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Optimizing thermoelectric efficiency of superlattice nanowires at room temperature

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ABSTRACT

It is known that the figure of merit (ZT) of thin nanowires can be significantly enhanced at room temperature due to the reduction of phonon thermal conductance arising from the increase of boundary scattering of phonons. It is expected that the phonon thermal conductance of nanowires filled with quantum dots (QDs) will be further reduced. Here we consider a superlattice nanowire (SLNW) modeled by a linear chain of strongly coupled QDs connected to electrodes. We study the dependence of ZT on the QD energy level (E_0) (relative to the Fermi level E_F in the electrodes), inter-dot coupling strength (t_c), tunneling rate (Γ), and temperature T in order to optimize the design. It is found that at room temperature the maximum power factor occurs when $(E_0 - E_F)/k_BT \approx 2.4$ and $\Gamma = t_c$, a result almost independent of the number of QDs in SLNW as long as $t_c/k_BT < 0.5$. By using reasonable physical parameters we show that thin SLNW with cross-sectional width near 3 nm has a potential to achieve $ZT \geq 3$.

1. Introduction

Extensive studies have shown that in bulk thermoelectric materials, it is difficult to achieve a figure of merit (ZT) larger than one at room temperature [1,2]. With the advances of nanostructure technology, many experiments nowadays can realize ZT larger than one at room temperature in low-dimensional structures [3,4]. The search of nanostructured materials with significantly improved ZT is still a subject of hot pursuit. If a material with $ZT \geq 3$ at room temperature (which corresponds to a Carnot efficiency around 30% [4]) can be found, it will brighten the scenario of thermoelectric devices tremendously [1,2]. For example, thermoelectric generators (TEGs) using human body as a heat source can be applied to wearable electrical powers, which are very useful for commercial wireless communication and low power electronics [5]. Thermoelectric coolers will also become a viable option for many applications [1,2]. It has been predicted theoretically that $ZT \geq 3$ can be achieved in thin semiconductor nanowires [6,7]. However, no experimental realization of such impressive TE devices has been reported [1,2].

The finding of $ZT = 1$ in silicon nanowires at room temperature [8] has inspired further studies of thermoelectric properties of silicon-based nanowires because of the advantages of low cost and the availability of matured fabrication technology in silicon industry [8–10]. Whether $ZT \geq 3$ exists in silicon-based nanowires at room temperature becomes an interesting topic. Monte Carlo simulations [11] have demonstrated that in heavily-doped Si naowires ZT does not increase dramatically with decreasing wire cross section since the electron conductance suffers stronger ionized-impurity scattering as the size reduces. Thus, to improve ZT it is better to use intrinsic nanowires. Silicon nanowire filled with quantum dots (QDs) may provide an alternative means to realize the values of $ZT \geq 1$ [1,2]. Furthermore, it is estimated that Si/Ge superlattice nanowire (SLNW) with an optimized period around 5 nm and cross-sectional area around 3 nm × 3 nm can lead to an reduction of phonon thermal conductance by one order of magnitude in comparison with pristine Si nanowires [12,13]. Therefore, it is desirable to study the dependence of ZT on relevant physical parameters of Si/Ge SLNWs near room temperature.

Here, we perform theoretical calculations of the thermoelectric properties of intrinsic SLNW connected with electrodes by using a linear chain of strongly coupled QDs. The electron carriers in SLNWs are provided by metallic electrodes with Fermi level below the conduction band minimum as proposed in Ref. [14]. The SLNW structure can

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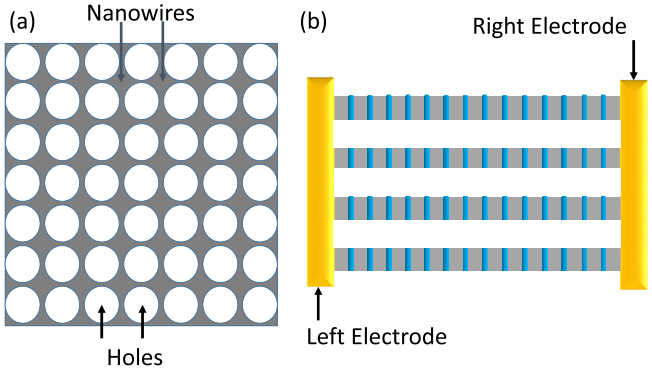

Fig. 1. (a) Schematic sketch of the creation of superlattice nanowires (SLNWs). (b) Side view of SLNWs connected to electrodes.

be realized by starting with a superlattice with optimized period to minimize the phonon thermal conductance. The creation of nanowires may be achieved by lithographically drilling a periodic array of closely-spaced holes [10], leaving an array of nanowires (with a star-shaped cross-section) as depicted in Fig. 1. To reduce the electron scattering from the rough surface, the side surfaces of the nanowires are oxidized to form a high electron barrier, which serves the purpose of confining electrons in the central region of the star-shaped nanowires. Due to the strong confinement of electrons, the electron-surface scattering can be reduced. At the same time the acoustic phonons are not so well confined in the central region which will then suffer more surface scattering. With such a design, we found that $ZT \geq 3$ may be achieved in a thin SLNW with reasonable physical parameters adopted. Our theoretical studies should provide a useful guideline for the design of future thermoelectric devices operating at room temperature.

2. Formalism

To model the thermoelectric properties of SLNWs, we consider a linear chain of strongly-coupled QDs with a system Hamiltonian given by an Anderson model $H = H_0 + H_{QD}$ [15], where

$$H_0 = \sum_{k,\sigma} \epsilon_k a^\dagger_{k,\sigma} a_{k,\sigma} + \sum_{k,\sigma} \epsilon_k b^\dagger_{k,\sigma} b_{k,\sigma} + \sum_{k,\sigma} V^L_{k,L} d^\dagger_{L,\sigma} a_{k,\sigma} + \sum_{k,\sigma} V^R_{k,R} d^\dagger_{R,\sigma} b_{k,\sigma} + c.c. \quad (1)$$

The first two terms of Eq. (1) describe the free electron gas in the left and right electrodes. $a^\dagger_{k,\sigma}$ ($b^\dagger_{k,\sigma}$) creates an electron of momentum k and spin σ with energy ϵ_k in the left (right) electrode. $V^L_{k,L}$ ($V^R_{k,R}$) describes the coupling between the left (right) lead with its adjacent QD. $d^\dagger_{L(R),\sigma}$ ($d_{L(R),\sigma}$) creates (destroys) an electron in the QD connected to the left (right) lead.

$$H_{QD} = \sum_{\ell,\sigma} E_\ell d^\dagger_{\ell,\sigma} d_{\ell,\sigma} + \sum_{\ell \neq j} t_{\ell,j} d^\dagger_{\ell,\sigma} d_{j,\sigma}, \quad (2)$$

where E_ℓ is the QD energy level in the ℓ-th QD and $t_{\ell,j}$ describes the electron hopping strength between the ℓ-th and j-th QDs. Here, for simplicity, we consider only one energy level for each QD, which is suitable for nanoscale QDs with no vally degeracy. For example, a cylidrical GaAs QD with high lateral potential barrier resulting from oxidation and vertical confinement via the band onset between GaAs and AlGaAs has a bound state (which is well separated in energy from the excited states) for diameter naer 3 nm and height near 5 nm [16]. For silicon QDs in the Si/Ge SLNW, we expect the valley degeneracy to lead to enhanced density of states in the energy range of interest, which can actually improve ZT further [17]. It should be noted that the Hubbard-like terms for Coulomb interactions between electrons in the SLNWs are neglected, since the electrons are delocalized along the transport direction in the strong hopping limit considered.

To study the transport properties of QDs junction connected with electrodes, it is convenient to use the Green-function technique. The electron and heat currents from reservoir α to its adjacent QD are calculated according to the Meir-Wingreen formula [18]

$$J^n_\alpha = \frac{ie}{h} \sum_{j\sigma} \int d\epsilon \left(\frac{\epsilon - \mu_\alpha}{e}\right)^n \Gamma_\alpha(\epsilon) [G^<_{\alpha,\sigma}(\epsilon) + f_\alpha(\epsilon)(G^r_{\alpha,\sigma}(\epsilon) - G^a_{\alpha,\sigma}(\epsilon))], \quad (3)$$

where $n = 0$ is for the electrical current and $n = 1$ for the heat current. $\Gamma_{L(R)}(\epsilon) = \sum_k |V_{k,L(R)}|^2 \delta(\epsilon - \epsilon_k)$ is the tunneling rate for electrons from the left (right) reservoir and entering the left (right) QD. $f_\alpha(\epsilon) = 1/\{\exp[(\epsilon - \mu_\alpha)/k_B T_\alpha] + 1\}$ denotes the Fermi distribution function for the α-th electrode, where μ_α and T_α are the chemical potential and the temperature of the α electrode. e, h, and k_B denote the electron charge, the Planck's constant, and the Boltzmann constant, respectively. $G^<_{\alpha,\sigma}(\epsilon)$, $G^r_{\alpha,\sigma}(\epsilon)$, and $G^a_{\alpha,\sigma}(\epsilon)$ denote the frequency-domain representations of the one-particle lessor, retarded, and advanced Green's functions, respectively.

In the linear response regime electrical conductance (G_e), Seebeck coefficient (S) and electron thermal conductance (κ_e) can be evaluated by using Eq. (3) with a small applied bias $\Delta V = (\mu_L - \mu_R)/e$ and temperature difference across junction $\Delta T = T_L - T_R$ [17]. For simplicity, we calculate these thermoelectric coefficients in terms of Landauer formula [19,20]. Here we have $G_e = e^2 \mathcal{L}_0$, $S = -\mathcal{L}_1/(eT\mathcal{L}_0)$ and $\kappa_e = \frac{1}{T}(\mathcal{L}_2 - \mathcal{L}_1^2/\mathcal{L}_0)$. Thermoelectric coefficients $\mathcal{L}_n$ are given by

$$\mathcal{L}_n = \frac{2}{h} \int d\epsilon \mathcal{T}_{LR}(\epsilon)(\epsilon - E_F)^n \frac{\partial f(\epsilon)}{\partial E_F}, \quad (4)$$

where $f(\epsilon) = 1/(\exp^{(\epsilon - E_F)/k_B T} + 1)$ is the Fermi distribution function of electrodes at equilibrium temperature T and $\mathcal{T}_{LR}(\epsilon)$ is the transmission coefficient. E_F is the Fermi energy of electrodes. The expression of $\mathcal{T}_{LR}(\epsilon)$ in Eq. (4) is given by Refs. [20,21]

$$\mathcal{T}_{LR}(\epsilon) = \frac{4\Gamma_L \Gamma^{eff}_R(\epsilon)}{\Gamma_L + \Gamma^{eff}_R(\epsilon)} (-Im(G^r_L(\epsilon))), \quad (5)$$

where $G^r_L(\epsilon) = 1/(\epsilon - E_1 + i\Gamma_L - \Sigma_{1,N}(\epsilon))$ denotes the one-particle retarded Green function of the leftmost QD with the energy level of E_1, in which the self energy $\Sigma_{1,N}(\epsilon)$ resulting from electron tunneling from the leftmost QD to the right electrode mediated by N-1 QDs is given by Ref. [21]

$$\Sigma_{1,N}(\epsilon) = \cfrac{t^2_{1,2}}{\epsilon - E_2 - \cfrac{t^2_{2,3}}{\epsilon - E_3 - \cdots \cfrac{t^2_{N-1,N}}{\epsilon - E_N + i\Gamma_R}}}, \quad (6)$$

where N denotes the total number of QDs. The rightmost QD is the Nth QD. The effective tunneling rate $\Gamma^{eff}_R = -Im(\Sigma_{1,N}(\epsilon))$. For simplicity, we assume $E_\ell = E_0$ and $t_{\ell,j} = t_c$ for all ℓ and j being the nearest neighbor of ℓ, and $\Gamma_L = \Gamma_R \equiv \Gamma$.

The figure of merit $ZT = S^2 G_e T/(\kappa_e + \kappa_{ph})$ contains the phonon thermal conductance (κ_{ph}) of SLNW, which can not be neglected at room temperature [17]. Many theoretical efforts have been devoted to the study of phonon thermal conductance of silicon nanowires [22,23]. Here, we adopt the formula of phonon thermal conductance as given in Ref. [23], which can well describe the experimental results of Si nanowires [23,24]. We have

$$\kappa_{ph,0}(T) = \frac{1}{h} \int d\omega \mathcal{T}(\omega)_{ph} \frac{\hbar^3 \omega^2}{k_B T^2} \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2}, \quad (7)$$

where ω is the phonon frequency and $\mathcal{T}_{ph}(\omega)$ the throughput function. In Refs. [12,13,25] it is theoretically demonstrated that $\kappa_{ph}(T)$ of Si nanowires filled with QDs is significantly reduced from the value

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