Physics Letters A 375 (2011) 2000–2006

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Ballistic phonon transport through a Fibonacci array of acoustic nanocavities in a narrow constriction

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ARTICLE INFO

Article history:
Received 7 December 2010
Received in revised form 13 February 2011
Accepted 26 March 2011
Available online 30 March 2011
Communicated by R. Wu

Keywords:
Phonons
Cavities
Ballistic transport
Heat conduction

ABSTRACT

We investigate the ballistic phonon transport through a Fibonacci array of acoustic nanocavities in a narrow constriction of a semiconductor nanowire at low temperatures. It is found that the transmission spectrum of such a system consists of quasiband gaps and narrow resonances caused by the coupling of phonon waves. Both phonon transmission and thermal conductance exhibit the similarity due to the Fibonacci sequence structure. The similarity is sensitive to the number n and parameters of nanocavities. The results are compared with those in a periodic acoustic nanocavities.

1. Introduction

The acoustic vibrational and phonon thermal transport properties of the nanoscale structures and materials have attracted an increasing amount of attention in recent years [1]. The introduction of the concepts of phononic crystals [2] and nanocavities [3] is the quintessence of these studies in order to manipulate acoustic waves. It has been demonstrated that acoustic nanocavities, which open the possibility of confinement and amplification of the acoustic phonons, can strongly confine the acoustical phonons [3–5], even selectively generate confined acoustic modes [6], and enhance the interaction between phonon and light [7]. When a large series of phonon cavities are coupled one after the other, the discrete confined energy states form phonon bands. As the energy of the ith cavity differs from that of the $(i-1)$th in a constant value, which introduces a phonon equivalent effective linear potential, phonon Bloch oscillation can exist in the acoustic cavity structures, while the acoustic-phonon pulses impinging on a structure with a parabolic effective potential will develop Bloch-like oscillation [8]. Very recently, Lanzillotti-Kimura et al. experimentally demonstrated that Bloch oscillations of acoustic phonons can be directly generated and probed [9]. In these studies, acoustic nanocavities must be inserted between two finite semiconductor superlattices acting as two acoustic Bragg mirrors. By using the multilayer structure consisting of two materials with contrasting acoustic properties, Lanzillotti-Kimura et al. verified that the coupling of the discrete energy states of two acoustic cavities leads to a splitting of modes [8]. Another phonon mode splitting behavior caused by one acoustic cavity has also been found in a Ψ-shaped semiconductor nanowire: different phonon modes transport selectively into different channels [10]. When more than one nanocavity is embedded in a narrow constriction, the nanowire has selective transmission and filter actions for the ballistic phonon [11].

Tailoring the acoustic-phonon spectrum to manage the phonon transport in nanoscale has also been the subject of intense interest at present due to its fundamental interest and critical role in controlling the performance and stability of nanostructural devices. An enormous theoretical and experimental researches on phonon heat transport of the nanoscale structures and materials has been reported [12–28]. The most remarkable examples in this domain are the observation of the quantization of the phonon band structure through an analysis of the specific heat [12], the discovery of ballistic phonon transport [13], and the measurement of the quantum of thermal conductance in a nanowire [14]. Another revolutionary discovery is the proposal and experimental verification of the solid-state thermal rectifier [15] and transistor [16]. In technological applications such as nanotube-based devices, thermal properties are of central importance for understanding and con-

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2011.03.046

trolling heat dissipation and self-heating effects [15,17,18]. More recently, we reported that phonon heat can be dissipated through different channels by properly tuning the parameters of the cavity in a Ψ-shaped semiconductor nanostructure [10], and introducing a nanocavity into a narrow constriction in a semiconductor nanowire, leads to an increase of the phonon transmission and to an enhancement of the thermal conductance at very low temperatures [11]. The material properties can also affect the ballistic phonon transport in the nanostructures [29], which is similar to the diffusive phonon transport.

The Fibonacci sequence (or quasiperiodic order) has been attracting a considerable interest since the experimental discovery of icosahedral diffraction pattern [33]. A fascinating feature of the quasiperiodic structures is that they exhibit collective properties not shared by their constituent parts. Furthermore, the long-range correlations induced by the construction of these systems are expected to be reflected to some degree in their various spectra (as in light propagation, electronic transmission, density of states, polaritons, etc.), defining a novel description of disorder [34–36]. Another important motivation for studying these structures comes from recognizing that the localization of electronic states, one of the most active fields in condensed matter physics, could occur not only in disordered systems but also in the deterministic quasiperiodic systems [37]. The most striking characteristic of the quasiperiodic structures is that they exhibit a highly fragmented energy spectrum displaying a self-similar pattern. Many interesting features have been uncovered due to the structures with Fibonacci sequence exhibiting some properties of the periodic order and some of the disordered systems [38–41]. For example, both electronic transmission coefficient and conductance exhibit self-similarity and the six-circle property in a Fibonacci magnetic superlattice [42], nonresonant Zener tunneling can be observed in a quasiperiodic lattices [43], the properties of the plasmon polaritons in photonic metamaterial Fibonacci superlattices strongly depend on the Fibonacci-sequence order m [44]. It is also reported that the Fibonacci structure acts as a filter for the phonon's transmission spectra [45]. In addition, the propagation bands separated by band gaps have been demonstrated in acoustic and photonic experiments [46,47]. These studies mainly focused on electronic or optical properties in multilayered structures with constituents arranged in a quasiperiodic fashion. In this Letter, we will examine the behaviors of ballistic phonon transport in acoustic nanocavities arranged according to the Fibonacci sequence. This 'special' arranged acoustic nanocavities is different from usual Fibonacci sequence, such as the multilayered structures with constituents arranged in a quasiperiodic fashion. Our results show some interesting physical properties such as the transmission spectrum consisting of quasiband gaps and narrow resonances, the similarity of phonon transmission and thermal conductance depending on the number n and parameters of nanocavities.

This Letter is organized as follows. In Section 2, a brief description of the model and the necessary formulae used in calculations is given. The numerical results are presented in Section 3 with analyses. Finally, we summarize our results in Section 4.

2. Model and formalism

A series of acoustic nanocavities embedded in a narrow constriction of a semiconductor nanowire is depicted in Fig. 1. The nanocavities are arranged serially according to a 'special' Fibonacci rule, i.e., the distance between them increases with the Fibonacci sequence, $dj = d(j-1) + d(j-2)$ with $d1 = d2$, where dj denotes the distance between the $(j-1)$th and jth cavities. D and $W1$ denote the cavity length and transverse width, respectively. $W1$ and $W2$ are the transverse widths of the nanowire and the narrow constriction, respectively. The system is considered to be a two-

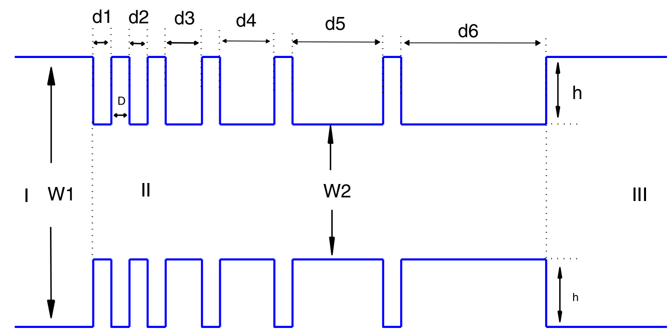

Fig. 1. (Color online.) A series of acoustic nanocavities embedded in a narrow constriction of a semiconductor nanowire. The nanocavities are arranged serially according to a 'special' Fibonacci rule, i.e., the distance between them increases with the Fibonacci sequence, $dj = d(j-1) + d(j-2)$ with $d1 = d2$. D and $W1$ denote the cavity length and transverse width, respectively. $W1$ and $W2$ are the transverse widths of the nanowire and the narrow constriction, respectively. $h = (W1 - W2)/2$.

dimensional system in the x–y plane. We divide the structure into two parts: one is the narrow constriction connected to left and right nanowires. The narrow constriction parameterized by transverse width $W2$ is continuously separated into sub-constriction by acoustic nanocavities. The other is the main wire, i.e., the left and right wires with uniform transverse width $W1$. It is assumed that the other ends of left and right wires are separately connected to two thermal reservoirs serving as phonon source and phonon sink (not shown in Fig. 1) with an infinitely small temperature gradient δT ($\delta T = T_L - T_R > 0$, and $\delta T \ll T_L, T_R$. Here, T_L (T_R) is the temperature of the left (right) reservoir.) So the mean temperature T $[T = (T_L + T_R)/2]$ can be adopted as the temperature of the left and right wires in following calculations. The reservoirs are at thermal equilibrium with phonon distribution in the Bose–Einstein form, $f_{BE}(\omega, T) = [\exp(\hbar\omega/k_B T) - 1]^{-1}$. It is also assumed that the thermal contacts between the wires and the reservoirs is *reflectionless*: all phonons going into reservoirs are assimilated by the reservoirs without being rebound back to the wires. At low temperatures, phonon–phonon interactions between different vibrational modes can be safely ignored [29–32]. Therefore the left and right wires act as phonon waveguides. Supposing that the incident phonon waves originate from the left wire, they then successively enter the converging and diverging regions where they suffer multi-reflection and interference, and finally, the phonon waves partially transmit to the right wire and partially rebound back to the left wire.

At low temperatures, ballistic phonon wavelengths are generally over several hundreds of angstroms which is much greater than the dimensions of the structure. Naturally, microscopic length such as the atomic bond length is much smaller than the wavelength of the ballistic phonon. Therefore, we use the scalar model of continuum medium theory to describe the ballistic phonon propagation in this work [29–32]. According to this theory, the displacement field $\mathbf{U}(x, y)$ satisfies the wave equation

$$v^2_{W,NC,C}\nabla^2\mathbf{U}(x, y) + \omega^2_{W,NC,C}\mathbf{U}(x, y) = 0, \tag{1}$$

where v is the wave velocity and ω is the frequency of phonon, W, NC, and C denote left and right nanowires, nanocavities, and the constrictions, respectively. Here, we take the stress-free boundary condition at the structure surfaces

$$\frac{\partial\mathbf{U}}{\partial\hat{n}} = 0, \tag{2}$$

where $\hat{n}$ is the unit vector perpendicular to the surface.

According to Eq. (1), the solutions of phonon displacement field equations in the nanowires, nanocavities, and the constrictions, can be written as follows: