Resonant Transmission of Acoustic Phonons in a Nanowire Superlattice with a Defect Layer

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Abstract. We study theoretically phonon transmission in a nanowire superlattice with a defect layer. We focus on azimuthally symmetric torsional modes and calculate the phonon transmittance. In frequency gaps, there exist transmission peaks originating from the resonant interaction with vibrational modes localized at the defect layer. It is shown that these peaks can be generated only above the critical frequency determined by the radius of the nanowire superlattice.

1. Introduction
Recently, nanowire superlattices (NWSLs) have been fabricated and their electronic and optical properties studied [1-4]. It is shown that the NWSLs are radically different from plain nanowires and quantum well structures in their electronic and optical properties [5]. Furthermore, this new structure leads to a variety of possible applications. For example, single electron transistors and one-dimensional resonant tunneling diodes were created [6, 7]. In addition, we can expect that this structure yields interesting physical effects on the phonon properties and is applicable to various phonon devices.

In the present study, we consider a nanowire superlattice with a defect layer. This structure acts as a double barrier for phonons, in which resonant transmission occurs. We focus on torsional modes whose displacement field and dispersion relations can be obtained analytically [8]. We calculate the transmittance of phonons and examine the effects of both the radial confinement and superlattice modulation on the phonon transmission.

2. Double barrier structure for phonons
The system we consider is illustrated in figure 1. We can regard this system as a double barrier structure for phonons. In a periodic NWSL, Bragg reflection occurs for phonons within the frequency gap determined by the periodicity of the NWSL. The wave vectors of these phonons have an imaginary part. In other words, the NWSL acts as a barrier for phonons. By connecting two NWSLs in series, a double barrier structure for phonons can be realized. This structure is similar to a double-barrier quantum-well structure for electrons, in which resonant transmission occurs. This analogy suggests that the resonant transmission of phonons occurs in the structure shown in figure 1 when the frequency of phonons coincides with a resonant frequency. The resonant frequency is equivalent to the eigenfrequency of the vibrational mode localized at a defect layer, because the layer sandwiched between two NWSLs can be regarded as a defect embedded in a periodic NWSL.
3. Transmission characteristics of phonons

The phonon transmittance is calculated with the use of the transfer matrix method. The detailed mathematical analysis will be given elsewhere [9]. As a numerical example, we consider a GaAs/AlAs NWSL with an AlAs defect layer. The unit period of the NWSL is assumed to be (GaAs)$_{15}$(AlAs)$_{15}$, i.e., $D=8.5$ nm. In NWSLs, the ratio between the radius $R$ and periodicity $D$ is important. In the present example, we assumed that $R=0.75D$. Because of the radial confinement of phonons, the wave number in the radial direction is discretized as

$$k = \frac{f_{2,s}}{R}.$$

Here, $f_{2,s}$ is the $s$th root of the equation $J_2 = 0$, where $J_2$ is the Bessel function of the first kind. Each value of $s$ corresponds to a different mode. In the present paper, we present the results calculated for $s=1$. In a paper [9], the results for $s=0, 1, 2$ will be shown.

The wave number $k$ has the same value in each constituent layer, because of the Snell’s law. On the other hand, the wave number in the longitudinal direction is given by

$$q_I = \sqrt{\left(\frac{\omega}{v_I}\right)^2 - \left(\frac{f_{2,s}}{R}\right)^2},$$

where $I$ denotes the constituent layer (i.e., $I = A, B, C$), $\omega$ is the frequency, and $v_I$ is the transverse sound velocity. When

$$\omega \geq \frac{v_I f_{2,s}}{R} \equiv \omega_I,$$

$q_I$ is a real number and the $z$-dependence of the phonon displacement has an oscillatory nature in the layer $I$. When $\omega < \omega_I$, on the other hand, $q_I$ becomes an imaginary number, and the displacement decays exponentially in the layer $I$. Thus, the displacement pattern is qualitatively different with the frequency range.

Figure 2 shows the transmittance calculated for various values of the thickness $d_c$ of the defect layer. In this calculation, both the substrate and detector layer are assumed to be GaAs, for simplicity. In the present example, $\omega_A < \omega_B = \omega_C$ is assumed (i.e., $A$ = GaAs and $B$ = C = AlAs). Furthermore, we chose $R=0.75D$ such that $\omega_C$ is located in the middle of the first (lowest) frequency gap. In figure 2, $\omega_C = \omega_B$ are indicated. On the other hand, the frequency $\omega_A$ is located below the first band, which is not shown in the figure. For $s \neq 0$, the corresponding phonon displacement has a node in the $r$ direction. As a result, the minimum frequency of this mode has a finite value.
Figure 2. Transmittance calculated for $s = 1$. The NWSL assumed is the (100) GaAs/AlAs NWSL with the AlAs defect layer. The unit period consists of $(\text{GaAs})_{15}(\text{AlAs})_{15}$. The ratio between the radius $R$ and the periodicity $D$ is assumed to be $R / D = 0.75$. The defect layer is sandwiched between two NWSLs (see figure 1). The number of periods of each NWSL is $N = 4$. The used parameters are as follows: the thickness of one monolayer is 2.83 Å in the (100) direction for both GaAs and AlAs; the mass densities and longitudinal sound velocities are 5.36 g/cm³ and 3.34 km/s for GaAs, and 3.76 g/cm³ and 3.97 km/s for AlAs.

We can see a sharp peak within the dip corresponding to the frequency gap. This peak is due to the resonant interaction of incident phonons with a vibrational mode localized at the defect layer. By increasing $d_C$, the resonant frequency decreases. Then, the other peak is extracted from the upper frequency band. However, the resonant frequencies cannot decrease across the critical frequency $\omega_c$. As a result, the number of peaks increases, and the resonant frequency is an aperiodic function of $d_C$. This behavior was not seen in one-dimensional superlattices. This is due to the effect of the radial confinement of phonons.

In the one-dimensional superlattices with a defect layer, the eigenfrequency of the localized mode is a periodic function of $d_C$ [10]. This periodicity is due to the fact that the number of nodes of the corresponding displacement in the defect layer increases by one when the width of the defect layer increases by the unit period. In the NWSL with the defect layer, the same situation occurs for $s = 0$. In this case, there is no region determined by $0 < \omega < \omega_c$ because $f_{2,0} = 0$. Thus, the wave number $q_i$ defined within each layer is always a real number, and the resonant frequency becomes a periodic function of $d_C$.

In the present example (i.e., $s = 1$), $\omega_c$ is located within the lowest frequency gap. In this frequency gap, the displacement pattern is different depending on whether the frequency is higher than $\omega_c$ or not. When $\omega < \omega_c$, the wave number $q_C$ defined within the defect layer becomes an imaginary number. The corresponding phonon displacement does not oscillate in the defect layer. That is, the
phonon displacement has no node within the defect layer, and the number of nodes can not increase. As a result, the resonant frequency becomes the aperiodic function of $d_c$.

In addition, it is found that the transmittance corresponding to the lowest frequency band depends on the width of the defect layer. By increasing $d_c$, the values of the transmittance decrease because the phonon displacement decays largely within the defect layer. For $d_c > d_A$, the value of the transmittance in the lowest frequency band is vanishingly small. As a result, the phonon transmission is prohibited below the critical frequency.

4. Summary
In the present paper, we calculated the transmittance of phonons in a NWSL with a defect layer. It is shown that resonant peaks appear within the frequency gaps. These peaks originate from the resonance with vibrational modes localized at the defect layer. In particular, we examined how the resonant frequency depends on the width of the defect layer. The radial confinement of the phonons generates a critical frequency, which is determined by the radius of the NWSL. When the frequency of phonons is lower than this critical frequency, the wave number defined in the defect layer becomes an imaginary number. Our results show that the localized modes can be generated only above the critical frequency.

Acknowledgments
This work was partially supported by a Grant-in-Aid for Scientific Research from the Japan Society for the Promotion of Science (Grant No. 17510093).

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