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Effect of structural defect on phonon transmission quantization in low-dimensional superlattices

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Abstract

Using the scattering-matrix cascading method, we investigate the effect of structural defect on the acoustic phonon transmission quantization in a low-dimensional superlattice quantum waveguide. In the present system, the phonon transmission exhibits rather complex resonant behaviors. It is found that a lateral defect in an otherwise periodic structure modifies the transversal phonon transmission spectra nontrivially and completely washes away the transmission quantization due to the strong additional scattering by defect. However, the appreciable quantization survives in the presence of a longitudinal defect. Our results also show that by adjusting the geometric parameters of the structural defect, one can control the phonon transport of the structure to match practical requirements in devices.
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1. Introduction

With the technological advances in nanoscale lithography and atom-layer epitaxy for fabricating artificial semiconductor nanoscale devices, the superlattices (SLs) with structural defects have attracted much attention due to the novel physical properties found in these kinds of structures in comparison with perfect SLs. The behaviors and properties of electron bound states [1–5], localized acoustic modes [6–9], interface optical-phonon modes [10–15], localized electron-optical-phonon interactions [16,17] in various kinds of quasi-two-dimensional SLs with structural defects have been extensively investigated, theoretically as well as experimentally. Their works show that the periodicity-broken coupling due to the existence of the inhomogeneous layers leads to the appearance of the new splitting levels which exhibit some interesting features such as localization effect, decaying behavior, mode evolution and magneto-coupling, which substantially depend on the structural parameters of the defect layer and SL cells. These results have found applications in energy-band tailoring and phonon engineering [4,16,18].

Recently, structural defects were introduced to the transport and transmission in quantum waveguide structures when system dimensions are comparable to or less than the wavelength of electron or phonon. It is well known that in one-dimensional systems electronic conductance has the feature of quantization [19,20]. Deo et al. [21] ever presented a theoretical research on the recovery of the conductance quantization in a periodically modulated quantum channel and indicate that even in the presence of defect, a periodic arrangement of double stubs gives remarkable quantization of conductance. As for phonon transport, since the thermal conductance at low temperature has been found to be quantized in a universal unit, $K/T = \pi^2 k_B^2/3h$, theoretically [22] and experimentally [23], the effect of discontinuity such as stubs [24–26], rough

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surfaces [27], abrupt junction [28], or the imperfect acoustic coupling between the wire and the reservoirs [29] on the phonon transmission and thermal conductance in a dielectric quantum waveguide has been studied in detail. It is found, in some cases, that the phonon transmission coefficient is still of quantum characteristic even in the presence of discontinuity. More recently, Chen et al. [30,31] exploited the thermal conductance in a nanowire with typical structural defects consisting of void or clamped material. Their results gave a possible exploration for the decrease in the thermal conductance below the quantized universal value in low temperatures presented in experiment [23]. Motivated by these works, in the present letter, we investigate the effect of structural defects on phonon transmission quantization in low-dimensional SL quantum waveguide where acoustic transport plays a critical role in controlling the performance and stability of the devices.

This letter is organized as follows. In Section 2, we present a brief description of model and necessary formulae used in calculations. The calculated results are given with analysis in Section 3. Finally, in Section 4, a summary is made.

2. Model and formalism

In general, the low-dimensional SL structures are confined in two or three directions. Here, we consider a quasi-one-dimensional quantum waveguide structure as shown in Fig. 1, in which a defect layer labeled as II (material AlAs) with a width of W_d and a height of H_II is sandwiched by two finite coupled SLs with a cell unit composed of a (GaAs) and b (AlAs) materials, and the channel connects to two semi-infinite heat reservoirs (material GaAs, labeled as I and III, respectively) which serve as heat sources and sink when a temperature difference is applied. W_a and W_b denote the widths of constituent layers a and b, respectively, and their perpendicular heights are both $H_\mathrm{I} = H_\mathrm{III}$. The number of the period at each side of the defect layer is m and n, respectively. h indicates the heights of both the lower and upper stubs of defect layer over the SL. Ignoring mode mixing effect that could occur at boundaries and interfaces [25,30], without any loss of generality, we only discuss the transmission of the horizontally polarized shear **SH** mode (polarized along the z direction) as in the previous papers.

In the elastic approximation, the displacement field ψ of **SH** mode satisfies the wave equation

$$\frac{\partial^2\psi}{\partial t^2} - v^2\nabla^2\psi = 0, \tag{1}$$

where the wave velocity v depends on the mass density ρ and elastic stiffness constant C_{44}

$$v^2 = C_{44}/\rho. \tag{2}$$

By matching the stress-free boundary condition, the solution to Eq. (1) in different subregions ξ can be written in the form

$$\psi^\xi(x,y) = \sum_{n=0}^{N} [A_n^\xi e^{ik_n^\xi x} + B_n^\xi e^{-ik_n^\xi x}]\phi_n^\xi(y), \tag{3}$$

where

$$\phi_n^\xi(y) = \begin{cases} \sqrt{\dfrac{2}{H_\xi}}\cos\dfrac{n\pi}{H_\xi}y & (n\neq 0), \\ \sqrt{\dfrac{1}{H_\xi}} & (n\equiv 0). \end{cases} \tag{4}$$

Here, k_n^ξ can be given by the energy conservation:

$$\omega^2 = v_\xi^2(k_n^\xi)^2 + \frac{n^2\pi^2 v_\xi^2}{H_\xi^2}, \tag{5}$$

ω is the incident phonon frequency.

By using the scattering matrix cascading method, the coefficients of the phonon wave functions in regions I and III can be correlated through the total scattering matrix S:

$$\begin{pmatrix} B^\mathrm{I} \\ A^\mathrm{III} \end{pmatrix} = \begin{pmatrix} S_{11}(\mathrm{I},\mathrm{III}) & S_{12}(\mathrm{I},\mathrm{III}) \\ S_{21}(\mathrm{I},\mathrm{III}) & S_{22}(\mathrm{I},\mathrm{III}) \end{pmatrix} \begin{pmatrix} I_l \\ 0 \end{pmatrix}, \tag{6}$$

where I_l is an $N^I \times 1$ vector with elements given by $(I_l)_m = \delta_{lm}$. Note that in subregion ξ, the corresponding scattering matrix is written as

$$S(\xi,\xi) = \begin{pmatrix} 0 & P \\ P & 0 \end{pmatrix}, \tag{7}$$

where P is an n-dimensional diagonal matrix with diagonal elements

$$P_{nn} = e^{ik_n^\xi W_\xi}. \tag{8}$$

Then, the flux transmission probability from incident mode m in region I to final mode n in region III across all the interfaces of the SL waveguide can be given as

$$\tilde{t}_{mn} = |t_{mn}|^2 \frac{k_n^\mathrm{III}}{k_m^\mathrm{I}}, \tag{9}$$

with

$$|t_{mn}|^2 = |S_{21}(\mathrm{I},\mathrm{III})_{nm}|^2. \tag{10}$$

Summing over all the active modes in regions III, we get the transmission coefficient $\tau_m(\omega)$ for the individual incident mode m (in region I

$$\tau_m(\omega) = \sum_{n,\omega_n<\omega} \tilde{t}_{mn}, \tag{11}$$

where $\omega_n (= n\pi v_\mathrm{I}/H_\mathrm{I})$ is the cutoff frequency of individual mode n in region I. So, the total transmission probability is calculated by

$$\tau = \sum_{m,\omega_m<\omega} \tau_m. \tag{12}$$

In the calculations, we employ those values of elastic stiffness constants and mass densities of GaAs and AlAs

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