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Influence of electron scatterings on thermoelectric effect

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In this work, we employed non-equilibrium Green's function to investigate the electron transport properties in a nanowire in the presence of scatterings. The scattering mechanism is modelled by the Büttiker probe. The effect of electron scattering is analyzed under three conditions: absence of external field; with a bias voltage; and with a finite temperature difference. It is found that weak and strong scattering strengths affect the electron transport in different ways. In the case of weak scattering strength, electron trapping increases the electron density, thereby boosting the conductance significantly. Although the increment in conductance would reduce the Seebeck coefficient slightly, the power factor still increases. In the case of strong scattering strength, electron diffraction causes the redistribution of electrons; accumulation of electrons at the ends of the wire blocks current flow; hence the conductance is reduced significantly. Although the Seebeck coefficient increases slightly, the power factor still decreases. The power factor is enhanced by 6% – 18%, at the optimum scattering strength. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4740235>]

I. INTRODUCTION

The thermoelectric (TE) device is a type of green energy device which has the potential to be widely used in near future. Since 1821, when the thermoelectric property of materials was first discovered by Seebeck, the development of TE material has been ongoing for almost two centuries,¹⁶ the energy conversion efficiency of current TE device is too low to be put into practice, and this problem has attracted much attention.^{1–7} The efficiency of a TE device is indicated by the dimensionless TE figure of merit (ZT), determined by the expression $S^2\sigma T/\kappa$ using its parameters Seebeck coefficient S , electric conductivity σ , thermal conductivity κ ($= \kappa_e + \kappa_{ph}$, contributed by electrons and phonons), and the temperature T . Among these parameters, S , σ , and κ_e are related to the electron transport and κ_{ph} is related to the phonon transport. Therefore, the strategies of developing high ZT device are improving the electronic TE efficiency and reducing the lattice thermal conductivity.¹⁵ Currently, most of the efforts are put in to reduce the lattice thermal conductivity by investigation the phonon transport, which can be found in our previous works.^{11–14} However, more attentions need to be paid on the electron transport, as the electronic TE efficiency limits the performance of TE device significantly.¹⁵ The best TE device has a Dirac delta shaped electron transmission function.⁸ Besides the TE efficiency, the power factor ($S^2\sigma$), related to the power rating, is another important index of TE device.

In nano-scaled device, electron transport becomes ballistic inside the channel, and the energy dissipation of electrons occurs in the contacts only. However, electron scatterings still take place for the reason of defects, grain boundaries, phonons, and charges in the device. It affects the transport properties of electron, hence further influences the TE effect.

A previous work has studied the effect of nano-particle scattering on TE power factor.⁹ It is found that the concentration of electron is usually higher in the sample with nano-particles, implying the Seebeck coefficient is usually unchanged and conductivity is increased at the optimum of the power factor. That work is based on low nano-particle concentration, and that work gave rise to our interest in the problem of the electron scattering strength on TE effect.

The non-equilibrium Green's function (NEGF) is a well developed tool to model the electron transport in nano-scaled device. To include the scattering effect in NEGF, the concept of the Büttiker probe is introduced. The Büttiker probe is a virtual probe, which extract and inject electrons, mimicking the electron scattering mechanism. So far, there are two options to handle the Büttiker probe in NEGF. The first option^{10,17,18} assumes that the Fermi level in the probe is well defined. It can be either position dependent only or both position and energy dependent, which is corresponding to the momentum relaxation or energy relaxation scattering process. The Fermi level is determined so that zero net current of the probe is achieved. The second option^{19–21} left the Fermi level undefined and express the scattering terms based on the Green's function (either the entire or the diagonal of the Green's function matrix, corresponding to the dephasing or the momentum relaxation scattering process). Therefore, a self-consistent procedure is required to determine the Green's function, and further development for this option is urged in order to handle the energy relaxation scattering process.

In this work, we employed NEGF method to investigate the electron transport properties in the nanowire in the presence of electron scatterings. We believe the energy exchange in the scattering mechanisms (such as electron-phonon and electron-impurity) is crucial at the scattering points, therefore the energy relaxation model in the first option for Büttiker probe is chosen. To reduce the computation time, only one or two scattering points are inserted in the nanowire.¹⁸ In the

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final analysis, the device is analysed and discussed under three different conditions with wide range of scattering strength: absence of external field, under a bias voltage, and a finite temperature difference.

II. THEORY

A silicon nanowire with square cross-sectional shape coupled by two contacts, which served as thermal and electric reservoirs, is considered as shown in Fig. 1. The wire is composed of several slices with the thickness (a_z) 0.3 nm parallel to the contact interface. For the slice at position z , the effective potential is given by

$$E_{n_1, n_2}(z) = \frac{\hbar^2 \pi^2}{2} \left[\frac{1}{m_x^*} \left(\frac{n_1}{l_x} \right)^2 + \frac{1}{m_y^*} \left(\frac{n_2}{l_y} \right)^2 \right] + V(z). \quad (1)$$

The variables $n_{1,2}$ is the quantum number for the energy in transverse direction; $l_{x,y}$ the side length of the cross-section (set to 5 nm in the computation); $V(z)$ the electric potential energy; m^* the effective mass of silicon; and $\hbar$ the Dirac constant. The Hamiltonian of the wire for the mode, denoted by the subscript (n_1, n_2) , is constructed as follows:

$$H = \begin{bmatrix} E_{n_1, n_2}(1) + 2t_z & -t_z & 0 & \dots \\ -t_z & E_{n_1, n_2}(2) + 2t_z & -t_z & \dots \\ 0 & -t_z & \ddots & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \quad (2)$$

where t_z is the coupling energy between two slices determined by the expression $\hbar^2/(2m_z^* a_z^2)$, which is about 461 meV in this model.

To reveal the effect of the electron scattering, the scattering points modelled by Büttiker probes are inserted into the wire. At a scattering point, the slice of the wire is coupled to the Büttiker probe with the coupling strength (U), as shown in Fig. 1. The coupling strength determines the electron scatterings strength. For the convenience in discussion, we define the scattering factor α , the relative scattering was respected to the coupling strength between two slices. Hence $U = \alpha \cdot t_z$, and α equal to 0.056 is equivalent to the thermal energy at 300 K, which is about 26 meV.

All the contacts in the system, including both virtual contacts (Büttiker probes) and two real contacts, are labeled by index i . The self-energy due to the contact i is given by

FIG. 1. The schematic of the modelled system: a nanowire coupled by two contacts at both ends, a scattering point denoted by the square box is coupled to the Büttiker probe through a virtual contact.

$$\Sigma_i(E) = U^2 \cdot \frac{-e^{i k_i(E) \cdot a_z}}{t_z \cdot a_z}, \quad (3)$$

where $k_i(E)$ is the longitudinal wave vector determined by

$$k_i(E) = \sqrt{\frac{2m_z^*}{\hbar^2} [E - E_{n_1, n_2}(z)]}. \quad (4)$$

The broadening function of the contact i is then obtained from its self-energy

$$\Gamma_i(E) = -2 \text{Im} [\Sigma_i(E)]. \quad (5)$$

The total self-energy of the wire Σ is the sum of the contribution from each contact. The retarded and advanced Green's function of the wire, G^R and G^A , are then determined by

$$G^R(E) = [E + i\epsilon - H - \Sigma(E)]^{-1}, \quad (6)$$

$$G^A(E) = [G^R(E)]^\dagger, \quad (7)$$

where ϵ is an infinitesimal positive number. With that, the electron transmission function between contact i and contact j is given by

$$T_{ij}(E) = \text{Tr} [\Gamma_i G^R \Gamma_j G^A]. \quad (8)$$

The electric current of contact i is determined by the Landauer-Büttiker formula

$$I_i = \frac{2e}{h} \int dE \sum_{j \neq i} T_{ij} \cdot (f_i - f_j), \quad (9)$$

where f_i is the Fermi-Dirac distribution at contact i with the Fermi level $E_{f,i}$, defined by

$$f_i = [e^{\frac{E - E_{f,i}}{k_B T}} + 1]^{-1}. \quad (10)$$

To fulfill the charge conservation, the net current of each Büttiker probe is set to zero by adjusting the Fermi levels of Büttiker probes using Jacobian method, (linear change in temperature is assumed in the wire). The Fermi levels in the left and right contacts are determined by assuming all donors are ionized, and the donor concentration 10^{18} cm^{-3} is used in the computation. The number of electrons in each slice of the wire are obtained from the diagonal elements of n , determined by the following expression:

$$n = \frac{1}{\pi} \int dE \sum_i f(E, E_{f,i}) G^R \Gamma_i G^A. \quad (11)$$

The potential energy $V(z)$ for each slice is updated by the Poisson equation using the electron density determined by the above formula, and the final status of the system is obtained after the self-consistent iteration process.

III. DISCUSSION

In the following, the system at room temperature under three conditions: (A) absence of external field, (B) with a

FIG. 2. The electron density in a nanowire with the length 18 nm, two scattering points are inserted at $z = 6$ nm and $z = 12$ nm, (a) is for the weak scattering strength region and (b) is for the strong scattering strength region. α is the relative scattering strength.

bias voltage, and (C) with a finite temperature difference, are discussed.

A. Absence of external field: Electron trapping and diffraction

In this section, the length of the nanowire is set to 18 nm, and two scattering points are inserted at the positions of $z = 6$ nm and $z = 12$ nm. With the absence of external

field, i.e., both temperatures and voltages at the two contacts are equal, the electron charge density along the wire determined by Green's function is shown in Fig. 2, in which the scattering points are denoted by "SP1" and "SP2." In the case of ballistic transport ($\alpha = 0$), electron scattering only occurs at the contact interfaces, but not in the wire. For this reason, electrons are accumulated at both ends of the wire, this incurs the repulsion of electron as the result of the Coulomb force. Therefore, a fluctuation of electron density is observed in the wire, as shown by the "Ballistic" curve in Fig. 2(a). When the scattering strength gets slightly stronger ($\alpha < 0.1$), the electron wave function in the wire is reconstructed due to the perturbation of the scattering points, but this effect is not significant. Electron scattering occurs when electron collides with the scattering points, and electrons are accumulated in the wire. Fig. 2(a) shows the stronger the scattering strength, the more electrons are trapped inside the wire, especially near the scattering points in the weak scattering strength region ($\alpha < 0.1$). This result is consistent with the previous work.⁹ However, in the strong scattering strength region, this effect vanished. This is because the electron wave function is significantly modified by the scattering points. The probability of finding an electron near the scattering points becomes much smaller, therefore the electron density near scattering points reduces (Fig. 2(b)), the chance of electron scatterings decreases. This phenomenon is known as the electron diffraction; electrons prefer avoiding the scattering points than being scattered.

B. A bias voltage

In the following, we discussed a 9 nm nanowire at room temperature in the presence of a bias voltage with a single scattering point located at the center of the wire. In the case of ballistic transport ($\alpha = 0$), due to the external field, the electron density tilts towards one end of the wire, as shown in Fig. 3(a). With slight increases in the scattering strength, more electrons are accumulated in the wire, especially near the

FIG. 3. A 9 nm nanowire with the presence of bias voltage ΔV , (a) the electron density and (b) the electric current in weak scattering strength region; (c) the electron density and (d) the electric current in strong scattering strength region. α is the relative scattering strength.

FIG. 4. A 9 nm nanowire with various bias voltages, the electric current is plotted with respect to the relative scattering strength α .

scattering point. This is consistent with the discussion in Sec. III A. With the bias voltage, the increment in electron density is conducive to boost the electric current as shown by Fig. 3(b). However, in strong scattering strength region, electrons bypass the scattering point by reconstructing their wave functions. This leads to the accumulation of electrons near the contact interfaces (Fig. 3(c)), which block current flow. So, a decrease in electric current is expected (see Fig. 3(d)).

With different bias voltages, the electric current with respect to the scattering strength shows a similar profile: a rise followed by a drop (Fig. 4). Also, the scattering strength at which the maximum current occurs, increases with the bias voltage. This phenomenon can be understood in the following way. The electrons are trapped in the wire in the weak scattering strength region. With the increase in the bias voltage, these electrons can be accelerated and contribute to the electric current. Higher bias voltage has stronger power in accelerating electron, therefore the scattering strength at which the maximum current occurs is increasing with the bias voltage. With sufficiently large scattering strength, the

diffraction of electron causes the accumulation of electrons at both ends of the wire, which blocks the electric current.

C. A finite temperature difference

To discuss the TE effect, a 9 nm nanowire under a temperature difference with single scattering point at the center is considered. The temperature difference is split into half and applied to the contacts, i.e., $T_L = T + \Delta T/2$ and $T_R = T - \Delta T/2$. In general, the TE effect is evaluated in the open circuit condition. Therefore, the net current is zero. For this reason, to offset the current produced by the temperature difference, an electric field is generated. The ratio of the voltage difference over the temperature difference gives the Seebeck coefficient. To determine the conductance of the wire in the presence of temperature difference, a testing current (a small current) is injected into the wire. From the change of the voltage difference, the conductance is obtained.

In the weak scattering strength region ($\alpha < 0.1$), Seebeck coefficient is smaller with stronger scattering. That is because the electric conductance increases (Fig. 5(b)), and a smaller electric field is sufficient to offset the current produced by temperature difference for the case of larger conductance. Similarly, in the strong scattering strength region, the Seebeck coefficient increases as a result of the decrease in the electric conductance, as shown in Figs. 5(c) and 5(d).

In Fig. 5(b), the conductance increases with the temperature difference, and starts to decrease after the critical point of temperature difference, also this point increases with the scattering strength. This is because, when temperature difference is small, the increment in temperature difference tends to inject more electrons into the wire; these electrons are trapped easily by the scattering point, which leads a higher electron density and a larger conductance. When the temperature difference is more than the critical value, more electrons are injected than the wire could conduct, which causes the redistribution of electrons, which limits current flow. Due to this effect on conductance, the Seebeck coefficient

FIG. 5. A 9 nm nanowire with temperature difference ΔT , (a) Seebeck coefficient and (b) electric conductance in weak scattering strength region; (c) Seebeck coefficient and (d) electric conductance in strong scattering strength region. α is the relative scattering strength.

FIG. 6. A 9 nm nanowire with temperature difference ΔT , the thermoelectric power factor is plotted with respect to the relative scattering strength α with (a) small temperature difference and (b) large temperature difference.

decreases at first and starts to increase after the critical point (Fig. 5(a)). In the strong scattering strength region, the fluctuations in conductance and Seebeck coefficient are not as much as that in weak scattering strength region. This is because the chance of electron scatterings is reduced due to the effect of electron diffraction and the number of electrons trapped in the wire is smaller than the case of weak scattering strength.

Fig. 6 shows the TE power factors with the change of scattering strength. The power factor has maximum value at about $\alpha = 0.1$, and it drops dramatically after that. The explanation of the change in power factor can be ascribed to the change in the conductance and Seebeck coefficient. At the optimum power factor ($\alpha = 0.1$), comparing to the ballistic case, for ΔT equals to 0 K, 20 K, and 50 K, the Seebeck coefficient drops by 8%, 13%, and 11% (Fig. 5(a)); but the conductance increases by 25%, 57%, and 35% (Fig. 5(b)), therefore the power factor is increased by 6%, 18%, and 7%, respectively. Due to the shifting of the critical point of temperature difference mentioned in previous paragraph, the power factor has the maximum enhancement when the temperature difference is about 20 K.

IV. CONCLUSION

Weak and strong scatterings strengths affect the electron transport in different manners. In the case of weak scattering strength, electron trapping increases the electron density and boosts the conductance significantly. The increment in conductance would reduce the Seebeck coefficient slightly, but overall the power factor increases. In the case of strong scattering strength, electron diffraction causes the redistribution of electrons, accumulation of electrons at the ends of the

wire block current flow, hence the conductance is suppressed significantly. Due to this effect, the Seebeck coefficient increases slightly, but the power factor decreases severely.

- ¹F. J. DiSalvo, *Science* **285**, 703 (1999).
- ²R. Venkatasubramanian, E. Siivola, T. Colpitts, and B. O'Quinn, *Nature* **413**, 597 (2001).
- ³T. C. Harman, P. J. Taylor, M. P. Walsh, and B. E. LaForge, *Science* **297**, 2229 (2002).
- ⁴K. F. Hsu, S. Loo, F. Guo, W. Chen, J. S. Dyck, C. Uher, T. Hogan, E. K. Polychroniadis, and M. G. Kanatzidis, *Science* **303**, 818 (2004).
- ⁵A. I. Hochbaum, R. Chen, R. D. Delgado, W. Liang, E. C. Garnett, M. Najarian, A. Majumdar, and P. Yang, *Nature* **451**, 163 (2008).
- ⁶A. I. Boukai, Y. Bunimovich, J. Tahir-Kheli, J.-K. Yu, W. A. Goddard III, and J. R. Heath, *Nature* **451**, 168 (2008).
- ⁷S. Volz, A. Shakouri, and M. Zebargadi, *Thermal Nanosystems and Nanomaterials* (Springer, Berlin/Heidelberg, 2009), Vol. 118, pp. 225.
- ⁸G. D. Mahan and J. O. Sofo, *Proc. Natl. Acad. Sci. U.S.A.* **93**, 7436 (1996).
- ⁹M. Zebargadi, K. Esfarjani, A. Shakouri, J.-H. Bahk, Z. Bian, G. Zeng, J. Bowers, H. Lu, J. Zide, and A. Gossard, *Appl. Phys. Lett.* **94**, 202105 (2009).
- ¹⁰R. Venugopal, M. Paulsson, S. Goasguen, S. Datta, and M. S. Lundstrom, *J. Appl. Phys.* **93**, 5613 (2003).
- ¹¹J. Li, T. C. Au Yeung, C. H. Kam *et al.*, *J. Appl. Phys.* **106**, 054312 (2009).
- ¹²J. Li, T. C. Au Yeung, C. H. Kam *et al.*, *J. Appl. Phys.* **106**, 014308 (2009).
- ¹³J. Li, T. C. Au Yeung, and C. H. Kam, *J. Appl. Phys.* **111**, 094308 (2012).
- ¹⁴X. Zhao *et al.*, *J. Appl. Phys.* **107**, 094312 (2010).
- ¹⁵J. Li, T. C. Au Yeung, and C. H. Kam, *J. Phys. D: Appl. Phys.* **45**, 085102 (2012).
- ¹⁶A. Bulusu and D. G. Walker, *Superlattices Microstruct.* **44**, 1 (2008).
- ¹⁷S. Datta, *Quantum Transport: Atom to Transistor* (Cambridge University Press, New York, 2005), Sect. 9.4.
- ¹⁸J. Xiong, G. Wang, and W. Mathis, *Int. J. Circuit Theory Appl.* (2012), doi:10.1002/cta.1805.
- ¹⁹S. Datta, *Lessons From Nanoelectronics* (World Scientific, 2012), Sect. 19.4.
- ²⁰A. Bulusu and D. G. Walker, *J. Heat Transfer* **129**, 492 (2007).
- ²¹A. Bulusu and D. G. Walker, *J. Appl. Phys.* **102**, 073713 (2007).