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Substrate Heat Resistance Engineering for Realizing High Performance Si Nanowires Thermoelectric Generator

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Abstract

We engineered the heat resistance of the substrate under the lateral Si nanowires (Si-NWs) thermoelectric (TE) generator for the performance enhancement in finite element method (FEM) simulations. The TE power density is enhanced greater than 100 times owing to the base-substrate heat resistance control. The presence of the SiO_2 insulating layer under Si-NWs is important to build a large temperature gradient across both ends of Si-NWs. This finding is crucial for designing the planar type high power TE generator.

1. Introduction

TE energy harvesters which utilize environmental heat energies are anticipated for the portable, wearable or swarmed sensor nodes in internet of things (IoT) systems. Since Si-NWs have both high electrical and low thermal conductivities, it can achieve a high TE figure of merit, ZT.

In previous works, we demonstrated both numerically and experimentally that the sub-μm class short Si-NWs lying on the SiO_2/Si-substrate of SOI wafer show high TE properties [1-3]. However, the TE performance was found to be limited by the parasitic heat resistance of the SiO_2 layer and the base-substrate. Most of the heat energy is dissipated in the thick substrate and thus the temperature difference in the short Si-NWs is drastically decreased. Further enhancement of the TE performance requires the engineering of the heat resistance in the substrate. In this study, we numerically investigated the effect of the thickness of the SiO_2 insulating layer underneath Si-NWs and the base-substrate under the SiO_2 layer by FEM simulations.

2. Structure of Si-NW TE generator

We investigated planar Si-NWs TE generator structure (Fig.1). Si-NWs (thickness 50nm, width 65nm, and length 250nm) is placed on the SiO_2 insulating layer and the base-substrate. The dopant concentration and Seebeck coefficient of the both n- and p-type Si-NWs is set as 1.0×10^{19} cm^{-3} and ±200 μV/K. 400nm-thick Al electrode pads are placed between the n- and p-type Si-NWs. 200nm-thick AlNs are placed as the heat conduction layer on alternate electrode pads. The open space is assumed to be a perfect vacuum. In this study, the substrate heat resistance is controlled by the following three parameters. 1) base-substrate material with different thermal conductivity (Si or diamond), 2) base-substrate thickness (50 μm - 745 μm), and 3) thickness of the SiO_2 insulating layer (0 nm - 1000 nm).

The temperature distribution and the TE characteristics of the Si-NWs TE generators were simulated by the multipurpose FEM software, COMSOL Multiphysics®. A periodic boundary condition is adopted in x and y directions, *i.e.*, the system is replicated throughout space to an infinite plane. The periodic pitch of x direction which is equal to NW pitch is 500 nm. The external temperature difference is set to 5 K. The thermal conductivity parameters are summarized in Table I [2]. The TE power density is normalized by the half area of the unit cell (Fig. 1) which is given by

$$A_{unit}/2 = 2L_{NW}P_{NW}, \tag{1}$$

where A_{unit}, L_{NW}, and P_{NW} are the area of the unit cell, the Si-NW length, and the Si-NW pitch, respectively, supposing that the pads and NW arrays have the same footprint.

3. Results and Discussion

The TE power density is enhanced by the base-substrate thickness thinning (Fig. 2(a)). Thinning the Si substrate is drastically effective to improve Si-NW TE generator performance which is enhanced to greater than 100 times. Further enhancement can be achieved by replacing the Si base-substrate with the diamond.

The TE power density depends on the base-substrate heat resistance θ_{area} (Fig. 2(b)). The base-substrate heat resistance is defined as the areal resistance given by

$$\theta_{area} = t/\kappa, \tag{2}$$

where κ and t are the thermal conductivity and the thickness of the base-substrate, respectively. A universal relation can be seen in Fig. 2(b) indicating that the performance of the TE generator is governed by θ_{area}.

The TE power density and the ΔT across the Si-NWs also depends on the SiO_2 layer thickness (Fig. 3 and 4), when the base-substrate thickness is 500 μm. The each dependence of TE power density and the ΔT on the SiO_2 layer thickness has a peak in the sub-micron region. Both the TE power density and the ΔT are steeply decreased in the thinner region. This result suggests that the SiO_2 layer is necessary to maintain the ΔT across the Si-NW.

The temperature distribution in the cross-sectional plane of the TE generator with the diamond base-substrate is shown in Fig 5. The Si-NW and the diamond layer (base-substrate) near the Si/diamond interface are entirely heated, and there is little ΔT across the Si-NW when the Si-NW lies directly on the 500μm thick diamond base-substrate (Fig. 5(a)). Sufficiently large ΔT is established in the Si-NW part when a thin SiO_2 layer is inserted between the Si-NW and the diamond layer (Fig. 5(b) and 5(c)). This large ΔT is due to the suppression of the lateral heat flow by the SiO_2 layer. Since the presence of the SiO_2 layer increases heat resistance of the substrate at the same time, there is an optimum thickness of the SiO_2 layer. 200 nm thick SiO_2 layer is the best case (Fig. 5(b)). Thus the TE performance of the planar Si-NW device can be effectively engineered by controlling the heat resistance distribution in the substrate.

4. Conclusions

We discussed how to control the substrate heat resistance to effectively improve the planar type Si-NW TE generator performance, comparing Si and diamond as the base-substrate material, based on a series of FEM analysis. Suppression of the base-substrate heat resistance is effective to increase the TE power density. Moreover, the tuning of the SiO_2 insulating layer underneath the Si-NWs is also indispensable to establish a temperature difference in Si-NW for the best TE performance.

Acknowledgements

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References

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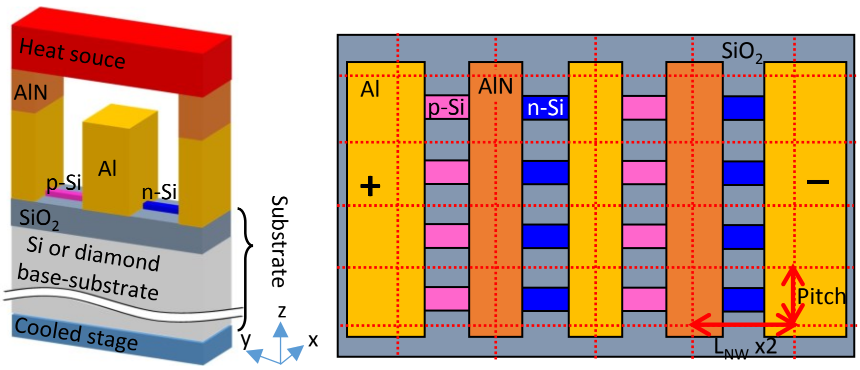

Fig. 1 Schematic and unit cell of simulated Si-NWs TE generator.

Table I thermal conductivities used in FEM simulation.

	κ (W/m·K)
Si-NW	1.4
Al	238
SiO_2	1.4
Si-sub	131
Diamond	2500

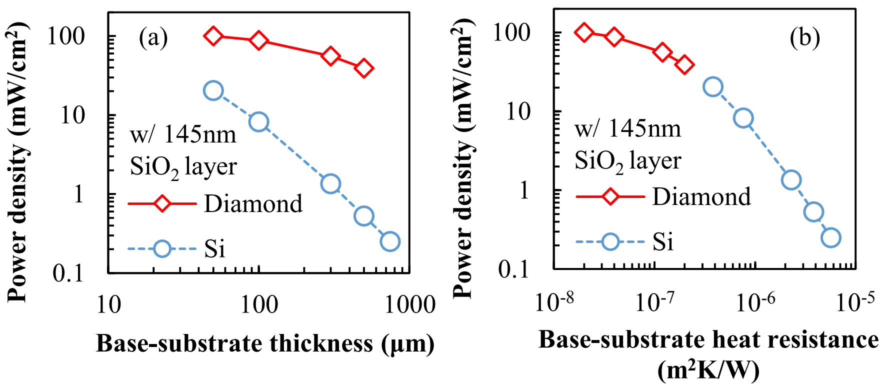

Fig. 2 Base-substrate thickness and heat resistance dependence of simulated TE power density.

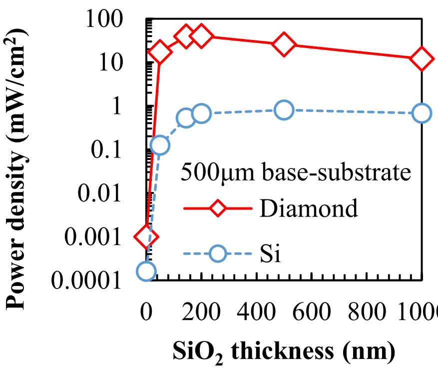

Fig. 3 SiO_2 thickness dependence of simulated TE power density.

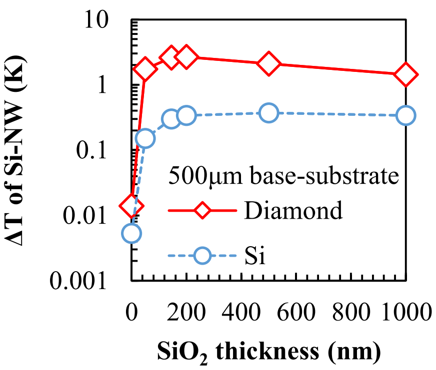

Fig. 4 SiO_2 thickness dependence of simulated ΔT.

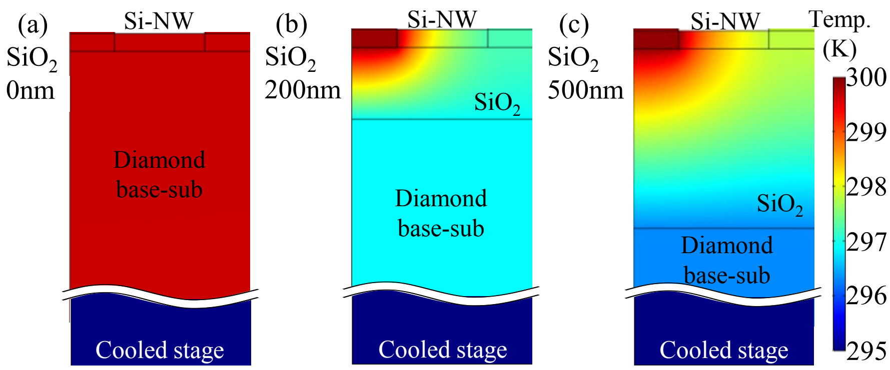

Fig. 5 Cross-section temperature profile simulation of the TE generator on 500-μm thick diamond base-substrate with 0-500nm thin SiO2 layer sample.