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Silicon Nanowire ForThermoelectric Applications: Effects of Contact Resistance

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***Abstract*—**Silicon nanowire (SiNW) based thermoelectric device (TED) has potential applications in areas such as chip level cooling/ energy harvesting. It is a great challenge however, to assemble an efficient device with these SiNW. The presence of parasitic in the form of interfacial electrical resistance will have a significant impact on the performance of the TED. In this work, we explore the effect of the electrical contact resistance on the performance of a TED. Numerical simulations are performed on SiNW to investigate such effects on its cooling performance. Intrinsically, SiNW individually without the unwanted parasitic effect has excellent cooling power density. However, the cooling effect is undermined with the contribution of the electrical contact resistance.

***Keywords*—**Thermoelectric; Silicon; Nanowire, Electrical contact resistance; Parasitics

I. Introduction

THe thermoelectric phenomenon has been an area of active area of research since the discovery of the Seebeck and Peltier effect. The Seebeck effect is the conversion of electrical differences into electricity. This effect can be harnessed to generate power from temperature differences. On the other hand, the Peltier effect is described as the removal of heat from a junction of two dissimilar conductors when a current is passed through it; it acts as a heat pump to cool one end as long as a current flow is maintained [1]. The efficiency of a thermoelectric material is characterized by a dimensionless figure of merit ZT which is defined as in (1)

$$ZT = \frac{S^2 \sigma T}{\kappa} \quad (1)$$

where S, σ, κ refers to the Seebeck Coefficient, electrical conductivity and thermal conductivity respectively. In 1993, Hicks and his team predicted that low dimensional material, such as a 2D quantum well and a 1D quantum wire, have enhanced ZT as compared to its bulk counterpart [2],[3],[4]. An even more interesting recent research finding reported that SiNW exhibited 2 orders improvement in ZT as compared to bulk silicon [5],[6],[7]. The κ of the SiNW was found to decrease drastically as its diameter is reduced. This resulted in an increase of the intrinsic ZT to 0.6 at room temperature [5]. Comparing bulk materials, current state of art thermoelectric materials Bi_2Te_3/Sb_2Te_3 have a ZT of ~1 as compared to bulk silicon of ~0.01 [5]. Hence, bulk silicon was never considered for thermoelectric applications previously. However, with the recent developments of SiNW which confirm ZT enhancement, the idea of a SiNW based TED is promising. It opens up opportunities for applications at the nano scale, i.e. microprocessor integration, or even as a power source for implantable medical devices (IMD). Fabricating a SiNW based thermoelectric device (TED) would invariably involve bundling hundreds of nanowires in an array to form respective N and P thermoelectric legs. It is a challenge, however, to form low resistivity ohmic contacts and to ensure good electrical contacts between all SiNW. Parasitic in the form of electrical contact resistance can be disastrous in all devices due to Joule heating (energy loss). SiNW with zero electrical contact resistance can be used to make an excellent device. However the achievement of zero contact resistance is impossible in reality. Electrical contact resistance, inevitably exist as long as there is an interface.The effect of electrical contact resistance is not so much of an issue for current bulk material TED; because of its large area (~mm^2), the electrical contact resistance is only a minute fraction of the material intrinsic resistance. This is however, not so for SiNW where this value can be comparable to the wire resistance. Nanowires have a large aspect ratio, which translates to a large contact resistance. This situation can be made worse if bad contacts are made between the electrodes and the SiNW. This situation can arise easily due to processing non-ideality that creeps in with the large number of SiNWs to be contacted.Zhang et al [8], have studied the cooling performance of individual SiNW using numerical simulations and reported parameters. However, it was assumed that there is no electrical contact resistance present. Hence, the results represent a best scenario case which deviates from what is achievable in reality. In this work, we provide another design perspective into understanding the performance of SiNW through numerical simulation. Using heat transfer model at the macro-scale and experimentally reported material's thermoelectric properties (S, σ, κ),the performance of SiNW as a thermoelectric material is re-evaluated in a realistic scenario here.

II. Simulations

Electrical contact resistance becomes more relevant as the size of the structure is scaled down to the nm range. Many groups have studied and reported the electrical contact resistance between silicon and metal; the electrical resistivity is largely dependent on the process conditions used to form the contact and also the method used to extract it [9],[10],[11]. The electrical contact resistivity as reported can be as low as 0.131 $\mu\Omega cm^2$ to as high as 5.02 $\mu\Omega cm^2$ [9],[11].As mentioned

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earlier there is a tremendous reduction of the κ of SiNW as the diameter decreases. The κ is further reduced depending on the surface roughness of the SiNW. One particular method to obtain SiNW of rough surface is the electroless etch (EE) method, which eventually leads to the best ZT reported. In this simulation, we make use of the parameters reported. In addition, we factor in the electrical contact resistance and investigate how such effect can prove detrimental to its thermoelectric performance. Table 1 shows the parameters used in the simulation which also corresponds to the best N-type EE SiNW of diameter ~50 nm and doping concentration ~1 x 10^{19}cm^{-3}; Table 1 also tabulates this list of contact resistance along with other parameters being included in the simulations. [5].

TABLE I
MATERIAL PARAMETERS USED IN SIMULATION

Size	ρ_c (μΩcm^2)	κ (W/mK)	S(μV/K)	σ (S)
50nm x 50nm (EE)	0.131	1.6	245	5.88x10^4
	0.173			
	0.261			
	3.74			
	5.02			

The simulation in this work aims to investigate the thermoelectric performance of SiNW in the cooling mode, subjected to the presence of electrical contact resistance. In the cooling model, we passed a current through the SiNW while taking adiabatic condition on all other surfaces. Upon electrical current flow, there will be four competing effects while achieving final steady state dT at both ends. The four effects are namely, Peltier effect which pumps the heat from the hot side to the cold side, heat conduction from the cold side to the hot side, joule heating of the SiNW, joule heating from the electrical contact resistance between the SiNW and the electrodes. The equation which describes the cooling and heat transfer is as in (2).

$$\nabla.(-\kappa.\nabla T + S.T.J) = J.(-\nabla.V) - c\frac{\partial T}{\partial t} \qquad (2)$$

We make use of a commercial finite element simulation tool – COMSOL Multiphysics[12] for this purpose. In our simulation model the structure is as shown in figure 1, we have a SiNW of length 1μm, which is contacted at both ends by copper electrodes. We used standard electrical and thermal parameters for the copper electrodes. In order to simulate the inclusion of an electrical contact resistance, a very thin layer of material with variable resistance is included in between the SiNW and the copper electrodes.

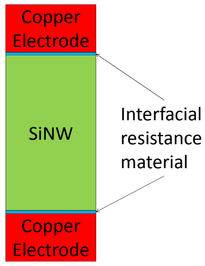

Fig. 1 Model of the structure used for simulation

First, we simulated the effect of the variation in the electrical contact resistivity on the maximum achievable dT under optimum current. In this case of a 50 nm x 50 nm EE SiNW with zero contact resistance, we simulated an optimum current of 7uA which resulted in a steady state dT of ~61 K across both ends of the SiNW (Figure 2).

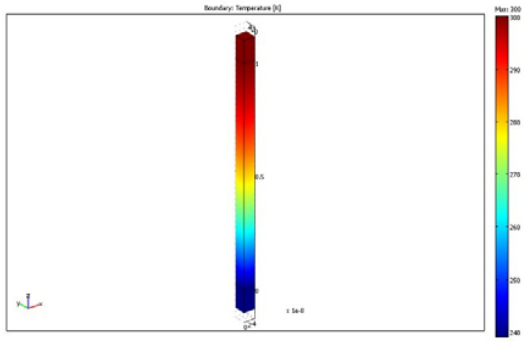

Fig. 2 Simulation result of the dT obtainable across the SiNW under an optimum current of 14 μA. Temperature bar on the left shows a range of 239K to 300K

We varied the interfacial layer's resistance according to that indicated in table 1 while keeping the other parameters (S, σ and κ) constant. From the thermoelectric equation as described in equation 2, we simulated the results of steady state dT across SiNW as the current through it is varied as shown in figure 3.In figure 3, we observed that for all 4 curves, as the current through the SiNW is increased, the dT generated across it increases to a maximum before decreasing to zero. Beyond that point, Joule heating dominates. As the electrical contact resistivity is increased, the curve started to scale downwards; correspondingly, the maximum achievable dT across the SiNW decreases as well. In figures 3, we omitted the data for electrical contact resistivity greater than 0.261μΩcm^{2}as the cooling curve cannot be observed.In figure 4, we plotted the relationship between the maximum achievable dT across SiNW with increasing electrical contact resistivity. It can be observed in figure 4 that there is a drastic drop of the maximum dT from ~61K to ~20K when the electrical contact resistivity is increased from 0 μΩcm^2 to 0.261 μΩcm^2. With further increase in the electrical contact resistivity, heating of the cold side takes place instead of the desired cooling. These results demonstrate the serious implication of contact resistance when SiNW based TED is intended to be used as a cooler.

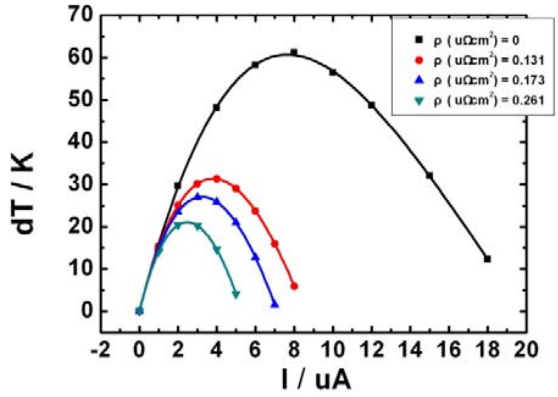

Fig. 3 Simulation result of the dTvs I curve as the electrical contact resistivity is varied

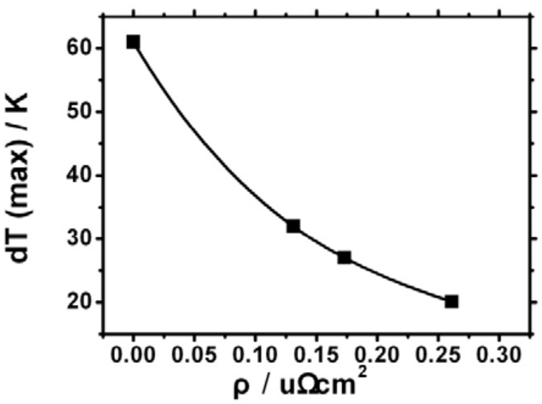

Fig. 4 Simulation result of the max dT obtainable across the SiNW when the contact resistivity is varied

Furthermore, we also investigated the effect of the maximum achievable dT when the SiNW size is varied. For this set of simulation, we assumed the thermal conductivities of different diameters of EE SiNW [5] while the other parameters (κ, S, σ) are kept constant; we keep the electrical contact resistivity constant at 0.131 μΩcm^2 for the 3 different SiNW. Table 2 shows the parameters of the SiNW which we used in this set of simulations.Similarly, in figure 5, we show the relationship between maximum cooling and wire diameter of SiNW as the current through it is varied. The 50 nm x 50 nm SiNW shows the best performance with the largest dT generated when optimum current is flowed. Hypothetically, the size of the SiNW will affect the contact resistance due to the difference in the area contacted to the metal electrodes, i.e. when the diameter of the SiNW is reduced, the electrical contact resistance should increase as well. This will in turn degrade the cooling performance of the SiNW. However, from equation 2, we observe that the cooling performance is a function of κ as well. Due to this competing effect, the 50 nm x 50 nm SiNW with a much smaller κ performs much better. Nevertheless, we should consider the presence of the electrical contact resistance when designing a TED for optimum performance.

TABLE II
PARAMETERS OF DIFFERENT DIAMETERS OF EE SINW AS USED IN SIMULATION

Size	κ (W/mK)	S(μV/K)	σ (S)
50nm x 50nm (EE)	1.6	245	5.88x10^4
98nm x 98nm (EE)	5		
115nm x 115nm(EE)	8		

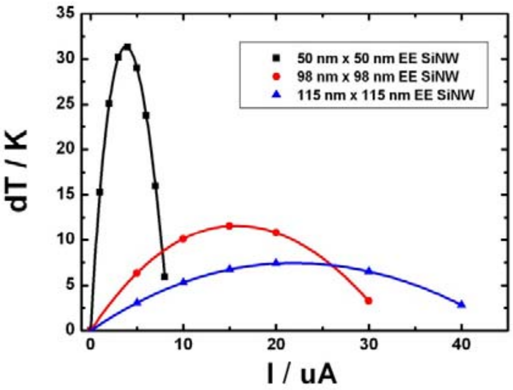

Fig. 5 Simulation result of the dTvs I curve for different diameters of EE SiNW

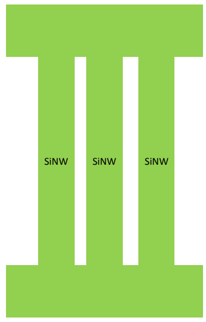

Fig. 6 Cascaded I structure to design SiNW based TED while keeping the electrical contact resistance low

Should a TED be fabricated using SiNW as the thermoelectric material, it is imperative in the fabrication process that steps be optimized to achieve an electrical contact resistance as low as possible. Some area of considerations can include doping considerations, metal electrodes considerations, or novel structure considerations. One of the proposals for novel structure is by having a cascaded I shape structure SiNW as shown in figure 5. This can ensure a large contact area while keeping the size of the middle SiNW small to exploit the benefits of enhancement of the thermoelectric performance at the nano-scale.

III. CONCLUSION

In this work, we investigated the effect of the electrical contact resistance on the cooling performance of a SiNW. The presence of the electrical contact resistance must be considered and accounted for while designing a TED. This is especially so when we are dealing with nanostructures such as SiNW where the magnitude of the electrical contact resistance is of magnitude larger than its bulk counterpart.

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REFERENCES

[1] Goldsmid, H.J. in *CRC Handbook of Thermoelectrics* (ed. Rowe, D.M.), CRC Press, Boca Raton, FL, Chapter 2& 19, 1995.

[2] L. D. Hicks, and M. S. Dresselhaus, "Thermoelectric figure of merit of a one-dimensional conductor", Physical Review B, vol. 47, no. 24, June 1993

[3] L. D. Hicks, and M. S. Dresselhaus, "Effect of quantum-well structures on the thermoelectric figure of merit", Physical Review B, vol. 47, no. 19, May 1993

[4] M. **S.** Dresselhaus, Y.M. Lin, G. Dresselhaus, X**.** Sun, Z. Zhang, S.B. Cronin, T. Koga and J.Y. Ying, "Advances in 1D and 2D Thermoelectric Materials", 18th International Conference of Thermoelectrics, 1999

[5] Allon I. Hochbaum, Renkun Chen, Raul Diaz Delgado, Wenjie Liang, Erik C. Garnett, Mark Najarian, Arun Majumdar and Peidong Yang, "Enhanced thermoelectric performance of rough silicon nanowires", Nature Letters, vol. 451, Janurary 2008

[6] L. Shi, D. Yao, G. Zhang, and B Li, "Size dependent thermoelectric properties of silicon nanowires", Applied Physics Letters, vol. 95, 063102, May 2009

[7] A. I. Boukai, Y. Bunimovich, J. Tahir-Kheli, J-K Yu, W. A. Goddardand J. R. Heath, "Silicon nanowires as efficient thermoelectric mateirals", Nature Letters, vol. 451, Janurary 2008

[8] G. Zhang, Q. Zhang, C. T. Bui, G. Q. Lo, and B Li, "Thermoelectric performance of silicon nanowires", Applied Physics Letters, vol. 94, 213108-1, May 2009

[9] Effects of Nanoscale Contacts to Silicon Nanowires on Contact Resistance: Characterization and Modeling, Joshua T. Smith et al, Proceedings, DRC 2010, 2010

[10] On the effect of the electrical contact resistance in nanodevices, T. Schwamb et al, APL, 92, 243106, June 2008

[11] Contact Resistance of Epitaxially Interfaced Bridged SiliconNanowires, A. Chaudhry et al, Proceedings, International conference on Nanotechnology, 2007

[12] COMSOL MULTIPHYSICS by COMSOL ©.