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Possibility of Thermoelectric Property Improvement by Non-uniformly Doped Si

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Abstract

We numerically demonstrate that a non-uniformly doped silicon (Si) has higher thermoelectric power factor (PF) compared to the uniformly doped Si. The PF is improved by decreasing the dopant concentration in the hot side and increasing that in the cold side. This is originated from the temperature dependency of the thermal conductivity of Si. The result shows that the adjustment of the dopant concentration distribution is effective to improve the performance of thermoelectric materials.

1. Introduction

Energy harvesting technology is the key to drive a great number of sensors in the future internet-of-things (IoT) society. One of the most anticipated energy harvester is the thermoelectric generator (TEG) which generates electric power from environmental heat energies. Recently, Si emerges as the promising material for the TEG, because Si nanowire was found to have a low thermal conductivity [1] and high thermoelectric property [2]. Si has a great advantage of matured manufacturing processes such as the doping and nanoscale fabrication, as well as the less environmental impact.

In this study, we pursued an optimal doping to bring out the best thermoelectric performance of Si by means of TCAD simulation [3].

2. Experiment

Fig. 1(a) shows the schematic illustration of the 2D device model which is n-type doped silicon with 80 nm thickness and 600 nm length. The Si layer is sandwiched between 10 nm thickness SiO_2 layers. Both ends of long side are connected to the electrodes. One end is set to 400 K and the other end is set to 300 K. In this 2D simulation, Fermi-Dirac statistics, Klaassen's unified low-field mobility, concentration dependent recombination, Selberherr's impact ionization model, and Giga simulation module [4] which treats thermal effects were applied. The dopant distribution is varied with keeping the mean concentration of whole system. The electro resistivity, Seebeck coefficient, and PF were derived from the I-V characteristic in each condition.

3. Results and Discussion

Fig. 2(b) summarizes the PF for different dopant concentration distributions when phonon drag effect is not considered. Here, the Si region is divided into three sections: H, M, and C as shown in Fig. 1(b). For example, sample "5-11" in Fig. 2 means donor concentration is $5 \times 10^{-18} cm^{-3}$ at section H, $8 \times 10^{-18} cm^{-3}$ at section M and $11 \times 10^{-18} cm^{-3}$ at section C. The result indicates that the PF is improved in a non-uniform dopant concentration distribution in which the hot side region (H) includes low concentration of dopant and cold side region (C) includes high concentration of dopant. The tendency is also confirmed when the simulation includes phonon drag effect as shown Fig. 2(c).

The dependence of the PF on the dopant distribution is explained by the nonlinear lattice temperature gradient in Si, which becomes steep at hot side and gentle at cold side, as shown in Fig. 3. This is caused by the temperature dependence of the thermal conductivity of Si. The thermal conductivity of Si is given by

$$\kappa = 1.48 \cdot (T_L/300)^{-1.65} W cm^{-1} K^{-1} \quad (1)$$

where T_L is lattice temperature. Therefore, the thermoelectric power is mainly generated at the region H, and the region C with small temperature gradient rather acts as merely a resistive load. The Seebeck coefficient is enhanced by decreasing the dopant concentration, and the electric conductance is enhanced by increasing the dopant concentration. Consequently, the lower dopant concentration in region H and higher dopant concentration in region C lead to the enhancement of the PF.

Fig. 4 shows an optimized dopant concentration distribution to maximize the PF keeping the mean dopant concentration in the device. It increases with 1.23% of that of the uniform doping shown in Table I. Although the increase is quite slight under the present restraint condition, the result suggests that the PF can be enhanced by changing the dopant concentration distribution according to the nonlinear temperature distribution.

4. Conclusions

The simulation performed in this work shows that a non-uniform dopant distribution of n-type Si enhances the PF compared to the uniform dopant distribution. It mainly caused by nonlinear temperature gradient in Si; the thermal conductivity decreases as the temperature increases, thereby the temperature gradient becomes larger near the hot side. The Seebeck coefficient of Si increases as the dopant concentration decreases, so that it is preferable to suppress the dopant concentration near the hot source with steep temperature gradient. Thus, the thermoelectric performance can be tuned by optimizing the dopant concentration distribution according to profile of temperature gradient.

Acknowledgements

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Reference

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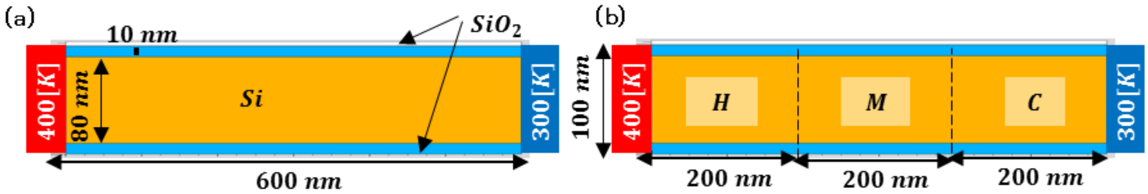

Fig.1 schematic illustration of the 2D device model

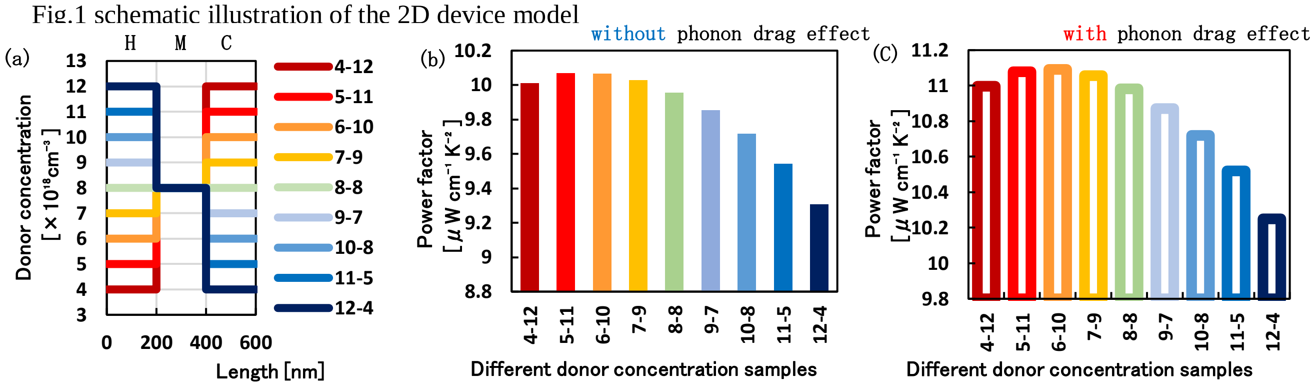

Fig.2 (a) Each non-uniform dopant samples, (b) PF of each dopant samples (without phonon drag effect) (c) PF of each dopant samples (with phonon drag effect)

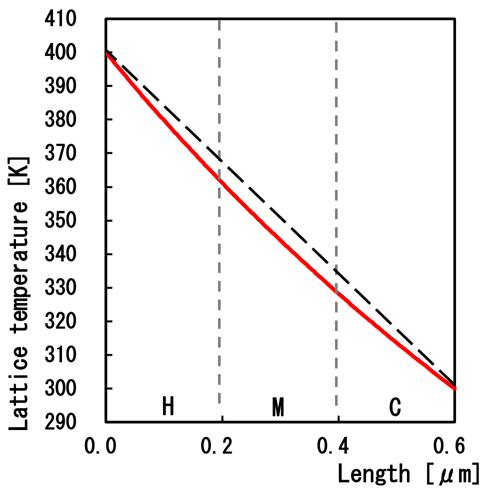

Fig.3.Temperature gradient by the function of thermal conductivity eq. (1)

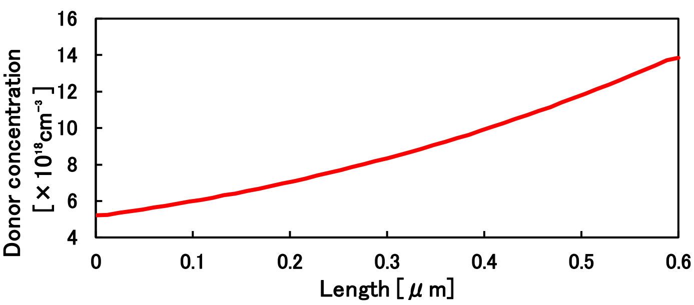

Fig.4 Optimum dopant concentration distribution at temperature gradient of Fig.3 (without phonon drag effect)

	Uniform ($7.727 \times 10^{18} cm^{-3}$)	Optimized
PF[$\mu W/K^2 cm$]	9.9557	10.0786
Increasing ratio of PF [%]		+1.234

Table.I Increase rate of PF by optimized dopant (without phonon drag effect)