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Phonon transport in nanowire with contacts: Size and doping

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The phonon transport in Lennard-Jones silicon wire with contacts is investigated using non-equilibrium Green's function. With the size decreasing, the significant reduction in the number of phonon modes leads to a smaller thermal conductance density. The dopant (Ge) atoms are used to substitute the atom in the wire to study the doping effect. For thin wire, its thermal conductance is very sensitive to the location of dopants. It is also found that the interior atom substitution has more impact on the thermal conductance over surface atom; substitution near contact surface reduces thermal conductance significantly; thermal conductance is suffering a 10%–20% variation due the random distribution of dopants; 17% of Ge content is sufficient to reduce thermal conductance by 80%. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4709755>]

I. INTRODUCTION

Much attention has been focused on improving the energy harvesting efficiency in thermoelectric (TE) devices.^{1–10} To date, the approaches for high TE efficiency can be categorized into two strategies: Depressing lattice thermal conductivity (contributed by phonon) and increasing the electronic TE efficiency.¹¹ Recently, high TE efficiency in silicon nanowire has been reported.¹ The reason is ascribed to the small lattice thermal conductivity, origin from the enhancement of phonon scatterings at the rough surface. To reduce the lattice thermal conductivity for silicon based device, an alternative and effective method is to dope germanium.^{10,12,13} The $\text{Si}_x\text{Ge}_{1-x}$ alloy has much lower lattice thermal conductivity than pure Si or Ge crystal. That rise our interest to study the doping effect in nanowire, in which the thermal conductance would depend on the position of the dopants. In this work, we employed non-equilibrium Green's function^{14–16} to investigate the phonon transport properties in the Lennard-Jones silicon (LJ-Si) nanowire with two contacts, similar to previous projects.^{17–19} The size effect and the Ge atom substitution effect (regarded as doping effect) on phonon transport properties of the system are discussed.

II. THEORY

In the modeled system, a short squared nanowire with the side length w (i.e., $w = l_x = l_y$) and length l , which are set to multiply integer of the lattice constant of silicon crystal a ($= 5.43 \text{ \AA}$), is aligned in z direction. This wire connects two semi-infinite thermal contacts with fcc lattice structure and $(0, 0, 1)$ plane as the contact surface. These two contacts serve as thermal reservoirs in which thermal equilibrium is assumed except for the regions near the joints of the wire. Together with the wire, the non-equilibrium regions denoted by LD and RD (in the left and right contacts, respectively) are treated as a whole wire (indicated by the dashed rectangular box in Fig. 1(a)). The regions LD and RD are defined

as the collection of atoms which are coupled to the wire through bonds or bond angles. Fig. 1(b) demonstrates the atom distribution of the whole wire with $w = 1a$ and $l = 3a$.

The elements of dynamical matrix, the elastic tensor (3×3 matrix) of atom i and atom j , is defined as

$$D_{ij} = \frac{1}{\sqrt{M_i M_j}} \cdot \frac{\partial^2 E}{\partial d_i \partial d_j}, \quad (1)$$

where E is the total potential energy, M_i the atom mass, and d_i the atomic position. For the potential energy, we considered the contribution from bonds and bond angles. The change of the potential energy due to bond stretching and contraction is described by the following equation with harmonic approximation:²¹

$$\delta E(i, j) = \frac{1}{2} C_0 \frac{(d_{ij} - d_0)^2}{d_0^2}, \quad (2)$$

where d_0 is the equilibrium distance and d_{ij} the distance between atom i and atom j . The constant C_0 is set to 49.1 eV, which is obtained from the harmonic term in the power series of the Lennard-Jones potential. The change of the potential energy due to the deformation of bond angle ($\delta\Theta_{ij,k}$ formed by atoms i, j , and k) is described by:

$$\delta E(i, j, k) = \frac{1}{2} C_1 (\delta\Theta_{ij,k})^2, \quad (3)$$

where the constant C_1 is set to 1.07 eV.²²

The following process is to determining the self-energy Σ_L , which describes the coupling of the whole wire to the rest part of the left contact. The Green's function for the first two layers (counting from contact surface) of the contact determined by decimation method²³ is with the expression

$$g_s(\omega, \vec{k}_{\parallel}) = \begin{bmatrix} g_{00}(\omega, \vec{k}_{\parallel}) & g_{01}(\omega, \vec{k}_{\parallel}) \\ g_{10}(\omega, \vec{k}_{\parallel}) & g_{11}(\omega, \vec{k}_{\parallel}) \end{bmatrix}, \quad (4)$$

where ω is the vibration frequency and $\vec{k}_{\parallel}$ the Bloch vector in transverse direction (paralleled to the contact surface).

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FIG. 1. (a) Schematic diagram of the modeled system: A nanowire connected two semi-infinite contacts, the parts LD and RD inside contacts are included into the whole wire. (b) Distribution of atoms for the whole wire with $w = a$ and $l = 3a$. Both LD and RD regions have 9 atoms, of which 3 are on the contact surface.

Then, the Green's function of the LD region is constructed in the following way:²⁰

$$g_{LD}(i, j, \omega) = \frac{1}{N} \sum_{\vec{k}_{\parallel}} g_{j,k}(\omega, \vec{k}_{\parallel}) \cdot e^{-i\vec{k}_{\parallel} \cdot (\vec{R}_i - \vec{R}_j)}, \quad (5)$$

where $g_{j,k}$ is the Green function of the layer j and layer k (j and k can be either 0 or 1, stands for the first layer and second layer, because atoms in LD region are on the first two layers), N ($= 200 \times 200$) is the number of sampling points in Brillouin zone (BZ) of the transverse plane. The self-energy of LD is then determined by:

$$\Sigma_{LD}(\omega) = \omega^2 I - D_{LD} - g_{LD}^{-1}(\omega), \quad (6)$$

where D_{LD} is the dynamical matrix of region LD. Finally, Σ_L is obtained by expanding Σ_{LD} to the dimension of the whole wire as

$$\Sigma_L(\omega) = \begin{bmatrix} \Sigma_{LD}(\omega) & 0 \\ 0 & 0 \end{bmatrix}. \quad (7)$$

Similarly, the self-energy of the whole wire due to the right contact Σ_R is determined, and the total self-energy of the whole wire Σ is the sum of Σ_L and Σ_R for harmonic phonon transport.

The retarded Green's function of the wire is given by

$$G^R(\omega) = [(\omega^2 + \delta i)I - D - \Sigma(\omega)]^{-1}. \quad (8)$$

The advanced Green's function G^A equals to $[G^R]^\dagger$; the broadening function due to the left contact Γ_L is determined by

$$\Gamma_L = -2\text{Im}[\Sigma_L], \quad (9)$$

similarly for Γ_R . The thermal conductance due to phonon transport is then determined:

$$K = \frac{1}{2\pi} \int d\omega \cdot T(\omega) \cdot \hbar\omega \cdot \frac{\partial f(\omega, T)}{\partial T}, \quad (10)$$

where f is Bose-Einstein distribution function,

$$f(\omega, T) = [e^{\frac{\hbar\omega}{k_B T}} - 1]^{-1}, \quad (11)$$

and $T(\omega)$ the phonon transmission function for harmonic phonon transport,

$$T(\omega) = \text{Tr}[\Gamma_L G^R \Gamma_R G^A]. \quad (12)$$

III. RESULT

The dynamical matrix $D_i(k)$ for the bulk LJ-Si is obtained from the equation

$$D_i(k) = \sum_j D_{ij} \cdot e^{i \cdot k \cdot a_{ij}}. \quad (13)$$

The phonon frequencies ω for the phonon wave with wave-vector k are the square root of the eigenvalues of $D_i(k)$ that determines the dispersion relation and the phonon density of states (DOS) of bulk LJ-Si (Fig. 2(a)). The phonon DOS can be obtained from the Green's function too,

$$\text{DOS} = -\frac{1}{\pi} \text{Im}[g(\omega)]. \quad (14)$$

Therefore, the surface Green's function g_{00} and Green's function of a layer deep inside the thermal contact, which is a by-product in the decimation method, give the phonon DOS at the contact surface and the DOS of bulk layer (Fig. 2(b)). Due to the termination of lattice structure at the contact surface, the surface atoms have less bonds (i.e., less coupling terms in

FIG. 2. (a) Phonon DOS for bulk LJ-Si and the dispersion relation (inset). (b) Phonon DOS for surface plane and the plane deep inside contact (treated as bulk layer). (c) Phonon DOS of squared silicon nanowires with side length $1a$, $2a$, $4a$, and $6a$.

FIG. 3. (a) Phonon transmission and (b) phonon transmission density of squared wires with various side lengths w and length $3a$. (c) Phonon transmission of wires with side length $2a$, and lengths $3a$ and $12a$.

dynamical matrix), many vibration modes are shifted to lower frequency,²⁴ therefore, a red-shift is noticed for the DOS at surface compared to the DOS of bulk layer.

A. Size effect

Generally, a thicker wire has more phonon states (Fig. 2(c)), larger phonon transmission (Fig. 3(a)), and larger thermal conductance (Fig. 5). The thermal conductance is proportional to the cross-sectional area of the wire except when the wire is sufficiently thin (refer to the conductance density D_K in Fig. 5). Furthermore, the DOS profile of the bulk LJ-Si (Fig. 2(a)) is similar to that of the thick wire ($w = 6a$ in Fig. 2(c)), but very different from that of the thin wire ($w = 1a$ or $2a$ in Fig. 2(c)). For this reason, transmission profiles of thin and thick wires are different (Fig. 3(b)).

FIG. 4. The possible phonon modes (considered to 10th nearest neighbor for the atom at the center of the wire) in Brillouin zone projected on k_x - k_y plane for (a) bulk LJ-Si (length of the wire is 0), (b)-(d) the wires with (the side length, the length) equal to ($1a$, $12a$), ($1a$, $12a$), and ($1a$, $12a$).

FIG. 5. Thermal conductance (dashed line) and thermal conductance density (solid line) respect to the cross-sectional area of squared wire.

A simpler explanation to these phenomena is the fcc crystal structure with the basis of two atoms vanished in thin wires.

To give an insight view of these phenomena, the possible phonon modes for the atom at the center of the wire are determined by transforming the surrounding atoms into the reciprocal lattice (the BZ), which correspond to the possible phonon wave vectors. For the convenience of visualization, the BZ is projected onto the k_x - k_y plane and is shown in Fig. 4. It is obvious that some of the phonon modes are missing compared with the phonon modes for bulk; the longer and thinner wire has less phonon modes. Thus, smaller phonon transmission density is expected for thinner and longer wire (Figs. 3(b) and 3(c)). The thermal conductance with linear area dependence (or constant conductance density) for thick or very short wire is expected (Fig. 5) because the number of phonon modes does not vary much.

In the previous work, the linear temperature dependence of thermal conductivity is found in low temperature range (20 to 100 K) for thin silicon nanowires with rough surface and is explained by the frequency dependent phonon-boundary scattering.⁵ In this work, the temperature dependence of thermal conductance (Fig. 6) is studied based on purely ballistic phonon transport in the wire (i.e., without phonon scatterings). The T^3 dependence is observed at low temperature ($T < 20$ K), and the linear temperature dependence is found especially for thin wire

FIG. 6. Thermal conductance of squared wire with various side lengths respect to temperature in (a) log scale and (b) linear scale.

FIG. 7. Four types of atomic layer (cross-section view) in the wire with side length $1a$, with number of bonds indicated for each atom.

($w = 1a$) at relatively higher temperature ($T > 20$ K). This phenomenon can be explained by analyzing phonon modes. The atom at the center of the wire receives phonon wave with relative short wavelength from the atoms in the wire (atoms within the distance $l/2$) and phonon wave with long wavelength from the atoms in the contacts (atoms with the distance more than $l/2$). Compared to the phonon modes in bulk LJ-Si (which has T^3 dependence properties for its thermal conductance), the phonon modes corresponding to the lattice points outside the boundary of wire are missing, that depress the thermal conductance due to short wavelength phonon (large wave vector k) significantly, but only slightly affect the thermal conductance due to long wavelength phonon (small wave vector k). In low temperature, the thermal conductance is dominated by long wavelength phonons (with low frequency, as $\omega = c \cdot k$, c is the sound speed); therefore, T^3 dependence is expected. When short wavelength phonons (with relative higher energy) contribute to lattice thermal conductance significantly at relatively high temperature, the T^3 dependence of lattice thermal conductance vanishes, and linear T dependence (which is the property of one dimensional system) appears.

B. Ge atom substitution

To investigate the doping effect, a wire with the values of $12a$ and $1a$ for its length and side length is used. To minimize the contact effect, 138 of 169 atoms (the total number of atoms in the whole wire) are allowed to be substituted. These atoms are completely in the wire, without direct coupling to the LD and RD region. Each of these atoms is labeled as 1, 2, or 4, which denotes the number of bonds connecting to the atom. As demonstrated in Fig. 7, the interior atoms are of 4 bonds, while the surface atoms are of either 1 or 2. The process of Ge atom substitution is carried out by replacing the atomic parameters (atomic mass and the constants for inter-atomic potential). The constants C_0 and C_1 in Eqs. (2) and (3) are set to 47.2 eV and 0.845 eV for (Ge-Ge) and (Ge-Ge-Ge).²⁵ The constants for (Si-Ge), (Si-Si-Ge), and (Si-Ge-Ge) are determined by interpolation with the values 48.1 eV, 0.989 eV, and 0.9142 eV, respectively.

The transmission function of a pristine wire (without Ge substitution) falls within the frequency range (from 0 to $100 T \cdot \text{rad/s}$) (Fig. 8(a)), and the transmission function of the wire with complete Ge substitution (138 atoms are substituted completely) falls within the frequency range (from 0 to $61 T \cdot \text{rad/s}$) (Fig. 8(c)). In Fig. 8(b), which is produced by scaling down the frequency of the transmission function of a pristine wire (Fig. 8(a)) by the factor 1.64 (determined by $\sqrt{C_0/M_{\text{Si}}}/\sqrt{C_0/M_{\text{Ge}}}$), the transmission peaks have almost the same locations, but different ampli-

FIG. 8. Phonon transmission of wires. (a) pristine LJ-Si wire; (b) pristine LJ-Si wire with the scale down of the frequency by a factor 1.64. (c) The wire with Ge substitutions for all atoms allowed to be substituted.

tudes with that in Fig. 8(c). This is because the lattice structure is assumed unchanged when Ge atom substitution takes place, and the two contacts remain in LJ-Si when the wire is completely substituted by Ge atoms.

In the following, a single Ge atom substitution is considered in the wire. Fig. 9(b) shows the changes of thermal conductance in percentage respect to longitudinal coordinate (z) of the Ge atom (the dopant). Substitution of surface atom (with 1 or 2 bond(s)) reduces conductance by 5% – 15%; substitution of interior atom (with 4 bonds) reduces conductance by 20% – 40%. The reduction in conductance is due to the differences in mass and bond strength between Si and Ge, which lead to damping effect: Decrease of phonon frequencies in the wire. Interior atom substitution affecting 4 atomic bonds has more impact in vibration modes, leads to stronger damping effect. Substitution near the contacts causes mismatch in phonon modes between wire and contacts, enhances phonon reflections, and reduces conductance significantly.

The variation of thermal conductance is found when N ($0 \leq N \leq 138$) atoms are substituted randomly in the wire

FIG. 9. (a) Percentage changes in thermal conductance with different Ge content. Maximum, mean, and minimum lines denote the variance of thermal conductance. Dashed line represents bulk Si-Ge alloy using the data from Garg's work.¹³ (b) Percentage change in thermal conductance due to single Ge atom substitution respect to the longitudinal direction z , the substituted atom is categorized by its labels 1, 2, or 4, the number of bonds with the atom.

(conductance is determined 10 times for each N). The maximum, mean, and minimum of the change in conductance with respect to the Ge content in the whole wire ($= \frac{N}{169} \times 100\%$) is shown in Fig. 9(a). Large variation of conductance (20%) is found when Ge content is less than 15%; and the variation of conductance is about 10% when Ge content is more than 15%. This is because it is likely that all the substituted atoms are on the surface or inside the wire when the number of substituted atoms is small. It leads to the variation of conductance 20% ($= 30\% - 10\%$), which is exactly the difference between the reduction in conductance for interior atom substitution and surface atom substitution (Fig. 9(b)).

The reduction in conductance with respect to Ge content of the system is compared with that of the bulk Si-Ge alloys (obtained from the previous work¹³) indicated by dashed line in Fig. 9(a). The atoms substituted in bulk material are always interior atoms; therefore, the dashed line is close to the minimum conductance, which is for the case of interior atoms substitution, when Ge content is less than 10%. The dashed line is close to the maximum conductance, when Ge content is greater than 20%. This is because a complete atomic layer in transverse direction of the wire can be substituted in the case of higher Ge content, which further depresses the conductance, but that is impossible in bulk material.

IV. SUMMARY

The proportionality between the thermal conductance and the cross-section area vanishes for thin wires due to the significant reduction of phonon modes. Ge atom substitution for interior atom has more impact over surface atom in reducing the thermal conductance. The thermal conductance

is with 10% – 20% variation for the wires with equal Ge content. Finally, the thermal conductance can be reduced by 80% with 17% of Ge content.

- ¹A. I. Hochbaum, R. Chen, R. Diaz Delgado *et al.*, *Nature* **451**, 163 (2008).
- ²T. Markussen, A.-P. Jauho, and M. Brandbyge, *Phys. Rev. Lett.* **103**, 055502 (2009).
- ³D. Donadio and G. Galli, *Phys. Rev. Lett.* **102**, 195901 (2009).
- ⁴P. Martin, Z. Aksamija, E. Pop, and U. Ravaioli, *Phys. Rev. Lett.* **102**, 125503 (2009).
- ⁵R. Chen, A. I. Hochbaum, P. Murphy, J. Moore, P. Yang, and A. Majumdar, *Phys. Rev. Lett.* **101**, 105501 (2008).
- ⁶J. Chen, G. Zhang, and B. Li, *Nano Lett.* **10**, 3978 (2010).
- ⁷P. E. Hopkins *et al.*, *Appl. Phys. Lett.* **99**, 133106 (2011).
- ⁸P. E. Hopkins *et al.*, *Appl. Phys. Lett.* **98**, 231901 (2011).
- ⁹K. Yamamoto, H. Ishii, N. Kobayashi, and K. Hirose, *Appl. Phys. Express* **4**, 085001 (2011).
- ¹⁰L. Shi, D. Yao, G. Zhang, and B. Li, *Appl. Phys. Lett.* **96**, 173108 (2010).
- ¹¹J. Li, T. C. Au Yeung, and C. H. Kam, *J. Phys. D: Appl. Phys.* **45**, 085102 (2012).
- ¹²W. Zhang, T. S. Fisher, and N. Mingo, *J. Heat Transfer* **129**, 483 (2007).
- ¹³J. Garg *et al.*, *Phys. Rev. Lett.* **106**, 045901 (2011).
- ¹⁴N. Mingo, *Phys. Rev. B* **74**, 125402 (2006).
- ¹⁵J. S. Wang, J. Wang, and N. Zeng, *Phys. Rev. B* **74**, 033408 (2006).
- ¹⁶T. Yamamoto and K. Watanabe, *Phys. Rev. Lett.* **96**, 255503 (2006).
- ¹⁷J. Li, T. C. Au Yeung, C. H. Kam *et al.*, *J. Appl. Phys.* **106**, 054312 (2009).
- ¹⁸J. Li, T. C. Au Yeung, C. H. Kam *et al.*, *J. Appl. Phys.* **106**, 014308 (2009).
- ¹⁹X. Zhao *et al.*, *J. Appl. Phys.* **107**, 094312 (2010).
- ²⁰W. Zhang, N. Mingo, and T. S. Fisher, *Phys. Rev. B* **76**, 195429 (2007).
- ²¹W. A. Harrison, *Electronic Structure and the Properties of Solids* (Dover, New York, 1989).
- ²²N. Mingo, *Phys. Rev. B* **68**, 113308 (2003).
- ²³F. Guinea, C. Tejedor, F. Flores, and E. Louis, *Phys. Rev. B* **28**, 4397 (1983).
- ²⁴C. Q. Sun, *Prog. Solid State Chem.* **35**, 1 (2007).
- ²⁵W. Zhang, T. S. Fisher, and N. Mingo, *J. Heat Transfer, Part B*, **51** 333 (2007).