Thermal Conductivity of Silicon Nanowire Using Landauer Approach for Thermoelectric Applications

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Abstract—The electronic and phononic band structure of silicon nanowires embedded in $SiGe_{0.3}$ is calculated and used to investigate its effect on the thermoelectric properties by Landauer approach. The contribution from elec-tron/hole on power factor and electronic thermal con-ductance is less than that from phonons on lattice ther-mal conductance.

Index Terms—Landauer Approach, Silicon Nanowire, Thermoelectric

I. Introduction

Thermoelectric (TE) energy conversion materials have been attracting attention for use in solid-state power generation devices. The dimensionless figure of merit (ZT) is the parameter used to indicate the performance of TE energy conversion materials. ZT is given by the equation:

$$ZT = \frac{S^2 \sigma T}{\kappa_{ph} + \kappa_{el}}, \tag{1}$$

where S is the Seebeck coefficient, σ the electrical conductivity, κ_{ph} the lattice thermal conductivity from phonon and κ_{el} the electronic thermal conductivity from electron. To achieve $ZT > 1$, the first is to reduce the lattice or electronic thermal conductivity in the denominator of Eq. (1) and the other is to enhance the power factor, $S^2\sigma$, in the numerator. These properties are determined by the details of the electronic and phonon structure with the scattering of charge carriers so that they are not independently controlled. Silicon (Si)-based nanostructure is one of attractive materials to realize low-cost TE devices. For example, Si nanowires (SiNWs) with a diameter of 50 nm have a much lower thermal conductivity of 1.6 W/mK than bulk Si (around 150 W/mK) [1].

In this paper, a high density array of silicon nanowires (SiNWs) with a 10-nm diameter embedded in matrix of $SiGe_{0.3}$ as shown in Fig. 1 is considered. We first calculate the electron band structure by solving the Schrödinger equation with Bloch theorem [2] and phonon energy dispersion by solving the Elastodynamic equation [3]. Then, the Landauer approach [4], which works in ballistic limit as well as quasi-ballistics and diffusive regimes, is used to investigate the quantum effect of nanostructure on the thermoelectric performance with different density of SiNWs by tuning space between SiNWs.

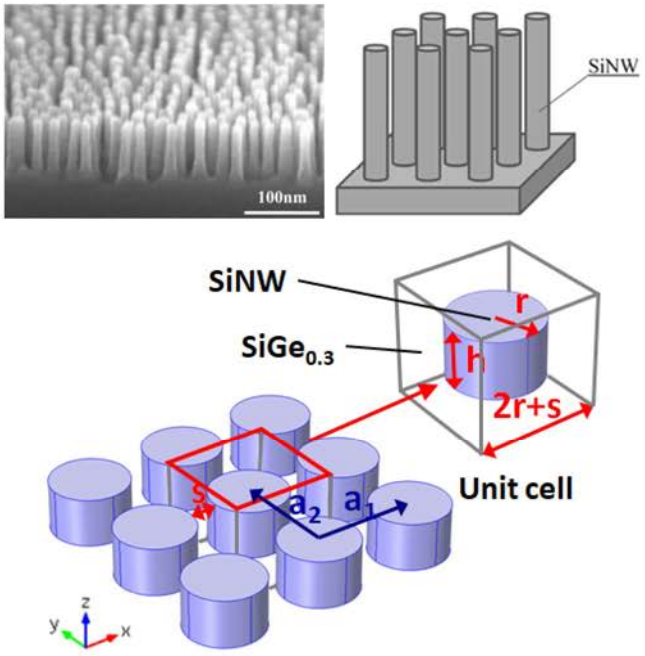

Fig. 1. A high-density array of SiNWs with a 10-nm diameter in SEM image is formed after neural beam etching using polyethylene glycol-modified ferritin as a mask, which is schematically illustrated as a square superlattice of SiNWs. The SiNWs is then embedded in $SiGe_{0.3}$ by thermal CVD techniques [5]. The SiNWs-$SiGe_{0.3}$ composite is simulated by a square superlattice with cuboid unit cell of radius r, height h and varied space s from 2 to 15 nm.

II. Modeling and Simulation Methodology

For the periodic SiNWs as shown in Fig. 1, the phonon energy dispersion is numerically solved by the elastodynamic wave equation as [6]

$$\nabla \cdot [\boldsymbol{C} \nabla u(\boldsymbol{r})] = -\rho \omega^2 u(\boldsymbol{r}), \tag{2}$$

where u is the displacement vector, ρ is the mass density, ω is the eigenfrequency and $\boldsymbol{C}$ is the elastic constant

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TABLE I
List of parameters used in the simulation of electronic band structure and phononic dispersion [8].

Materials	Electron mass (m_e)		Hole mass (m_e)		Bandgap
	m_l^*	m_t^*	m_{hh}^*	m_{lh}^*	eV
Si	0.98	0.19	0.49	0.16	1.12
$SiGe_{0.3}$	1.14	0.12	0.41	0.10	1.00

Materials	Elastic constants (GPa)		
	C_{11}	C_{12}	C_{44}
Si	165.8	63.9	79.6
$SiGe_{0.3}$	154.6	59.2	75.8

matrix which describes second-order strain energy density [3]. Here $\boldsymbol{C}$ is a 6×6 symmetric matrix that has 21 independent elements. Since the silicon have a cubic symmetry, the number of independent elastic constants reduced to three, C_{11}, C_{12}, and C_{44}.

On the other hand, the electron band structure is numerically solved by the Schrödinger equation with the effective mass approximation under the Bloch theorem [2] as

$$\nabla\left[-\frac{\hbar}{2m^*}\nabla u_{\boldsymbol{k}}(\boldsymbol{r})\right] - \frac{i\hbar}{m^*}\boldsymbol{k}\cdot\nabla u_{\boldsymbol{k}}(\boldsymbol{r}) + \left[V(\boldsymbol{r}) + \frac{\hbar^2 k^2}{2m^*}\right] u_{\boldsymbol{k}}(\boldsymbol{r}) = E_{n,k}u_{\boldsymbol{k}}(\boldsymbol{r}), \tag{3}$$

where $\hbar$, m^*, $V(\boldsymbol{r})$, $E_{n,k}$, $u_{\boldsymbol{k}}(\boldsymbol{r})$ are the reduced Plank's constant, the effective mass, the position-dependent potential energy, quantum energy levels, and the corresponding wave function respectively.

Since SiNW-$SiGe_{0.3}$ composite is modeled by a square superlattice with cuboid unit cell as Fig. 1, both Eq. (2) and Eq. (3) follow specific boundary conditions based on the periodicity. The displacement vector u in Eq. (2) satisfies the Floquet periodic condition, $u(\boldsymbol{r}) = u_{\boldsymbol{q}}\exp(\boldsymbol{q}\cdot\boldsymbol{r})$, at boundary of a unit cell [7]. Here $\boldsymbol{q}$ is a wave vector. Meanwhile, the wave function $u_{\boldsymbol{k}}$ in Eq. (3) satisfies the periodic condition, $u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = u_{\boldsymbol{k}}(\boldsymbol{r})$, where $\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$ is the lattice vector with integer n_1 and n_2. Thus, Both Eq. (2) and Eq. (3) are discretized within a unit cell formed by the primitive vectors ($\boldsymbol{a}_1$ and $\boldsymbol{a}_2$) and then solved by a finite element method (FEM) solver for each sampling q-point or k-point in the irreducible Brillouin zone. The parameters used to calculate the electron band structure and phonon energy dispersion are listed in Table I.

With the calculated electron band structure $E(\boldsymbol{k})$ from Eq. (3) and phonon energy dispersive relation $\omega(\boldsymbol{q})$ from Eq. (2), the Landauer approach [9], [10] is adopted to describe the electron and phonon transport in nanostructures and investigate the quantum effect of nanostructure on the thermoelectric performance [4] because of its physical insight in ballistic limit as well as quasi-ballistic and diffusive regimes. The transport coefficients for thermoelectricity in Eq. (1) are expressed as

$$\begin{aligned}
\sigma &= \int_{-\infty}^{\infty}\sigma'(E)dE \\
S &= \frac{k}{q\sigma}\int_{-\infty}^{\infty}(E-E_F)\,\sigma'(E)dE \\
\kappa_0 &= T\left(\frac{k}{q}\right)^2\int_{-\infty}^{\infty}(E-E_F)^2\,\sigma'(E)dE\text{'} \\
\kappa_{el} &= \kappa_0 - S^2\sigma T \\
\kappa_{ph} &= \int_{-\infty}^{\infty}\kappa'_{ph}(E)dE
\end{aligned} \tag{4}$$

where E_F is the Fermi level, σ' and κ'_{ph} are differential conductivity for electron and phonon, respectively. For bulk materials [11], [12]

$$\begin{aligned}
\sigma'(E) &= q^2\Sigma(E)\left(-\frac{\partial f_0}{\partial E}\right) \\
\kappa'_{ph}(E) &= \frac{E^2}{T}\Sigma_{ph}(E)\left(-\frac{\partial n_0}{\partial E}\right)
\end{aligned}, \tag{5}$$

where $\Sigma(E)$ and $\Sigma_{ph}(E)$ are are transport distribution functions for electron and pho-non respectively that depends on both band structure or phonon dispersion (the number of modes) and scattering (mean free path).

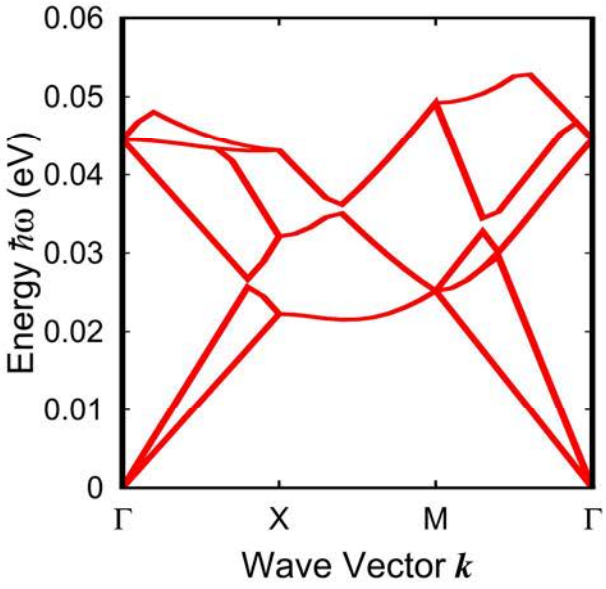

Fig. 2. Phonon Energy dispersion for bulk silicon along with the specific symmetric k-points.

III. Results and Discussion

Figure 2 shows the calculated phonon energy dispersion for bulk silicon using Eq. (2) and parameters in Table I. The result approximates the experimental data [3] well under the same order with only three independent elastic constants in Table I.

Figure 3 shows the calculated conductance as function of the Fermi level using Eq. (4). P-type SiNW has larger

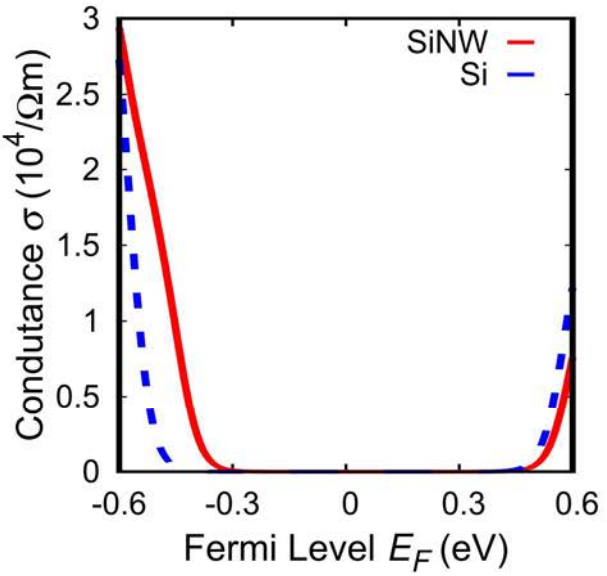

Fig. 3. Calculated conductance as function of the Fermi level for SiNW (solid red line) and bulk silicon (dash blue line).

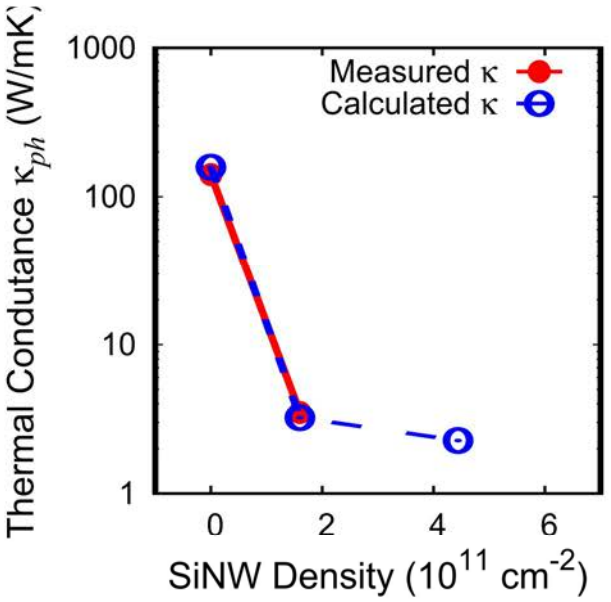

Fig. 4. Thermal conductance contributed from lattice dynamic for bulk silicon (zero SiNW density at x-axis) and SiNW-$SiGe_{0.3}$ superlattice from experiment (solid symols) [5] and simulation (open symols).

conductance than bulk p-type silicon since the $SiGe_{0.3}$ has lower bandgap energy than Si as list in Table I and more energy band offset between SiNW and $SiGe_{0.3}$ for hole that induces quantum confinement and higher tunneling probability. However, the energy band offset between SiNW and $SiGe_{0.3}$ for electron is small so that the difference to bulk silicon for the conductance is little.

Based on the Elastodynamic wave equation Eq. (2), the phonon energy dispersion for SiNW-$SiGe_{0.3}$ superlattice is also calculated and then used to simulate the lattice thermal conductivity by Eq. (4) and Eq. (5). Fig. 4 shows the lattice thermal conductivity with a comparison between bulk silicon (zero SiNW density at x-axis) and SiNW-$SiGe_{0.3}$ superlattice. The simulation shows reduction of thermal conductivity around almost two orders for SiNW-$SiGe_{0.3}$ superlattice as the experiment results [5].

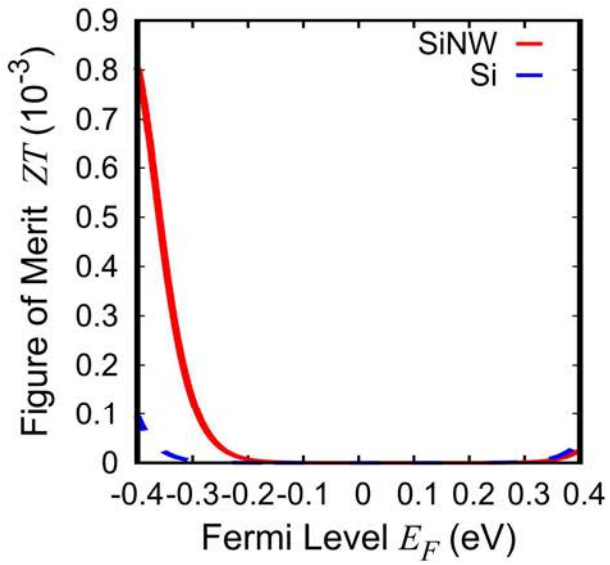

Fig. 5. ZT as function of the Fermi level for SiNW-$SiGe_{0.3}$ superlattice (solid red line) and bulk silicon (dash blue line).

Figure 5 shows the calculated ZT as function of the Fermi level with contribution of electronic and lattice thermal conductivity. The main difference comes from the lattice thermal conductivity so that the ZT can reach around 0.01 for SiNW-$SiGe_{0.3}$ superlattice (at the Fermi level around -0.4 eV) and ZT is in value of less than 10^{-4} for bulk silicon, which is also two order smaller than that SiNW-$SiGe_{0.3}$ superlattice as Fig. 4.

IV. Conclusion

In this paper, we take use of the Landauer approach to investigate the quantum effect on thermoelectric properties for SiNWs embedded in matrix of $SiGe_{0.3}$. The impact of SiNWs on thermoelectric from electron, such as power factor and electronic thermal conductance, is less than that that from phonon, which is consistent with the observation in the experiment.

Acknowledgment

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References

[1] A. I. Hochbaum, R. Chen, P. D. Delgado, W. Liang, E. C. Garnett, M. Najarian, A. Majumdar, and P. Yang, "Enhanced thermoelectric performance of rough silicon nanowires," Nature, vol. 451, pp. 163–167, 2008.

[2] M.-Y. Lee, Y. Li, and S. Samukawa, "Miniband calculation of three-dimensional nanostructure array for solar cell applications," IEEE Trans. Elec. Devices, vol. 62, pp. 3709–3714, 2015.

[3] W.-W. Zhang, H. Yu, S.-Y. Lei, and Q.-A. Huang, "Modelling of the elastic properties of crystalline silicon using lattice dynamics," J. Phys. D, vol. 44, p. 335401, 2011.

[4] J. Maassen and M. Lundstrom, "The landauer approach to electron and phonon transport," ECS Trans., vol. 69, pp. 23–36, 2015.

[5] A. Kikuchi, A. Yao, I. Mori, T. Ono, and S. Samukawa, "Composite films of higly ordered Si nanowires embedded in $SiGe_{0.3}$ for thermoelectric applications," J. Appl. Phys., vol. 122, p. 165302, 2017.

[6] R. Anufriev and M. Nomura, "Thermal conductance boost in phononic crystal nanostructures," Phys. Rev. B, vol. 91, p. 245417, 2015.

[7] M. Collet, M. Ouisse, M. Ruzzene, and M. N. Ichchou, "Floquet–bloch decomposition for the computation of dispersion of two-dimensional periodic, damped mechanical systems," Int. J. Solids and Structures, vol. 48, pp. 2834–2848, 2011.

[8] F. Schaffler, "Silicon-Germanium," in Properties of Advanced Semiconductor Materials: GaN, AIN, InN, BN, SiC, SiGe, M. E. Levinshtein, S. L. Rumyantsev, and M. S. Shur, Eds. New York: Wiley, Inc., 2001, pp. 149–188.

[9] R. Landauer, "Spatial variation of currents and fields due to localized scatterers in metallic conduction," IBM J.Res. Dev., vol. 1, no. 3, pp. 223–231, 1957.

[10] S. Datta, Electronic Transport in Mesoscopic Systems. New York: Cambridge University Press, 1997.

[11] C. Jeong, S. Datta, and M. Lundstrom, "Full dispersion versus Debye model evaluation of lattice thermal conductivity with a Landauer approach," J. Appl. Phys., vol. 109, p. 073718, 2011.

[12] ——, "Thermal conductivity of bulk and thin-film silicon: A Landauer approach," J. Appl. Phys., vol. 111, p. 093708, 2012.