Ballistic thermoelectric transport in structured nanowires

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Abstract
Thermoelectric (TE) devices are solid-state energy converters that can be used for power generation through the Seebeck effect and TE cooling through the Peltier effect. Nanostructures give great opportunities to engineer TE energy conversion efficiency. In this work, we investigate TE transport properties in structured nanowires (NWs) in the ballistic transport regime, where the NWs are bent, kinked, stubbed and segmented like a superlattice nanowire using the Green’s function method and the Landauer–Büttiker formula. A large Seebeck coefficient is found when the transmission gap appears due to the quantum interference effect of electrons. The sign of the Seebeck coefficient can be controlled by the geometries of these structured NWs. This finding is helpful for the design of nanoscale TE devices, such as thermocouple, with the same type of material doping rather than those comprised of n-type and p-type materials.

Keywords: thermoelectricity, nanowire, structure, ballistic, Green’s function
1. Introduction

Solid-state thermoelectric (TE) devices can be used for both power generation and refrigeration based on the two fundamental TE effects, the Seebeck effect and the Peltier effect [1, 2]. The energy conversion efficiency of TE material is characterized by the dimensionless figure of merit (ZT):

$$ZT = \frac{GS^2}{\kappa} T,$$  \hspace{1cm} (1)

where $G$ is the electrical conductance, $S$ is the Seebeck coefficient, $T$ is the absolute temperature, and $\kappa$ is the thermal conductance. $\kappa = \kappa_e + \kappa_p$, where $\kappa_e$ and $\kappa_p$ are the electronic and lattice (phonon) contributions, respectively. A larger ZT means higher energy conversion efficiency. ZT needs to be significantly improved to be competitive with the conventional energy converters such as vapor-compression refrigerators. Different approaches have been explored to enhance the performance of TE materials: (a) one is to develop new families of advanced bulk TE materials, such as skutterudites [3, 4]; (b) the other is nanostructuring of conventional TE materials and non-TE materials [5, 6], such as nanowires (NWs) [7–9], superlattices [10, 11], and quantum wells [12, 13]. More recently these two approaches have converged to generate nanostructured bulk materials such as nanocomposites [14]. Physically, ZT could be greatly enhanced by utilizing nanostructured materials [15, 16] from the following aspects. On the one hand, the introduction of quantum confinement effect or low-energy electron filters can enhance the power factor $GS^2$ [17]. On the other hand, the introduction of numerous interfaces can reduce the thermal conductance [8, 9]. Simultaneous enhancement of electronic power factor and reduction of thermal conductivity can be achieved in many nanostructured TE materials including quantum dot nanocomposites and organic inorganic nanocomposites [18].

Significantly enhanced ZT has been experimentally demonstrated in NWs [8, 9], owing mostly to the reduction of thermal conductance due to surface phonon scattering [8, 9]. Besides the straight NWs, ZT enhancement in structured NWs has somewhat been explored. For example, molecular dynamics study showed that the thermal conductance of kinked NWs [19] is much smaller than that of straight NWs, which might enhance the ZT [20]. The electron subband formation in superlattice NWs could enhance the Seebeck coefficient within the diffusive regime while significant thermal conductance reduction due to interfaces is expected between superlattice segments, both lead to the enhancement of ZT [21–24].

When the temperature- and material-dependent characteristic lengths, de Broglie wave length of electron, mean free path of electron scattering and phase coherence length are larger than the dimension of the conductor [25], electron transport, especially at low temperature, could be ballistic. These lengths could be as long as tens of microns at liquid helium temperature in high mobility semiconductors. In the ballistic regime, the phase of electron is maintained during transport, which would result in quantum interference effect. The electrical conductance due to ballistic transport in NWs has been widely studied [25], although the Seebeck coefficient has not been studied in depth. Abundant interference and resonance effects can induce oscillation of transmission probability in NWs, which provide a pathway to enhance the Seebeck coefficient, which is proportional to the slope of transmission spectrum. Recently, Zianni [26] studied ballistic TE transport in diameter-modulated NWs. In her work, the strong energy-dependent transmission probability is tuned by the diameter of NWs, which comes from
the interference between propagating electron states and confined electron states, i.e. the Fano resonance. This Fano resonance effect has been experimentally observed by Wu et al.\textsuperscript{[27]} in InAs NWs with diameter modulations. Zhou and Yang investigated the ballistic TE transport properties of double-bend NWs\textsuperscript{[7]}, where quantum confinement is not necessary for the strong energy dependence of transmission probability. The interference of electron wave in such structured NW is analogous to the interference of electromagnetic wave in a waveguide which can be explained as follows: the transmission probability is the modular square of the total transmission amplitude, which is the sum of transmission amplitudes associated with particular Feynman paths\textsuperscript{[25]}. The Feynman paths are very sensitive to the geometry of NWs. If the transmission amplitudes are in phase, the transmission probability shows a peak. In contrast, if the transmission amplitudes are out of phase, the transmission probability shows a gap. This feature provides a pathway to control the transmission spectrum and TE transport properties by changing the geometry of NWs. Both above researchers pointed out that the Seebeck coefficient could be positive and negative without changing the doping type in NWs due to the ballistic transport. Here we investigate systematically the geometry effect on the ballistic TE transport in NWs with various structures such as bent\textsuperscript{[28]}, kinked\textsuperscript{[19]}, stubbed\textsuperscript{[29]} and superlatticed\textsuperscript{[30]} NWs, where such crystalline structured NWs have been experimentally synthesized.

This paper is organized as follows. We present the tight-binding model and the Green’s function method in section 2. The calculation results obtained from the Landauer–Büttiker formula for a variety of structured NWs are presented in section 3. Section 4 concludes the paper.

2. Model

The tight-binding approach is used to describe the electrons in NWs. The Hamiltonian $H$ with the nearest-neighboring approximation is written as:

\[ H = \sum_{m,n} \left( \varepsilon_{m,n} a_m^\dagger a_m + t a_{m+1,n}^\dagger a_m + t a_{m,n+1} a_m^\dagger + t a_{m,n+1}^\dagger a_{m,n} + t a_{m,n}^\dagger a_{m+1,n} + t a_{m+1,n}^\dagger a_{m,n+1} \right), \]  

where $m$ and $n$ denote discrete lattice sites that are located at $(x, y) = (ma, na) \equiv [m, n]$ with $m, n$ being integers, and $a$ standing for the lattice constant of grid. There is no variable $z$ in this Hamiltonian since only the lowest subband in the $z$-direction is considered in our model. $\varepsilon_{m,n}$ denotes the on-site energy with $\varepsilon_{m,n} = -4t + V(m, n)$, where a hard wall boundary condition is applied by choosing $V(m, n) = 0$ inside the NW and $V(m, n) \to \infty$ outside the NW. $t$ is the hopping energy between the nearest-neighboring sites with $t = -\hbar^2/2m^*a^2$, where $m^*$ is the effective mass of electrons and $\hbar$ is the Planck constant. $a_m^+$ and $a_m$ are the creation and annihilation operators of electron on site $[m, n]$, respectively.

In order to calculate the TE transport properties in the ballistic regime, the Green’s function method is used, which is written as

\[ G^+ = \left[ EI - H - \Sigma_L^+ - \Sigma_R^+ \right]^{-1}, \]  

where $G^+$ is the retarded Green’s function, $E$ is the electron energy, $I$ is identity matrix, $\Sigma_L^+$ and $\Sigma_R^+$ are the self-energy functions due to attached left and right leads, respectively. When the NW is long, the computation could be very costly since inverting a large matrix as shown in equation (3) requires tremendously large memory. We use the recursive Green’s function.
method [31], which divides the NW layer by layer along the transport direction, to address this computational challenge.

The total transmission probability \( T_{\text{tot}}(E) \) of electron can then be calculated using obtained Green’s function as [25]

\[
T_{\text{tot}}(E) = \text{Tr} \left[ G_L^+ G_R^- \right]
\]  
(4)

where \( G_{L(R)} = -2 \text{IM} \left[ \Sigma_{L(R)} \right] \) with \( \text{IM}[...] \) taking the imaginary part of self-energy functions, \( G^- \) is the advanced Green’s function of the NW.

The electrical conductance \( G \) and the Seebeck coefficient \( S \) are calculated using the Landauer–Büttiker formalism [25, 32, 33]:

\[
G(\mu, T) = \frac{2e^2}{h} \int_0^\infty T_{\text{tot}}(E) \left[ -\frac{\partial f}{\partial E} \right] dE
\]  
(5a)

\[
S(\mu, T) = -\frac{k_B}{e} \frac{\int_0^\infty T_{\text{tot}}(E) \left[ -\frac{\partial f}{\partial E} \right] E - \mu}{\int_0^\infty T_{\text{tot}}(E) \left[ -\frac{\partial f}{\partial E} \right] dE}
\]  
(5b)

where \( e \) represents the absolute value of the unit electron charge, \( k_B \) is the Boltzmann constant, \( \mu \) is the chemical potential and \( f \) is the Fermi–Dirac distribution function, respectively.

3. Results and discussions

We perform numerical calculations for the bent, kinked, stubbed and superlatticed NWs as shown in figures 1(a)–(d) to study their TE properties along the x-direction, when the electron transport is in the ballistic regime. The y-direction is confined by a hard wall, which determines various geometries. In our study, only the lowest subband along the z-direction is considered. The NWs are connected to two electron reservoirs through two ideal leads with perfect Ohmic contact.

The parameters used in calculation are chosen as follows: \( m^* = 0.067 m_e \), which is the effective mass of conduction band in GaAs, where \( m_e \) is the free electron mass, and \( a = 1.906 \text{ nm} \), which results in a hopping energy \( t = -1/4 \text{ eV} \). In order to simplify the discussion, we fix the width \( W \) of NWs to be \( 7a \) throughout the paper. All the calculations are performed when temperature is at \( T = 10 \text{ K} \), which ensures the electron transport is in the ballistic regime. Higher temperatures, such as room temperature, would smear the variation of transmission probability [7], which makes the ballistic effect on TE transport properties difficult to observe [25]. The main objective of this paper is the geometry effect. Therefore, the temperature dependences of the electrical conductance, the Seebeck coefficient and the power factor are not presented here while interested readers are referred to [7].

3.1. Bent NWs

Figure 1(a) shows the schematics of a bent NW along the x-direction while the transverse direction is confined by hard walls. The bend angle is \( \theta \), the width is \( W \) and the inter-bend length is \( h \).
Figure 2(a) shows the transmission probability $T_{\text{tot}}$ plotted as a function of electron energy $E$ in bent NWs with bend angle $\theta$ varying from 0° to 90° when $h=18a$. Oscillation of transmission probability with multiple gaps occurs when the bend angle increases. These transmission gaps are the results of anti-resonance of electron wave near the bent areas [7]. The variation of transmission probability changes slightly when the bend angle varies from 0° to 30°. When the bend angle increases to beyond 30°, the transmission gaps become steeper and more significant, which indicates a much stronger quantum interference in bent NW with sharper bend angle. Figures 2(b)–(d) show the electrical conductance, the Seebeck coefficient and the power factor varying with chemical potential $\mu$ for different bend angles when $h=18a$.

Similar to the transmission probability, the electrical conductance also exhibits oscillating behavior, which becomes more significant with the increase of bend angle as shown in figure 2(b). In figure 2(c), the sign change of the Seebeck coefficient is observed when the bend angle increases. The maximum value of the absolute Seebeck coefficient, denoted as $|S|_{\text{max}}$, also increases as the bend angle increases, since the transmission probability varies more sharply for larger bend angle as shown in figure 2(a). Typical $|S|_{\text{max}}$ is larger than 200 $\mu$V K$^{-1}$ when the bend angle is over 80°. Figure 2(d) shows the peaks of power factor obtained when the chemical potential is close to the edge of the transmission gap. The power factor reaches about $2k_B^2/h$ when the bend angle is 80°.

Figure 3(a) shows the transmission probability $T_{\text{tot}}$ versus electron energy $E$ in bent NWs for different $h$ when bend angle is 80°. Larger $h$ results in more transmission peaks and gaps. There are two transmission gaps when $h=14a$, three gaps when $h=18a$ and four gaps when $h=22a$. The reason is that the transmission probability would be close to 1 when resonance occurs once an integer multiple of electron wavelength matches $h$. The transmission probability
reaches its minimum when anti-resonance occurs once a half-integer multiple of electron wavelength matches $h$. The Seebeck coefficient describes the average entropy carried by each charge carrier and is approximately proportional to the slope of transmission probability at low temperature [7]. The resonance and anti-resonance enable us to control both the sign and the amplitude of the Seebeck coefficient by modulating the inter-bend length $h$. Figures 3(b)–(d) show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential $\mu$ for different bend lengths $h$ when the bend angle is 80°. Figure 3(b) shows that there are more gaps of electrical conductance when $h$ increases. This is a consequence of the appearance of more transmission gaps. Moreover, according to equation (5b), a large positive Seebeck coefficient can be found when the chemical potential is close to the lower edge of the transmission gap since only the electrons whose energies are smaller than the chemical potential ($E < \mu$) contribute to transport. Similarly, large negative Seebeck coefficient could be found when the chemical potential is close to the upper edge of the transmission gap since only the electrons whose energies are larger than the chemical potential ($E > \mu$) contribute to transport. In figure 3(c), the sign of the Seebeck coefficient changes more frequently when chemical potential changes with the increase of $h$. The largest $|S|$ of 250 $\mu$VK$^{-1}$ is obtained when $h = 18a$. In figure 3(d), the highest peak of power factor appears when $\mu \sim 0.14$ eV and $h = 18a$. 

Figure 2. (a) Total transmission probability plotted as a function of electron energy $E$ in bent NW for different bend angles when $h = 18a$. (b) Electrical conductance, (c) Seebeck coefficient and (d) power factor versus chemical potential $\mu$. 

New J. Phys. 16 (2014) 065018 B Wang et al
The variation of the transmission probability and the sign change of the Seebeck coefficient due to the geometric interference obtained above are similar to the TE transport in molecules [34–36], which is largely determined by the electronic structure of the molecule. Similar behavior can also be found for other NWs studied in this paper.

3.2. Kinked NW

Figure 1(b) shows the schematics of a kinked NW. The width of NW is $W$, the length of each serration is $2L$ and the bend angle is $\theta$. This kinked NW is a periodic structure with the number of periods $p$. We fix $W=7a$ and $L=18a$ to focus on the influences of the bend angle $\theta$ and the number of periods $p$.

Figure 4(a) shows the transmission probability $T_{tot}$ as a function of electron energy $E$ in kinked NWs with bend angles 30°, 45° and 60° when there is only one period, i.e. $p=1$. A transmission gap is obtained when the bend angle is 30° because of anti-resonance of electron wave at bend areas. When the bend angle in kinked NW becomes large, the electron transmission probability decreases rapidly since more wave function is reflected back due to stronger interference. Figures 4(b)–(d) respectively show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential $\mu$ for different bend angles.

![Figure 3](image.png)

Figure 3. (a) Total transmission probability versus electron energy $E$ in bent NW for different inter-bend length $h$ when $\theta=80^\circ$. (b) Electrical conductance, (c) Seebeck coefficient and (d) power factor versus chemical potential $\mu$ in bent NW for different inter-bend length $h$ when $\theta=80^\circ$. The variation of the transmission probability and the sign change of the Seebeck coefficient due to the geometric interference obtained above are similar to the TE transport in molecules [34–36], which is largely determined by the electronic structure of the molecule. Similar behavior can also be found for other NWs studied in this paper.
angles when \( p = 1 \). Figure 4(b) shows that the electrical conductance has a similar gap as transmission probability showed in figure 4(a). In figure 4(c), we find a sign change of the Seebeck coefficient in kinked NW. The largest \( |S|_{\text{max}} \) of 160 μV K\(^{-1}\) is obtained when the bend angle is 60° in comparison with 30° and 45°. However, the power factor shown in figure 4(d) is not a large value around \( \mu = 0.06 \) eV and \( \theta = 60° \) even though the corresponding Seebeck coefficient is maximized. The maximum power factor reaches 1 \( k_B^2/\hbar \) when bend angle is 30° at \( \mu = 0.11 \) eV.

Figure 5(a) shows the transmission probability \( T_{\text{tot}} \) plotted as a function of electron energy \( E \) in kinked NWs for different \( p \) with fixed bend angle \( \theta = 45° \). Figure 5(a) shows that a larger \( p \) leads to more transmission gaps. As \( p \) increases, the transmission gaps become deeper and fine structures of transmission probability appear. When \( E = 0.08 \) eV, there is a major transmission gap for all three cases. Figures 5(b)–(d) respectively show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential \( \mu \) for different \( p \) with bend angle 45°. Figure 5(b) shows that there are minimum electrical conductance when \( \mu \sim 0.08 \) eV for all three cases. This is a consequence of transmission gaps near \( E \sim 0.08 \) eV as shown in figure 5(a). In figure 5(c), when \( p \) increases, \( |S|_{\text{max}} \) is enhanced remarkably when \( p > 1 \) because of the fine structures of the transmission probability. \( |S|_{\text{max}} \) reaches 600 μV K\(^{-1}\) when \( \mu \sim 0.08 \) eV. There are multiple peaks of power factor as shown in figure 5(d) due to the fine structures of the transmission probability. It is found that the power factor is not maximized.
even though the Seebeck coefficient reaches maximum values when $\mu = 0.08$ eV. This is mainly because the electrical conductance decreases. After all, kinked structure enables us to obtain a large absolute Seebeck coefficient with reasonable large power factor.

### 3.3. Stubbed NWs

Figure 1(c) shows the schematics of a stubbed NW. The height of stub is $h$ and the width is $W$, which is the same as the width of NW.

Figure 6(a) shows the transmission probability $T_{\text{tot}}$ plotted versus electron energy $E$ in stubbed NWs for different $h$, which demonstrates resonant behavior. Moreover, the existence of transmission gaps means that incident electrons with certain energy can be reflected back due to the anti-resonance occurring due to the stub. When the height increases, the number of transmission gaps increases since more anti-resonance modes appear: there are two transmission gaps when $h=5a$, three transmission gaps when $h=9a$ and four transmission gaps when $h=14a$. Figures 6(b)–(d) respectively show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential $\mu$ for different heights of stub $h$. Figure 6(b) shows the gaps of conductance when the chemical potential approaches the transmission gap. The larger $h$ is, the more gaps appear. In figure 6(c), two extremes of the Seebeck coefficient are obtained when chemical potential is close to the edge of the

![Figure 5](image_url)
transmission gap. The positions of the extremes of the Seebeck coefficient are symmetric to the center of the transmission gap. The peak of the positive Seebeck coefficient at low energy is close to the lower edge of the transmission gap. The gap of the negative Seebeck coefficient at high energy is close to the upper edge of the transmission gap. $|S|_{\text{max}}$ is larger than $140 \mu V K^{-1}$ when $h=5a$. With increasing $h$, more peaks and gaps of the Seebeck coefficient that corresponds to the transmission gap can be obtained: there are two peaks and gaps when $h=5a$, three peaks and gaps when $h=9a$, and four peaks and gaps when $h=14a$. In figure 4(d), the peaks of the power factor could be larger than $1k^2_F/\hbar$. Each peak is related to an extreme of the Seebeck coefficient. It is not surprising that more peaks show up when $h$ is 9a and 14a because of the existence of more anti-resonance modes.

### 3.4. Superlatticed NWs with periodic potential modulations

There has been great interest in growing superlatticed NWs for TE applications. For example, NWs with multiple heterostructures have been synthesized in Bi$_2$Te$_3$ based materials [37–39]. Wu et al fabricated Si/SiGe superlatticed NWs [30]. Theoretically, Lin and Dresselhaus [21] have calculated the diffusive TE transport properties of superlatticed NW using the Boltzmann transport equation. TE transport properties in NWs with several quantum dots serially embedded have been studied in the Coulomb blockade regime [40–42]. The Coulomb
interaction was found to be important. Here, we study the ballistic TE transport in superlatticed NWs that differs from the above theoretical studies. We focus on the transmission gap induced by Bragg reflection when the propagating wavelength of electron and the period length of NW satisfy Bragg’s law. Figure 1(d) shows the schematics of a superlatticed NW along the $x$-direction while the $y$-direction is confined by hard walls. The superlatticed NW is modulated by a periodic potential, which can be written as $V(x)$:

$$V(x) = \begin{cases} u, & n(A + B) \leq x < A + n(A + B) \\ 0, & A + n(A + B) \leq x < (n + 1)(A + B) \end{cases},$$

where $n = 0, 1, 2 \ldots N$. $N$ is the number of periods of modulation, $u$ is the height of potential barrier, $A$ is the width of the potential barrier and $B$ is the distance between two adjacent potential barriers. The total length of NW along the $x$-direction is denoted as $N(A + B)$.

Figure 7(a) shows the total transmission probability $T_{\text{tot}}$ as a function of electron energy $E$ in superlatticed NWs with different numbers of potential barriers when $A = B = 5a$ and $u = 0.01$ eV. The transmission probability exhibits a gap near $E \sim 0.07$ eV. An increasing number of potential barriers (larger $N$) leads to a deeper transmission gap. This effect comes from the well-known Bragg scattering in periodic potential [43]. Larger $N$ implies stronger Bragg scattering. Figures 7(b)–(d) respectively show the electrical conductance, the Seebeck coefficient.
coe\textit{f}cient and the power factor as a function of chemical potential $\mu$ for different numbers of potential barriers when $A = B = 5a$ and $u = 0.01$ eV. Figure 7(b) shows that the electrical conductance decreases drastically when the chemical potential gets closer to the transmission gap. Therefore, there is a conductance gap that corresponds to the transmission gap for all three cases. Figure 7(c) shows that there are two extremes of the Seebeck coefficient when the chemical potential is close to the transmission gap, one extreme is positive when chemical potential is smaller than the energy of transmission gap and the other is negative when the chemical potential is larger than the energy of transmission gap. $|S|_{\text{max}}$ becomes larger as $N$ increases, since the gap of transmission probability becomes deeper. $|S|_{\text{max}}$ reaches a maximum 250 $\mu$V K$^{-1}$ when $N = 20$. At the same time, the peak values of power factor become larger with $N$ increasing as shown in figure 7(d). The largest power factor could reach $1.8 k_B^2/\hbar$.

Figure 8(a) shows the total transmission probability $T_{\text{tot}}$ plotted as a function of electron energy $E$ in superlatticed NWs with different widths of potential barriers when $N = 20$ and $u = 0.01$ eV. The transmission gap shifts from $E \sim 0.08$ eV to 0.068 eV and 0.06 eV when the width of potential barrier increases from $A = B = 4a$ to $5a$ and $6a$, respectively. This is analogous to the shift of band gap due to the energy band theory. Figures 8(b)–(d) respectively show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential $\mu$. In figure 8(b), the gap of electrical conductance shifts along with the transmission gap.
In Figure 8(c), the chemical potential corresponding to extreme values shifts to lower energy with increasing width of the potential barriers. \(|S|_{\text{max}} \) is as large as 250 \(\mu V\) K\(^{-1}\). The peaks of power factors shift to lower chemical potentials while the peak values change little, as shown in Figure 8(d).

Figure 9(a) shows the total transmission probability \(T_{\text{tot}}\) plotted as a function of electron energy \(E\) in superlatticed NWs with different heights of potential barriers when \(N=20\) and \(A=B=5a\). The width of transmission gap increases with increasing barrier height because of stronger modulation effect. Figures 9(b)–(d) respectively show the electrical conductance, the Seebeck coefficient and the power factor as a function of chemical potential \(\mu\). The gap of electrical conductance shown in figure 9(b) becomes wider when \(u\) increases, due to the widening transmission gap as shown in figure 9(a). Figure 9(c) shows that \(|S|_{\text{max}}\) increases as \(u\) increases. When \(u=0.005\) eV, \(|S|_{\text{max}}\) is about 100 \(\mu V\) K\(^{-1}\), when \(u=0.01\) eV, \(|S|_{\text{max}}\) increases to about 300 \(\mu V\) K\(^{-1}\) and when \(u=0.015\) eV, \(|S|_{\text{max}}\) is about 400 \(\mu V\) K\(^{-1}\). This is because the edge of the transmission gap grows steeper with increasing \(u\). Figure 9(d) shows the properties of the power factor for different \(u\). When \(u=0.005\) eV, the maximum value of the power factor is about 1.10 \(k_{B}^{2}/h\) at \(\mu=0.06\) eV with the positive Seebeck coefficient (100 \(\mu V\) K\(^{-1}\)), and reaches 1.14 \(k_{B}^{2}/h\) at \(\mu=0.067\) eV with the negative Seebeck coefficient (–98 \(\mu V\) K\(^{-1}\)). The largest power factors exist when \(u=0.01\) eV rather than \(u=0.015\) eV, even though the Seebeck coefficient for the latter case is much larger than the former one. This is because when the energy gap in
transmission probability becomes wide enough, the reduction of electrical conductance is more significant than the increase of Seebeck coefficient.

4. Conclusion

We have investigated the TE transport properties of structured NWs in the ballistic regime with special geometries such as bent, kinked, stubbed and superlatticed NWs by using the Green’s function method and the Landauer–Büttiker formula. In these structured NWs, one can tune the sign and the amplitude of Seebeck coefficient by controlling the structure parameters such as bend angle, inter-bend length, stub height and potential barrier height. A large Seebeck coefficient and power factor can be obtained in these structured NWs by utilizing the transmission gap induced by geometry-related quantum interference of electron wave. Our study provides a promising way to design nanoscale TE devices with the same type of material in which both positive and negative Seebeck coefficients can be obtained, which differs from the traditional TE devices that consist of both p-type and n-type materials.

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References

[1] DiSalvo F J 1999 Thermoelectric cooling and power generation Science 285 703–6
[2] Bell L E 2008 Cooling, heating, generating power, and recovering waste heat with thermoelectric systems Science 321 1457–61
[3] Snyder G J and Toberer E S 2008 Complex thermoelectric materials Nat. Mater. 7 105–14
[4] Nolas G S, Morelli D T and Tritt T M 1999 Skutterudites: a phonon-glass-electron crystal approach to advanced thermoelectric energy conversion applications Annu. Rev. Mater. Sci. 29 89–116
[5] Kim R, Datta S and Lundstrom M S 2009 Influence of dimensionality on thermoelectric device performance J. Appl. Phys. 105 034506
[6] Dresselhaus M S et al 2007 New directions for low-dimensional thermoelectric materials Adv. Mater. 19 1043–53
[7] Zhou J and Yang R G 2011 Ballistic thermoelectricity in double-bend nanowires Appl. Phys. Lett. 98 173107
[8] Boukai A I et al 2008 Silicon nanowires as efficient thermoelectric materials Nature (London) 451 168–71
[9] Hochbaum A I et al 2008 Enhanced thermoelectric performance of rough silicon nanowires Nature (London) 451 163–7
[10] Whitlow L W and Hirano T 1995 Superlattice applications to thermoelectricity J. Appl. Phys. 78 5460–6
[11] Broido D A and Reinecke T L 2000 Thermoelectric power factor in superlattice systems Appl. Phys. Lett. 77 705–7
[12] Hicks L D and Dresselhaus M S 1993 Effect of quantum-well structures on the thermoelectric figure of merit Phys. Rev. B 47 12727–31
[13] Hicks L D and Dresselhaus M S 1993 Thermoelectric figure of merit of a one-dimensional conductor Phys. Rev. B 47 16631–4
[14] Poudel B et al 2008 High-thermoelectric performance of nanostructured bismuth antimony telluride bulk alloys Science 320 634–8
[15] Vineis C J, Shakouri A, Majumdar A and Kanatzidis M G 2010 Nanostructured thermoelectric: big efficiency gains from small features Adv. Mater. 22 3970–80
[16] Zhang G Q, Yu Q X, Wang W and Li X G 2010 Nanostructures for thermoelectric applications: synthesis, growth mechanism, and property studies Adv. Mater. 22 1959–62
[17] Harman T C, Taylor P J, Spears D L and Walsh M P 2000 Thermoelectric quantum-dot superlattices with high ZT J. Elec. Mater. 29 L1–2
[18] Zhou J, Li X B, Chen G and Yang R G 2010 Semiclassical model for thermoelectric transport in nanocomposites Phys. Rev. B 82 115308
[19] Tian B Z et al 2009 Single-crystalline silicon antimony telluride superlattices Nat. Nanotechnology 4 824–9
[20] Jiang J W, Yang N, Wang B S and Rabczuk T 2013 Modulation of thermal conductivity in kinked silicon nanowires: phonon interchanging and pinching effects Nano Lett. 13 1670–4
[21] Lin Y M and Dresselhaus M S 2003 Thermoelectric properties of superlattice nanowires Phys. Rev. B 68 075304
[22] Yang N, Zhang G and Li B W 2008 Ultra-low thermal conductivity of isotope-doped silicon nanowires Nano Lett. 8 276–80
[23] Hu M and Poulikakos D 2012 Si/Ge superlattice nanowires with ultralow thermal conductivity Nano Lett. 12 5487–94
[24] Shi L H, Jiang J W, Zhang G and Li B W 2012 High thermoelectric figure of merit in silicon–germanium superlattice structured nanowires Appl. Phys. Lett. 101 233114
[25] Datta S 1992 Electronic Transport in Mesoscopic Systems (Cambridge: Cambridge University Press)
[26] Zianni X 2010 Diameter-modulated nanowires as candidates for high thermoelectric energy conversion efficiency Appl. Phys. Lett. 97 233106
[27] Zianni X 2011 Efficient thermoelectric energy conversion on quasi-localized electron states in diameter modulated nanowires Nanoscale Res. Lett. 6 286
[28] Wu P M et al 2013 Large thermoelectric power factor enhancement observed in InAs nanowires Nano Lett. 13 4080
[29] Smith C G et al 1990 One dimensional electron tunneling and related phenomena Surf. Sci. 228 387–92
[30] Wu Y, Fan R and Yang P 2002 Block-to-block growth of single-crystalline Si/SiGe superlattice nanowires Nano Lett. 2 83–6
[31] Ferry D K and Goodnick S M 1997 Transport in Nanostructures (Cambridge: Cambridge University Press)
[32] Büttiker M 1986 Four-terminal phase-coherent conductance Phys. Rev. Lett. 57 1761–4
[33] Proetto C R 1991 Thermopower oscillations of a quantum-point contact Phys. Rev. B 44 9096–9
[34] Reddy P, Jang S, Segalman R A and Majumdar A 2007 Thermoelectricity in molecular junctions Science 315 1568–71
[35] Paulsson S and Datta S 2003 Thermoelectric effect in molecular electronics Phys. Rev. B 67 241403
[36] Dubi Y and Di Ventra M 2011 Colloquium: heat flow and thermoelectricity in atomic and molecular junctions Rev. Mod. Phys. 83 131–55
[37] Wang W, Lu X, Zhang T, Zhang G, Jiang W and Li X 2007 Bi2Te3/Te multiple heterostructure nanowire arrays formed by confined precipitation J. Am. Chem. Soc. 129 6702
[38] Zhang G, Fang H, Yang H, Jauregui L, Chen Y and Wu Y 2012 Design principle of telluride-based nanowire heterostructures for potential thermoelectric applications Nano Lett. 12 3627
[39] Fang H, Feng T, Yang H, Ruan X and Wu Y 2013 Synthesis and thermoelectric properties of compositional-modulated lead telluride bismuth telluride nanowire heterostructures Nano Lett. 13 2058

[40] Kuo D 2011 Thermoelectric properties of double quantum dots embedded in a nanowire Japan J. Appl. Phys. 50 025003

[41] Kuo D and Chang Y 2013 Thermoelectric properties of a chain of coupled quantum dots embedded in a nanowire J. Vac. Sci. Technol. B 31 04D108

[42] Tseng Y, Kuo D, Chang Y and Lin T 2013 Heat rectification effect of serially coupled quantum dots Appl. Phys. Lett. 103 053108

[43] Zhou J, Shi Q W and Wu M W 2004 Spin-dependent transport in lateral periodic magnetic modulations: scheme for spin filters Appl. Phys. Lett. 84 365–7