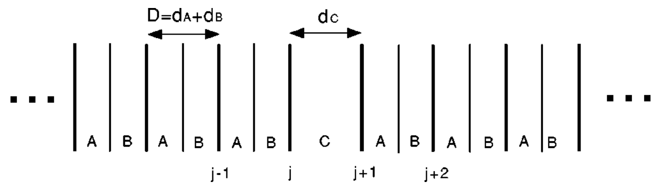

FIG. 2. Schematic of a superlattice with a defect layer.

$$\frac{1}{\sigma_n}U_{n+1}+\frac{1}{\sigma_{n-1}}U_{n-1}=\left(\frac{\lambda_n}{\sigma_n}+\frac{\mu_{n-1}}{\sigma_{n-1}}\right)U_n. \tag{3}$$

Here, U_n is the displacement at the nth interface, which is numbered in Fig. 2. Here λ_n, σ_n, and μ_n are the elements of the transfer matrix of the segment between nth and $(n+1)$th interfaces: if the jth segment is a defect layer consisting of the single layer C (see Fig. 2), $\lambda_j=\mu_j=\cos\gamma$ and $\sigma_j=\sin\gamma$, where $\gamma=\omega d_C/v_C$ and d_C is the thickness of the defect layer; if the $n(\neq j)$th segment is a constituent bilayer of SL,

$$\lambda_n=\cos\alpha\cos\beta-\frac{Z_A}{Z_B}\sin\alpha\sin\beta\equiv\lambda, \tag{4}$$

$$\sigma_n=\sin\alpha\cos\beta+\frac{Z_A}{Z_B}\cos\alpha\sin\beta\equiv\sigma, \tag{5}$$

$$\mu_n=\cos\alpha\cos\beta-\frac{Z_B}{Z_A}\sin\alpha\sin\beta\equiv\mu, \tag{6}$$

where $\alpha=\omega d_A/v_A$ and $\beta=\omega d_B/v_B$, and d_A (d_B) is the thickness of layer A (B). More explicitly, Eq. (3) can be written as

$$U_{j-1}-(\mu+\sigma\cot\gamma)U_j+\frac{\sigma}{\sin\gamma}U_{j+1}=0,$$

$$\frac{\sigma}{\sin\gamma}U_j-(\lambda+\sigma\cot\gamma)U_{j+1}+U_{j+2}=0,$$

$$U_{n-1}-(\mu+\lambda)U_n+U_{n+1}=0 \quad (n\neq j,j+1), \tag{7}$$

where we assumed that the material of the impurity layer is the same as that of layer A (i.e., $Z_C=Z_A$), for simplicity. In Ref. 3, Eqs. (7) are examined in terms of the transfer matrix method and Green's function method. In the present paper, after reproducing the fundamental results with intuitive method without the Green's function, we will derive the explicit expressions for the eigenfrequency and decay factor of the localized phonons, which were not obtained in the previous papers.

We seek the solution to Eqs. (7) of the form

$$U_n=\begin{cases}\Lambda^{n-j-1}U_{j+1} & \text{for } n\geqslant j+1,\\ \Lambda^{-(n-j)}U_j & \text{for } n\leqslant j,\end{cases} \tag{8}$$

where

$$|\Lambda|<1. \tag{9}$$

Equation (9) ensures that the phonon displacement is localized at the defect layer. Substituting Eq. (8) into Eq. (7), we have the equations

$$\Lambda^2-(\mu+\lambda)\Lambda+1=0, \tag{10}$$

$$\Lambda^2-(\mu+\lambda+2\sigma\cot\gamma)\Lambda+\mu\lambda-\sigma^2+(\mu+\lambda)\sigma\cot\gamma=0. \tag{11}$$

Equation (10) leads to the expression for the decay parameter,

$$\Lambda=\frac{\mu+\lambda}{2}\pm\sqrt{\left(\frac{\mu+\lambda}{2}\right)^2-1}, \tag{12}$$

and therefore the condition (9) requires that

$$\left|\frac{\mu+\lambda}{2}\right|>1. \tag{13}$$

In this case, the decay parameter Λ can be written in a simpler form

$$\Lambda=\pm e^{-\theta} \tag{14}$$

by defining the positive variable θ as

$$\frac{\mu+\lambda}{2}=\pm\cosh\theta, \tag{15}$$

where the upper sign corresponds to the case $(\mu+\lambda)/2>1$ and the lower sign to $(\mu+\lambda)/2<-1$. This positive value θ represents the decay factor or the imaginary part of the wave number, because the complex wave number k can be expressed as $kD=m\pi+i\theta$, by putting Eq. (14) in the form $\Lambda=e^{ikD}$, where $D=d_A+d_B$ is the length of a unit period of the SL. The frequency range satisfying Eq. (13) defines the frequency gap (or phonon stop band) because the corresponding phonon displacement decays exponentially away from the defect layer. On the other hand, for the phonon whose frequency satisfies the inequality

$$\left|\frac{\mu+\lambda}{2}\right|\leqslant 1, \tag{16}$$

it is easily shown that $|\Lambda|=1$ (i.e., the phonon displacement does not decay), and therefore Eq. (16) defines the frequency band.

With the use of Eq. (14), Eq. (11) becomes

$$\pm\frac{\zeta-\sigma}{2\sinh\theta}=-\cot(\omega d_C/v_C), \tag{17}$$

where

$$\zeta=-\sin\alpha\cos\beta-\frac{Z_B}{Z_A}\cos\alpha\sin\beta. \tag{18}$$

The solution of Eq. (17) gives the eigenfrequency of the localized mode. The right-hand side of Eq. (17) depends only on the parameters of the defect layer, and the left-hand side depends on those of the unit period of the SL. In Ref. 3, Eq. (17) was graphically examined.

Our aim in the present paper is to derive the explicit expressions for the decay factor θ defined in Eq. (15) and the solution to Eq. (17). From Eqs. (4) and (6), we have

$$\frac{\mu+\lambda}{2}=\cos\left(\frac{\pi\omega}{\omega_1}\right)-\frac{\varepsilon^2}{2(1+\varepsilon)}\sin\alpha\sin\beta, \tag{19}$$

where $\omega_1=\pi(d_A/v_A+d_B/v_B)^{-1}$ is the first-order Bragg frequency and $\varepsilon=Z_B/Z_A-1$ represents the acoustic mismatch between constituent layers A and B.[7] For the majority of SL's, this acoustic mismatch is small, i.e., $|\varepsilon|\ll 1$. Therefore, Eq. (13) is satisfied for the frequencies close to the mth Bragg frequency $\omega_m\equiv m\omega_1$, which corresponds to the center of the mth frequency gap. Expanding Eq. (19) around ω_m and also neglecting the higher order of ε, we obtain

$$\frac{\mu+\lambda}{2}\cong(-1)^m\left[1-\frac{\pi^2}{2\omega_1^2}(\omega-\omega_m)^2+\frac{\varepsilon^2}{2}\sin^2(\omega_m d_A/v_A)\right]. \tag{20}$$

From this equation, it is shown that Eq. (13) is satisfied for the frequency window:

$$\omega_m-\Delta_m\leqslant\omega\leqslant\omega_m+\Delta_m, \tag{21}$$

where

$$\Delta_m=(\omega_1/\pi)|\varepsilon\sin(\omega_m d_A/v_A)|. \tag{22}$$

In other words, Eq. (22) gives half of the width of the mth-frequency gap. In this frequency gap, the right-hand side of Eq. (15) can be also expanded as

$$\frac{\mu+\lambda}{2}\cong(-1)^m\left[1+\frac{1}{2}\theta^2\right]. \tag{23}$$

Here, the sign $\pm$ in Eq. (15) has been replaced by $(-1)^m$, because Eq. (20) ensures that the sign of $(\mu+\lambda)$ near ω_m is $(-1)^m$. Comparing Eqs. (20) and (23), we have the expression of θ:

$$\theta=\sqrt{\varepsilon^2\sin^2(\omega_m d_A/v_A)-\frac{\pi^2}{\omega_1^2}(\omega-\omega_m)^2}. \tag{24}$$

Next, we examine Eq. (17). Within the present approximation, we have

$$\frac{\sigma-\zeta}{2}\cong(-1)^m\frac{\pi}{\omega_1}(\omega-\omega_m), \tag{25}$$

and Eq. (17) becomes

$$\frac{\pi}{\omega_1}(\omega-\omega_m)=\theta\cot(\omega d_C/v_C), \tag{26}$$

where $\sinh\theta$ has replaced by θ because the maximum value of θ is an order of $\varepsilon(\ll 1)$ within the frequency gap [see Eqs. (21), (22), and (24)]. Substituting Eq. (24) into Eq. (26), we have an expression for the eigenfrequency of localized phonon:

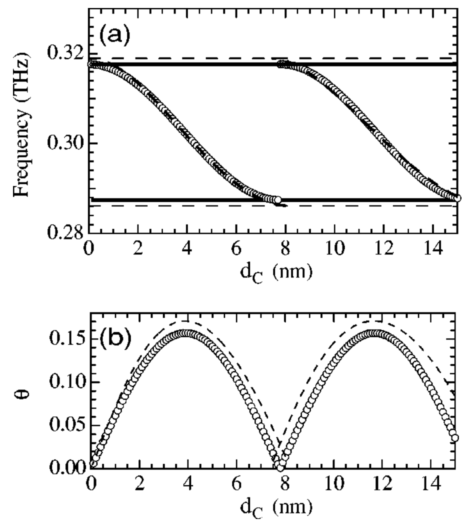

FIG. 3. Eigenfrequency (a) and decay factor θ (b) versus the width of the defect layer. The open circles are calculated from the approximated expressions [Eqs. (29) and (30)] and broken lines are calculated from the exact expressions [Eqs. (17) and (15)]. The region between two solid (dotted) horizontal lines means frequency gap calculated from the approximated formula (21) [exact formula (13)].

$$\omega_{defect}=\omega_m\pm(\omega_1/\pi)\varepsilon\sin(\omega_m d_A/v_A)\cos(\omega_m d_C/v_C), \tag{27}$$

where

$$\pm\varepsilon\sin(\omega_m d_A/v_A)\sin(\omega_m d_C/v_C)>0 \tag{28}$$

should be satisfied because θ is defined to be positive so that Eq. (8) represents the localized solution. Combining Eqs. (22), (27), and (28), we obtain a final expression for the eigenfrequency:

$$\omega_{defect}=\omega_m+\Delta_m|\sin(\omega_m d_C/v_C)|\cot(\omega_m d_C/v_C). \tag{29}$$

Also, by inserting Eq. (29) into Eq. (24), the decay factor of this localized mode can be written in the simple form

$$\theta=|\varepsilon\sin(\omega_m d_A/v_A)\sin(\omega_m d_C/v_C)|. \tag{30}$$

As a numerical example, we consider a (100)GaAs/AlAs SL with a defect layer consisting of GaAs. The unit period of the SL is assumed to be $(\mathrm{GaAs})_{15}(\mathrm{AlAs})_{15}$. In Fig. 3(a), we plot the eigenfrequency of the localized phonon within the lowest-frequency gap as a function of the width d_C of the defect layer C. The dashed lines are calculated from Eq. (17) and open circles are calculated from the approximated formula, Eq. (29). The region between two solid (dashed) horizontal lines means the lowest-frequency gap calculated from the approximated formula (21) [exact formula (13)]. The approximated results are in good agreement with the exact one. By increasing d_C, the eigenfrequency decreases and this localized mode merge into the lower-frequency band. Then, the other mode is extracted from the upper-frequency band. Figure 3(b) shows the d_C dependence of the decay factor θ. This decay factor has the maximum value when the eigenfrequency is located in the center of the frequency gap. This is clearly understood with the use of Eqs. (29) and (30). Figure 3 shows that ω_{defect} and θ are periodic functions of d_C. This periodicity was first pointed out in Ref. 6, and similar periodicity was seen in Refs. 8 and 9 of the modes localized at a free surface, when varying the width of the surface layer. This periodic behavior can be well explained with our formulas. From Eqs. (29) and (30), it is found that the period of ω_{defect} or θ is given by

$$d_p=\frac{\pi}{\omega_m}v_C=\frac{1}{m}\left(\frac{d_A}{v_A}+\frac{d_B}{v_B}\right)v_C. \tag{31}$$

In the lowest-frequency gap, Eq. (31) can be written as

$$d_p=(t_A+t_B)v_C, \tag{32}$$

where $t_A=d_A/v_A$ ($t_B=d_B/v_B$) is the time needed for a phonon to go through layer A (B). This result means that a width increase of d_p is equivalent to an increase of a constituent bilayer of SL's, for a change in the phase of the phonon displacement. In other words, the number of nodes of the phonon displacement within the defect layer increases by 1 if the width of the defect layer increases by d_p. The factor m^{-1} in Eq. (31) is due to the fact that in the mth-frequency gap the number of the standing waves in a constituent bilayer is m.

In the present numerical example, we show only the results within the lowest-frequency gap, but our formulas are applicable to not only the lowest-frequency gap but also the other gaps. In fact, it is confirmed that the previous results calculated numerically for the second gaps of some SL's with a defect layer[4] are well reproduced from our formulas. Similarly, the dependence of the eigenfrequency and decay factor on the parameters of the constituent bilayer of SL can be well explained by using our general formulas.

In conclusion, we have derived the explicit expressions for the eigenfrequency and corresponding decay factor of the phonon localized at the defect layer embedded in SL's. From these expressions, we can clearly understand how the eigenfrequency depends on the parameters of the defect layer and also constituent bilayer of SL's. In particular, their periodic behavior was discussed, based on the expression of the period we derived. Our results suggest the potential for designing phonon tunneling device to be used for the detection or generation of quasimonochromatic acoustic phonons.

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