Miniaturized Thermoelectric Generators Based on Poly-Si and Poly-SiGe Surface Micromachining

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SUMMARY

We report on miniaturized thermoelectric generators which are being developed to convert waste heat into a few µW of electrical power sufficient to supply microelectronic circuitry. A BiCMOS realization using standard materials is favored to make these generators amenable to low cost applications. In order to optimize our device, the design and the material properties have been studied. The use of micromachining techniques allowed us to improve the thermal efficiency of the generator significantly. Low thermal conductivity of the thermoelectric materials proved to be the most important factor to increase the output power. The materials we have investigated are poly-Si and poly-SiGe. Experimental results of the fabricated devices show good agreement with the predictions of thermal simulations.

Keywords: thermoelectric generator, surface micromachining, poly-SiGe

INTRODUCTION

For the operation of small electronic devices and systems, often power sources of some few µW are sufficient. If there is a thermal gradient between the location of the device and the ambient, the batteries of such systems could be replaced by attached thermoelectric generators (TEGs). For example, there should always be a temperature difference of some degrees between the surface of the human body and its environment. Exploiting this temperature gradient, wrist watches can be powered thermoelectrically [1]. Some other environments such as heating appliances (e.g. radiators) or engines in the automotive field provide even higher thermal differences.

Our goal is to develop a micro-machined thermoelectric generator that matches the needs of low cost, small size and low power systems. Therefore, we explore BiCMOS materials such as poly-Si and poly-SiGe for our thermoelectric applications. Since these materials are compatible with the fabrication process, our generator can easily be integrated on chip level.

BASIC CONSIDERATIONS

As usual for TEGs, our device consists of couples of legs made of n- and p-type thermoelectric materials (see Fig. 3). These legs are electrically connected in series via metal bridges and are arranged in meanders to make best use of the given area. The actual generator layer is sandwiched between the silicon substrate below and a convection-cooled heat sink mounted on top. A thermal gradient between the bottom of the device and the ambient on top of it effects a vertical heat flow a part of which can be converted into electrical energy by the thermoelectric effects. The main difference to conventional, large scale applications of TEGs lies in the small internal thermal resistance of the device itself compared to the large thermal resistors enclosing the actual generator. Because of the dominance of the thermal resistors covering the device, the system is operated under constant heat flux conditions rather than at a constant temperature difference. In order to understand this behavior, the thermoelectric network of the device (see Fig. 1) has to be solved.

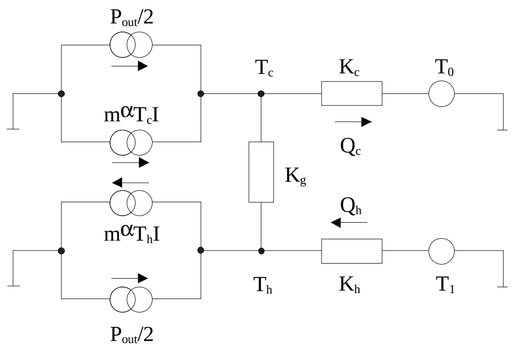

Fig. 1. Thermal network of a thermoelectric generator including the Peltier effect and Joule heating acc. to [2].

For a given relative Seebeck coefficient α of the two thermoelectric materials employed, the generated voltage U_0 can be expressed by the number m of couples of thermoelectric legs and the temperature difference ΔT_g between the hot and the cold junctions:

$$U_0 = m \alpha \Delta T_g \,. \qquad (1)$$

As the system shall be operated at maximum electrical power output P_{out} the case of matched impedances is considered where the ohmic resistance of the generator is equal to the electrical resistance of the load:

$$P_{out} = U_{out} I = \frac{U_0^{\,2}}{4R_g} = \frac{m^2\alpha^2}{4R_g}\left(\Delta T_g\right)^2 , \qquad (2)$$

where U_{out} is the output voltage, I is the electrical current and R_g is the electrical resistance of the generator.

Solving the thermoelectric network for the case of a matched electrical load resistor, the solution for the maximum electrical power output of the generator can be calculated in dependence of the external temperatures T_0 and T_1, the material properties and geometry only [2]. This solution also reveals that a low power thermoelectric generator (LPTG) operates in another regime than conventional large scale TEGs (see Fig. 2).

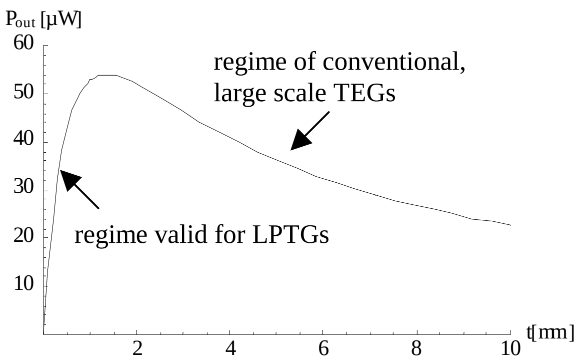

Fig. 2. Calculated output power of a typical TEG as a function of the height t of the thermoelectric legs. LPTGs are operated in the regime shown on the left.

For an ideal thermoelectric generator that fulfills the requirements of a LPTG, i.e. the length of the thermoelectric legs lies in the µm range, the following approximation for the maximum electrical power output applies [2]:

$$P_{out} = \frac{1}{16}\frac{\alpha^2}{\lambda^2\rho}\, t\, \frac{A_0 + A_{sp0}}{A_0}\, \frac{\lambda_c^{\,2}\lambda_h^{\,2}}{\left(t_c\lambda_h + t_h\lambda_c\right)^2}\left(\Delta T\right)^2 A_g \,. \qquad (3)$$

Here, A_g is the total area of the generator, λ_c and λ_h are the thermal conductivities and t_c and t_h the thicknesses of the thermal resistors on the cold and hot side, respectively. A_{sp0} denotes the free area between neighboring legs in a unit cell.

This result shows that the maximum output power per area of the generator is limited by the Seebeck coefficient α, the electrical resistivity ρ and the thermal conductivity λ. P_{el} increases with the height t of the thermoelectric couples and it decreases with the cross-sectional area A_0 of the legs. The above relation for maximum power output also suggested to define a modified figure of merit, Z*, characterizing the performance of a LPTG as:

$$Z^* = \frac{\alpha^2}{\lambda^2\rho} \,. \qquad (4)$$

Since the square of the thermal conductivity λ enters this expression, the importance of a high internal thermal resistance of a LPTG is evident. Hence, this modified figure of merit Z* is an appropriate criterion to find suitable materials for low power thermoelectric devices.

For the derivation of the modified figure of merit Z* as introduced above the contact resistances R_c of the metal junction have been neglected. To describe the system for non-vanishing R_c the electrical resistance of the generator would be:

$$R_g = \frac{2m\left(\rho t + 2R_c A_0\right)}{A_0} \qquad (5)$$

Note that each thermocouple implies four metal contacts. It will be discussed below that the contact resistances can amount up to more than half of the total electrical resistance.

MATERIAL PROPERTIES

The Seebeck coefficient α and the electrical resistivity ρ have been measured for both pure poly-Si and poly-$Si_{70\%}Ge_{30\%}$ (see Tab. 1). The Seebeck coefficients have been extracted using special planar test structures [3]. The values of the electrical resistivity have been determined from van-der-Pauw Greek cross structures [4]. From these results, the most efficient material combination can be selected.

Tab. 1: Measured data for 400 nm thick poly-Si and poly-SiGe layers. Z* is calculated assuming an average thermal conductivity of $\lambda = 20\ Wm^{-1}K^{-1}$ for poly-Si and an average $\lambda = 5\ Wm^{-1}K^{-1}$ for poly-SiGe [5].

material	doping concentration c [10^{20} cm^{-3}]	Seebeck coef. α [μVK^{-1}]	el. resistivity ρ [mΩcm]	figure of merit Z* [μW^{-1}]
n poly-Si (-)	0.25	-183 ± 3	9.71 ± 0.01	0.86
p poly-Si (-)	0.25	165 ± 5	6.8 ± 0.1	1.01
n/p poly-Si couples (-)	0.25	348 ± 6	8.2 ± 0.1	3.68
n poly-Si (+)	2.5	-57 ± 9	0.813 ± 0.001	1.00
p poly-Si (+)	2.5	103 ± 17	2.214 ± 0.004	1.19
n/p poly-Si couples (+)	2.5	160 ± 19	1.514 ± 0.004	4.21
n poly-SiGe (-)	0.25	-249 ± 19	117 ± 2	2.11
p poly-SiGe (-)	0.25	105 ± 7	8.8 ± 0.1	4.97
n/p poly-SiGe couples (-)	0.25	354 ± 20	63 ± 2	7.93
n poly-SiGe (+)	2.5	-77 ± 7	2.37 ± 0.04	9.90
p poly-SiGe (+)	2.5	59 ± 9	1.87 ± 0.01	7.46
n/p poly-SiGe couples (+)	2.5	136 ± 11	2.12 ± 0.04	34.70

The advantage of employing poly-SiGe instead of pure poly-Si lies in its expected lower thermal conductivity [5]. However, in agreement with earlier work [6], the electrical resistivity of phosphorous-doped poly-SiGe was found to be higher than that of identically n-doped pure poly-Si. This finding limits the gain in performance of poly-SiGe as thermoelectric material compared to poly-Si because it leads to a higher total electrical resistance of the generator.

DEVICE REALIZATION

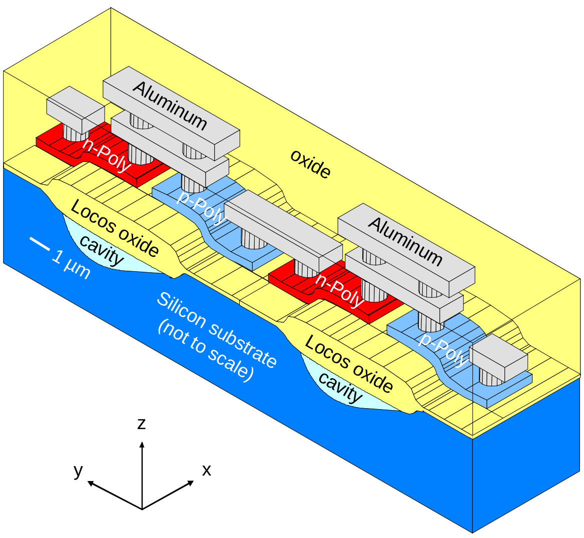

Fig. 3: Schematic view of two thermoelectric couples of the BiCMOS realization. Additionally, the cavities which can be etched into the Si-substrate are shown.

The generators were fabricated in a BiCMOS production facility, each one consisting of 59.400 thermocouples integrated on an area of about 6 mm^2. A schematic view onto the cells of the generator is displayed in Fig. 3. The thermal isolation between the cold and the hot side of the thermoelectric legs is achieved by means of a 1.6 µm thick thermal barrier made of LOCOS oxide (see Fig. 4). A 400 nm thick polysilicon layer is partly phosphorous-implanted to generate the n-legs and partly boron-implanted in other regions to form the p-legs. Afterwards, the polysilicon layer is patterned to release the thermoelectric legs. Both, samples with pure polysilicon as well as others containing poly-$Si_{70\%}Ge_{30\%}$ have been produced. The poly-SiGe layers were grown in a conventional chemical vapor deposition (CVD) reactor, commonly used for poly-Si deposition. For the deposition a mixture of disilane (Si_2H_6) and germane (1% GeH_4 in H_2) was used. The carrier gas was hydrogen. The poly-SiGe layers were grown at a temperature of 670 °C and a pressure of 19 Torr. With these parameters a high deposition rate of 100 nm/min was achieved. To avoid big grains that may result from bad nucleation of germanium on oxide, a thin polysilicon wetting layer of about 5 nm was deposited prior to the deposition of poly-SiGe. Aluminum bridges are used to avoid pn-junctions which otherwise would exist between adjacent thermoelectric legs. A second metal bridge is added to every other junction to improve the thermal coupling to the surface of the device.
Additionally, cavities can be etched into the silicon substrate using isotropic CF_4 dry etching (see Figs. 3 and 4). These measures help to optimize the heat flux direction within the generator.

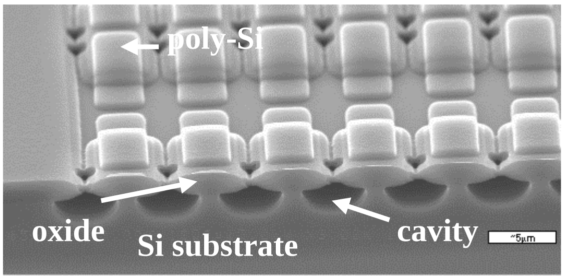

Fig. 4: SEM-micrograph showing cavities etched into the Si-substrate through an oxide mask using CF_4 dry etchant. View before metallization into the y-direction as displayed in Fig. 3.

DEVICE TESTING

The devices have been tested on wafer-level, placed on a heatable thermochuck and a cooler mounted on top. In agreement with the results of the thermal simulations previously performed using the FEM tool ANSYS [3], the micromachining steps improved the output voltage of the generator significantly. The output gain of the poly-SiGe type combined with substrate etching was even higher than expected. An output efficiency of about 100 mV/K was obtained which means a factor of 2.3 increase compared to the basic type. Measured output voltages for each type of thermoelectric generator are shown in Fig. 5.

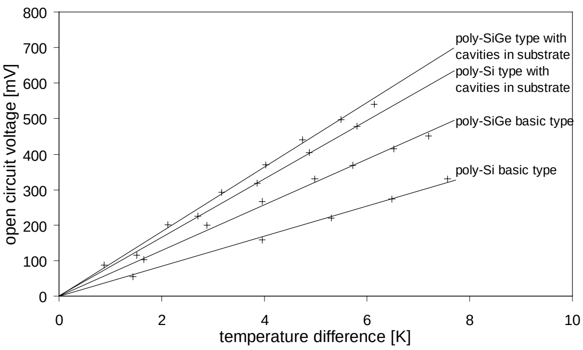

Fig. 5: Measured open circuit voltages of different highly doped types of thermoelectric generators versus the temperature drop between bottom and top of the entire chip.

The output power is limited mainly by the electrical resistance of the generators. We found that for generators with highly doped poly-Si the resistance of a contact was 23±1 Ω. That means that about half of the total resistance of about 10 MΩ results from the contacts. In the case of poly-SiGe, the resistance of a contact was found to be 119±4 Ω. As the electrical resistivity of n-doped poly-SiGe is undesirably high, too, measures have to be taken to reduce those resistances. Experiments focussing on these matters are in progress.

CONCLUSION

The difference between conventional TEGs and low power thermoelectric generators (LPTGs) has been elaborated. A modified figure of merit Z* for LPTGs was introduced which reveals the importance of a high internal thermal resistance of the generator. Z* can be used as a valuable criterion to find suitable materials for these specific thermoelectric devices. The relevant thermoelectric properties of our BiCMOS materials were measured and compared. In order to optimize the heat flux within the device, special surface micromachining techniques have been used. Generators made of poly-Si as well as poly-SiGe have been fabricated in our facility and were tested successfully. The output voltage was in the range of about 100 mV/K. Further efforts will still have to be made in order to reduce the electrical resistance of the generators.

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