Optimization of Doping Concentration for Three-Dimensional Bulk Silicon Microrefrigerators

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Abstract

We designed and fabricated a three-dimensional (3D) silicon microrefrigerator, which demonstrates a cooling power density over 200W/cm^2 with only ~1^{0}C cooling. The high cooling power density is mainly due to the high thermal conductivity and heat spreading effects. These devices have potential application in hot-spots management to reduce the chip peak temperature and realize on chip thermal management. A finite element model is developed to study and optimize these 3D devices. The simulation results showed that the optimized doping concentration to achieve the maximum cooling for these 3D silicon microrefrigerators (5e18 cm^{-3}) is different from the conventional 1D device, where $S^2\sigma$ achieves the maximum at the doping of 5e19 cm^{-3}. At its optimized doping concentration, these silicon microrefrigerators could reach a maximum cooling of 3^{0}C. Further studies prove that this deviation is due to the non-idea factors inherent within the device, e.g. semiconductor-metal contact resistance, Joule-heating from probe contact resistance etc… Thus to optimize the real device, it is necessary to chose a full model considering all the non-ideal factors.

Keywords

Silicon microrefrigerators, hot spots, on-chip thermal management, doping concentration, Seebeck coefficient, electrical conductivity

1. Introduction

Silicon has been the heart of microelectronics for over 50 years since the discovery of transistors in the early 1950s. However, it has been completely ignored in the thermoelectric field because of its high thermal conductivity and low figure

$$ZT = \frac{S^2\sigma T}{\kappa}$$

of merit, ZT, which has the expression of, S: Seebeck coefficient; σ, electrical conductivity; κ, thermal conductivity; and T is the absolute temperature. Since the early work in thermoelectric field in 1950's, most researchers have been focused on high ZT materials, like BiTe and its alloys. The high ZT of BiTe and its alloys is mostly due to its very low thermal conductivity (κ), ~1.4 W/mK at a reasonably good electrical conductivity, which contributes to higher ZT. The higher ZT is desirable because it can produce larger temperature gradient and more efficient heat pumping. However, ZT was lingering around 1 for the past fifty years. The difficulty in increasing ZT lies in the fact that Seebeck coefficient (S), electrical conductivity (σ), and thermal conductivity (κ) are not independent, it is extremely difficult to alter one without affecting the other. In 1993, Hicks and Dresselhaus first proposed that the low dimensional semiconductor structures could overcome bulk materials' intrinsic limit. [1,2] Subsequently, Venkatasubramanian reported ZT of 2.4 for BiTe superlattice structure in 2001[3] and Harman reported ZT of 2.0 for PbTe quantum dots in 2002. [4] Interestingly, the main advantage of these state-of-the-art nanostructured material is in the reduction of lattice thermal conductivity compared to bulk BiTe. Si/SiGeC and Si/SiGe superlattice microcoolers have also been demonstrated with a maximum cooling of 7^{0}C at a 100^{0}C stage temperature and a cooling power density of 600 W/cm^2. [5, 6, 7] The multibarrier hot electron filters were used which could increase the Seebeck coefficient without reducing the electrical conductivity. The focus on Si-based microrefrigerators is targeted to provide on-chip hot spot cooling solution without the hassle of dealing with incompatibility of materials, additional thermal interface resistances when dissimilar materials are integrated, and reliability issues.

Currently, thermal budget is mostly driven by the "hot spots", where the heatflux could be 3-4 times higher than the average, and temperature could be up to 50^{0}C higher than the average. Thus if we could reduce the hot spots temperature even at the cost of marginal average temperature increase, it is still could be a cost-saving approach. That is the idea of developing on-chip microrefrigerators. Here we investigated the idea of using three-dimensional device geometry based on bulk silicon and utilize the thermoelectric effect to spread the localized heatflux away from hot spots. [8] In this case high thermal conductivity is needed in order to reduce the effect of background heating on the silicon die. [9] The device geometry with indicated current and heat flow is illustrated in Figure 1. When we apply a positive current to p-type material, at the cathode interface, there will be thermoelectric cooling. Current flow through the silicon substrate carries the heat flux (this is the average transport energy of holes). When holes reach the anode interface, the heat is released to the lattice. One can locate the anode in a region where there is less overall heating or to make the anode metal contact area large in order to reduce temperature rise at that location. Due to the current flow, Joule-heating is generated inside the silicon, but the substrate temperature increase will be very modest, in the order of 0.1-0.2 ^{o}C because the current required to reach the maximum cooling is minimal. The generated cooling power at the cathode interface could be used to absorb the localized transistor heating. Most importantly, in this case the capability of removing heatflux is not directly constrained by the low ZT of the material. So silicon came across to be a good candidate considering its high thermal conductivity, in the order of 125W/cm^2 and its wide applicability in semiconductor industry.

In previous studies [8], we studied the device geometry effects on achieving the maximum cooling and pointed that a three-dimensional structure is necessary to achieve a better maximum cooling power density contributing from the current non-uniformity distribution and heat spreading effects. In this paper, we will focus on optimizing the silicon doping concentrations, which affects the materials' properties, mainly Seebeck coefficient and electrical conductivity.

2. Current experimental devices performance

A typical P-type 3D silicon microrefrigerator is demonstrated in Figure 1, Boron-doped to 5e19cm^{-3} with device sizes ranging from 40x40~100x100 µm^2 using standard lithography, dry etching and metal evaporation technique. Experimentally it demonstrates a maximum cooling power density of 220 W/cm^2 though the maximum cooling is less than 1^{0}C as illustrated in Figure.

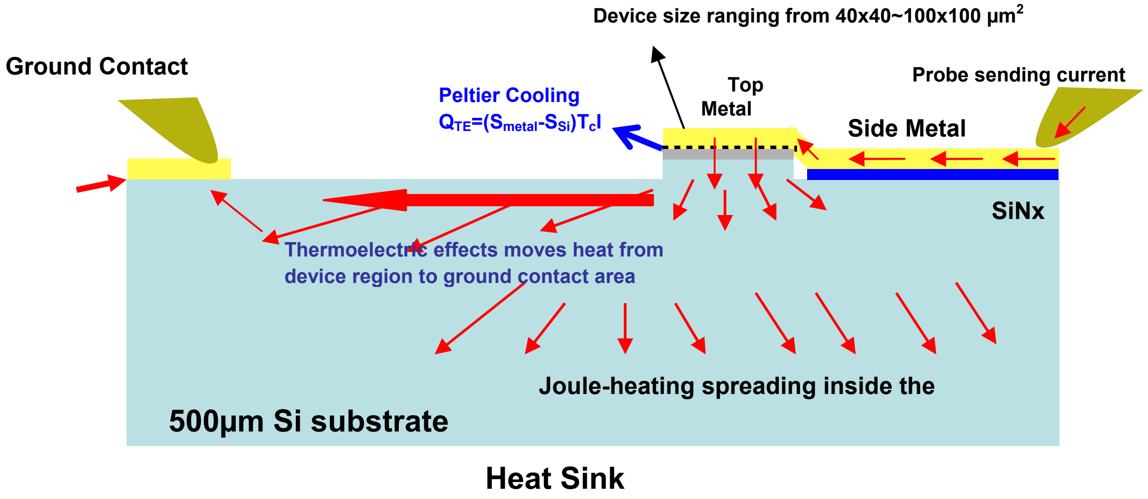

Figure 1: Schematic of silicon microrefrigerator with indicated current and heat flow

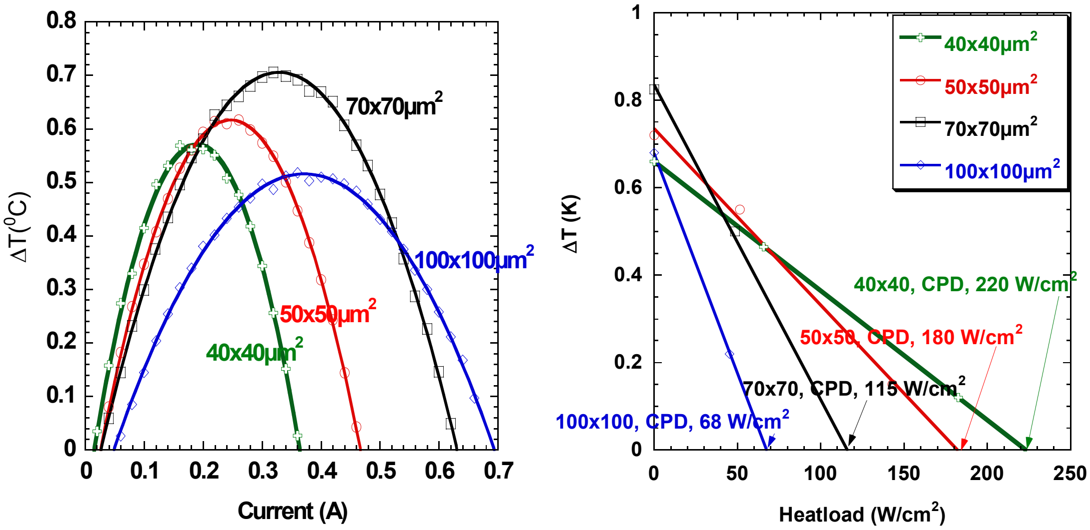

Figure 2: (Left) cooling versus supplied current; (right) maximum cooling versus supplied heatload, with indicated maximum cooling power densities for various device sizes. (Experimental data)

Doping(cm-3)	S (μV/K)	σ (ohm-cm)$^{-1}$	S^{2}σ (*10^{-4}W/mK)	ZT	T$_{max}$
1.00E+18	850	75	0.5	0.0130	2.0
5.00E+18	750	100	0.6	0.0135	2.0
1.00E+19	600	180	0.6	0.0156	2.3
5.00E+19	400	500	0.8	0.0192	2.9
1.00E+20	250	1150	0.7	0.0173	2.6

Table 1: List of Seebeck coefficient, electrical conductivity, power factor ($S^2\sigma$), ZT and estimated maximum cooling for different doping concentration, data from Gaballe's paper. [13]

3. 3D finite element modeling

In order to capture all the non-ideal factors, heat and current spreading effect inside the real devices, we developed a 3D electrothermal model using finite element analysis ANSYS™ software, which is powerful in solving coupled-field problems. [10] Figure 3 shows the device model with finite element meshing. Due to the large aspect ratio of the device— the thinnest insulating layer composed of SiN_x is only 0.3μm compared to the substrate with 500μm thickness—the meshing of this device was very challenging. The element was tetrahedral-shaped with element size ranging from 0.15 -- 50μm depending on the location of the device, for example, the metal/semiconductor contact region has a much finer meshing than the substrate.

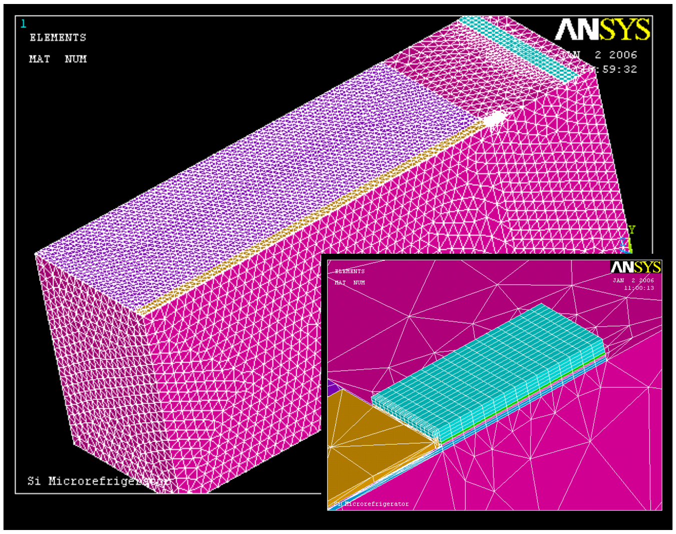

Figure 2: Silicon microrefrigerator device model with finite meshing, right corner is the enlarged picture shows the finer meshing at metal/semiconductor contact region

Different from the conventional thermoelectric modules, where heat and current are both transport in one-dimension, the silicon microrefrigerator has the unique 3D device geometry. Both the current and heat spread in 3D, thus it is necessary to use a 3D electrothermal transport model to replace the conventional 1D balance equation. In the current model, the bulk Joule heating and heat conduction are automatically calculated by solving Fourier heat conduction equation, Poisson equation for electrostatics and current continuity equation with the defined materials' properties. The heat conduction is described by the equation:

$$\rho(\vec{x})c(\vec{x})\frac{\partial T(\vec{x},t)}{\partial t} = H(\vec{x},t) + \nabla_{\vec{x}} \cdot \left(\kappa(\vec{x})\nabla_{\vec{x}} T(\vec{x},t)\right),$$

where, T, H, ρ, c, κ denote temperature, heat generation density, mass density, specific heat and thermal conductivity respectively. This study is in steady-state, thus the left part of the equation equals to zero. The Poisson equation is represented by $\nabla^2 \mu = -\frac{\rho}{\varepsilon}$, where, μ is potential, ρ is charge density and ε is permittivity of the material. The current continuity equation for electrons is defined as: $q\frac{\partial n}{\partial t} = \nabla \cdot \vec{J} - q(R-G)$, where q is the electron charge, n is the electron concentration, t is the time, $\vec{J}$ is the current density, and G,R represents the generation and recombination rates respectively. A similar equation could be written for holes. The Peltier effect is modeled as an interface cooling/heating source at the designated interfaces, as illustrated in Figure 1. The accuracy of the program has been verified with experimental results. [11] In addition, similar methodology also applied to calculate the cooling of commercial BiTe thermoelectric elements and the results are consistent to the manufacturer data. [12]

4. Simulation Results

Using this model, we studied the effect of doping concentration influence on silicon microrefrigerators. The change of doping concentration affects the Seebeck coefficient as well as the electrical conductivity. With the increasing doping concentration, the semiconductor will have a higher electrical conductivity but a smaller Seebeck coefficient. Figure 3 illustrates the correlation of Seebeck coefficient and electrical conductivity versus doping concentration from literature. [13] For conventional 1D TEC devices, the optimized doping concentration is determined by the maximum ZT, where the $S^2\sigma$ reaches maximum. Table 1 listed the doping concentration, Seebeck coefficient, electrical conductivity, power factor ($S^2\sigma$), ZT and the estimated maximum cooling by 1D electrothermal model, ½ ZT_c^2. As we could see, the maximum cooling for 1D device is at the maximum power factor, 5e19 cm^{-3}, where silicon estimated to cool up to 2.9^{0}C. However, for our current 3D silicon microrefrigerators, the optimum doping is different. Figure 4 illustrates the maximum cooling of a 40x40µm^2 silicon microrefrigerator with different doping concentration ranging from 1e18 ~1e20 cm^{-3}. The maximum cooling that the device reaches, ~3^{0}C occurs at 5e18 cm^{-3}, which is an order of magnitude lower than the 5e19 cm^{-3}, where 1D device reaches its maximum cooling. Figure 5 illustrates the maximum cooling of si microrefrigerator with optimized doping concentration in finite element model. This optimized doping change is due to the non-ideal factors which affect a realistic device. In this case, metal-semiconductor contact resistance and the side metal contact add additional sources of Joule heating which affects the overall device performance and shift the optimum doping to a lower value. When we remove the Joule heating induced by the probe heating and the metal semiconductor contact resistance in the model, we found that the optimized doping concentration move back to 5e19cm^{-3} as illustrated in Figure 6.

Also from Figure 5 and Figure 7, we also noticed that the maximum cooling that the 3D Si microrefrigerator could achieve exceed the maximum cooling predicted by the 1D theory, ½ ZT_c^2. This improvement is contributed from the non-uniform current distribution, which causes the non-uniform temperature distribution, thus in center region, the maximum cooling of 3D device could exceed the 1D device. The detailed analysis of the 3D geometry effect had been explained elsewhere. [8, 12, 14]

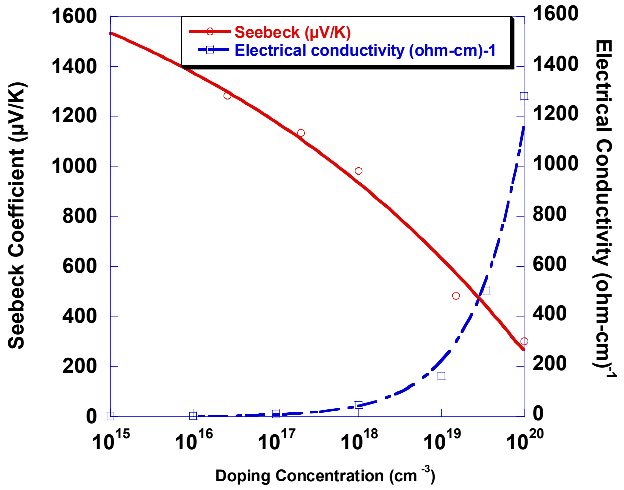

Figure 3: P-type Silicon Seebeck coefficient and electrical conductivity versus doping concentration. [Error! Bookmark not defined.]

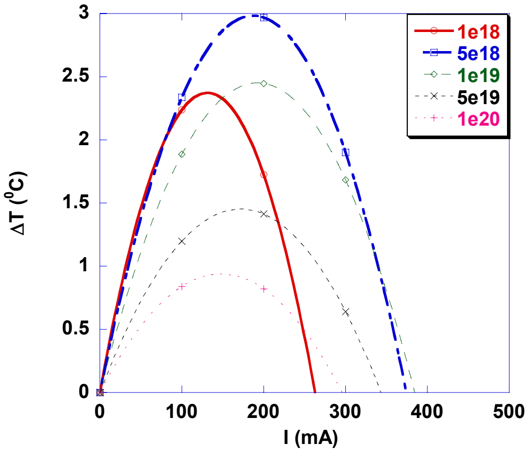

Figure 4: Maximum cooling versus supplied current for Si microrefrigerator (40x40µm^2) device with different doping concentration varying from 1e18 to 1e20 cm^{-3}.

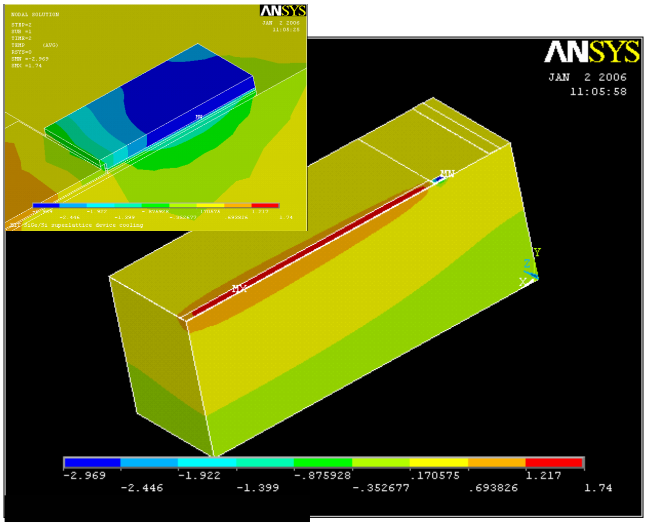

Figure 5: Demonstrated maximum cooling for 3D silicon microrefrigerator with 5e18 cm-3 doping in finite element model.

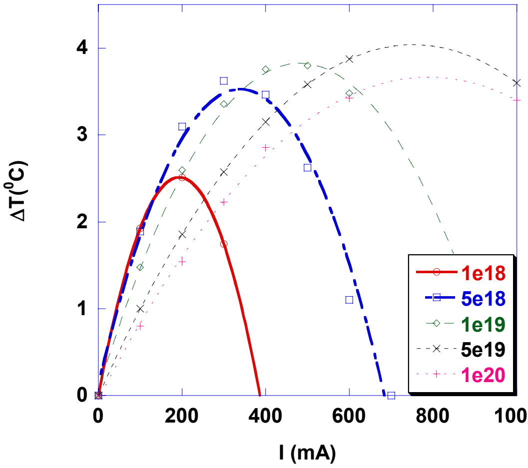

Figure 6: Maximum cooling versus supplied current for "ideal" Si microrefrigerator (40x40 µm2) with different doping concentration --- no probe Joule heating, no semiconductor contact resistance.

5. Conclusions and Future Work

We developed a 3D electrothermal model to study and optimize silicon microrefrigerators. We studied p-type silicon microrefrigerators with different doping concentrations and found out that silicon microrefrigerator could cool up to 3^0C with supplied 0.2A at the optimized doping concentration, 5e18 cm^{-3}. It is interesting to find that this optimized doping concentration is different from the expected value where, $S^2\sigma$ reaches the maximum value (5e19 cm^{-3}). This shift is due to the non-ideal factors inside the devices. It is important to consider these non-ideal factors, mainly metal-semiconductor contact resistance and Joule heating from side probe in real device designs. Silicon microrefrigerator could be used as a potential on-chip thermal management solution to remove hot spots because of its localized cooling with high cooling power density. Next, we plan to experimentally test samples with different doping concentrations and verify the simulation results.

Acknowledgments

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