Monte Carlo Simulation of Thermoelectric Properties in Si Nanostructures

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To further improve the material's thermoelectric figure-of-merit $ZT = (S^2\sigma/\kappa)T$, where S is the Seebeck coefficient, σ the electrical conductivity, κ the thermal conductivity, and T the temperature, much interest is now attracted to the enhancement of the power factor ($S^2\sigma$) by engineering the nanostructures [1]. Since this property is related to the carrier transport physics, the simulation techniques developed to investigate the nanoscale semiconductor devices are expected to contribute to this field; e.g., thermoelectric simulations for 1D nanostructures have been demonstrated by using the Monte Carlo (MC) [2] and NEGF [3] methods. In this work, we carried out the MC simulation to study the power factor of Si nanostructures considering the 2D non-uniformity of the doping density.

Fig. 1 schematically explains the present MC simulation. A finite difference mesh of 2D Poisson equation was coupled with the particles using cloud-in-cell scheme to solve the electrostatic potential and the electron distribution self-consistently. The models for the non-parabolic band structure and the phonon scattering were based on [4], while the third body exclusion model was employed for the ionized impurity scattering [5]. A linear temperature gradient was applied to the sample by changing the phonon scattering rate depending on the position, which induces the thermopower as shown in Fig. 2. By measuring the open-circuit voltage $V_{\rm op}$ and short-circuit current $I_{\rm sh}$, we evaluated S and σ. $V_{\rm op}$ was obtained by measuring the difference of quasi-Fermi levels at both ends of the opened sample, while $I_{\rm sh}$ was measured by forcing the quasi-Fermi levels at both ends to be equal.

The validity of our simulation was verified as shown in Fig. 3. Although the lower values compared to experiments [6], [7] were obtained (probably due to the lack of the phonon drag mechanism in the present simulation), the diffusion component of S depending on the doping density was well reproduced.

We then analyzed thermoelectric properties for various nanocomposite structures of heavily and lightly doped regions (Fig. 4). An example of the simulated result to calculate $V_{\rm op}$ is shown in Fig. 5. In Fig. 6, the simulated thermoelectric properties are plotted against volume fraction x of lightly doped region in each structure. Note that the obtained results are not necessarily explained by the simple averaging over S and σ of each region [1] (dashed lines). Structure (c) features one layer of low doping region to introduce the potential barrier for enjoying the S enhancement through the energy-filtering effect [3], but at the same time hinders σ. The incomplete barrier structure (c) caused moderate filtering. In (e) we elongate this incomplete barrier demonstrating better σ compared to average of volume fraction. We employed a slaloming path in (f); despite having similar x, (e) and (f) showed a radically different σ, which is probably caused by the straight shape of (e).

In summary, we have investigated the trade-off of S and σ modulation to enhance the power factor by using the MC method. The simple averaging of the thermoelectric properties of two-phase regions was not necessarily a good approximation for the nanocomposite structures, and the device simulation techniques would provide a useful approach to design the high ZT materials.

REFERENCES

[1] M. Zebarjadi et. al., Nano Lett., vol. 11, 2225, (2011).
[2] B. S. Ramin et. al., J. Electronic Materials, vol. 41, no. 2, 1370, (2012).
[3] R. Kim et. al., J. Appl. Phys., vol. 111, no. 2, 024508 (2012).
[4] C. Jacoboni et. al., Rev. Mod. Phys., vol.55, 645, (1983).
[5] B. K. Ridley et. al., J. Physics C. , vol. 10, no. 10, 1589, (1977).
[6] T. H. Geballe et. al., Phys. Rev., vol.98, 940, (1955).
[7] F. Salleh et. al., Appl. Phys. Express, vol. 2, no. 7, 071203, (2009)

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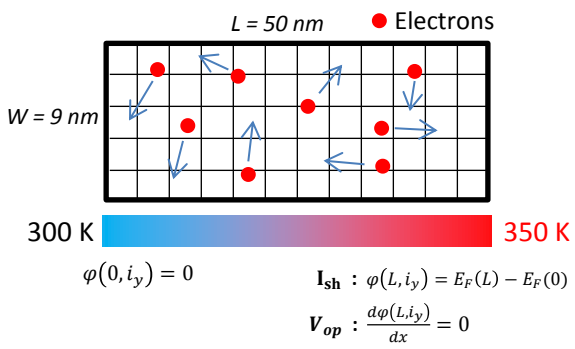

Fig. 1. Schematic explanation of the simulation method used in this study. A linear temperature gradient was applied to the sample, and the carrier density and the electric static potential were self-consistently calculated by the MC simulator coupled with 2D Poisson equation solver. The boundary condition of poisson eq. is different for V_{op} and I_{sh} calculation (see Fig. 2). The quasi-Fermi level $E_F(x, y)$ was evaluated from the carrier density n and carrier temperature T_e.

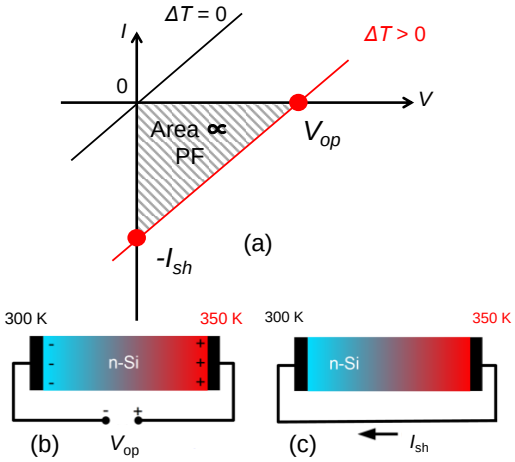

Fig. 2. Schematic illustration of the simulation method to evaluate the thermoelectric properties. The shift of *I-V* characteristics is induced by the temperature gradient applied to the sample (a). The open voltage V_{op} (b) and short-circuit current I_{sh} (c) were measured, and then the Seebeck coefficient S (= V_{op} / ΔT) and the electrical conductivity σ (= I_{sh} L / $V_{op}A$) were evaluated, where L and A are the length and the cross section of the sample, respectively.

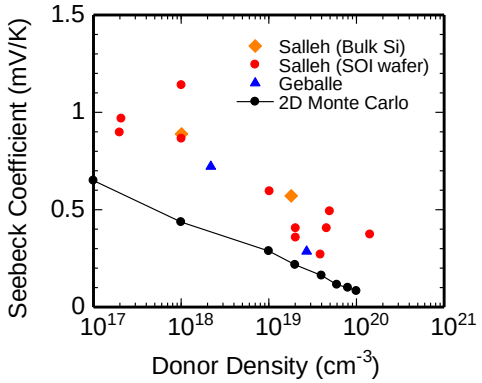

Fig. 3. Simulated results of Seebeck coefficient S plotted as a function of the doping density N_D compared to the experimental data [6-7].

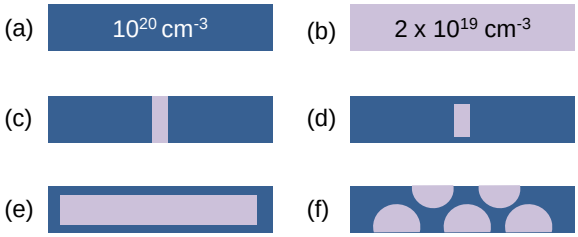

Fig. 4. Schematic illustration of simulated device structures, showing distribution of heavily (N_D = 10^{20} cm^{-3}) and lightly (N_D = 2 x 10^{19} cm^{-3}) doped regions. The device dimension is 50 nm x 9 nm. (a) and (b): homogeneously doped structures. (c): 1D barrier structure. (d): incomplete 1D barrier structure. (e): high doping near walls structure. (f) slalom path structure.

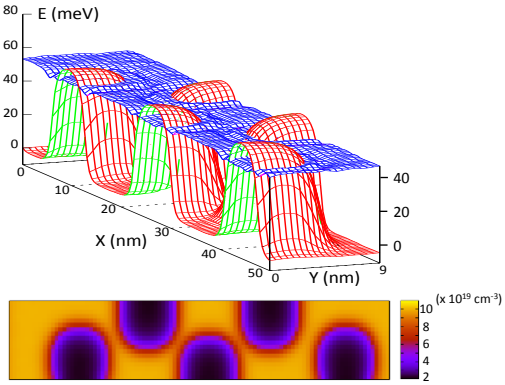

Fig. 5. An example of the simulated results for measuring V_{op} (see, Fig. 3) of the structure (f). (top) Potential (red) and quasi-Fermi level (blue) distributions. (bottom) Carrier density distribution.

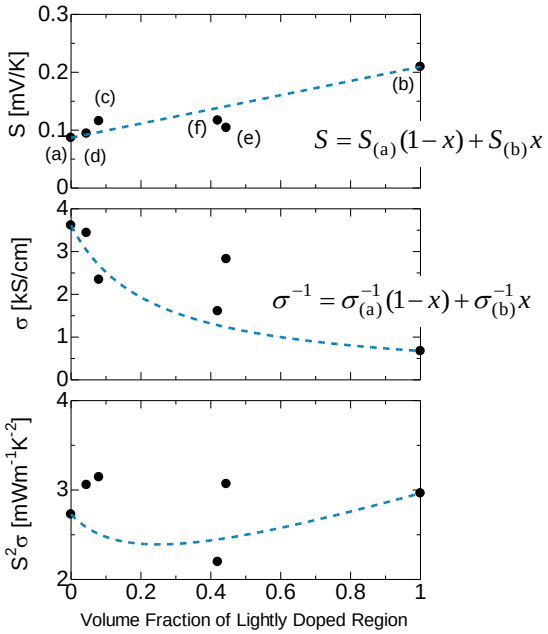

Fig. 6. Simulated results of the Seebeck coefficient S, the electrical conductivity σ, and the power factor $S^2\sigma$ plotted against the volume fraction x of lightly doped region in each structure shown in Fig. 4. Blue lines show the characteristics estimated by simply averaging over S and σ of each region [1].