Thermoelectric Power Generation Using Large Area pn-Junctions

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Abstract

A new approach to thermoelectric power generation using large area pn-junctions is presented [1]. Thermally generated electron-hole pairs are separated by the built-in potential gradient of the pn-junction. A temperature gradient applied along this pn-junction causes a flux of both carrier types from the hot to the cold region. This principle allows us to use layer structures similar to solar cells as thermoelectric elements. Thermoelectric modules can be manufactured by stacking these elements. Effective development and optimization of thermoelectric elements and modules depend on a strong simulation environment based on accurate models. We use the device and circuit simulator Minimos-NT of the Institute for Microelectronics / TU Vienna for both two- and three-dimensional simulations of thermoelectric devices. Its open description language and sophisticated model server enables us to easily implement models for new materials as well as for extended temperature ranges. The models are calibrated with measured data and results from full band Monte-Carlo simulations. Experimental results for Silicon based thermoelectric elements and modules are presented and compared to simulation results.

Introduction

Using large area pn-junction similar to solar cells as shown in Figure 1 for thermoelectric power generation has one main advantage: the strong correlation of thermal and electrical properties can be overcome. The generation of electron-hole pairs and the transport of the carriers are spatially separated and therefore both effects can be optimized independently from each other.

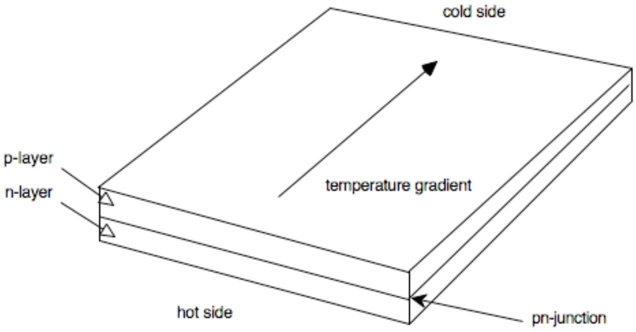

Figure 1: Large area pn-junction with temperature gradient

To understand why a temperature gradient within this structure leads to the generation of an electrical current we have to consider the effect of the temperature on the electrostatic potential of a pn-junction (Figure 2). Basically, the higher temperature T_1 leads to the smaller step ΔE_1 from the potential of the n- to the p-layer compared to the step ΔE_2 at the lower Temperature T_2.

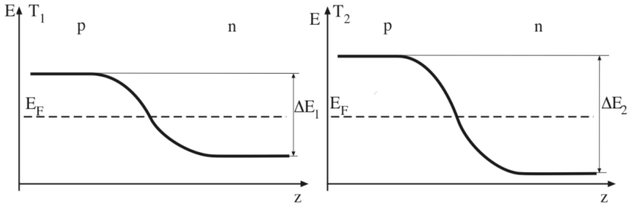

Figure 2: Temperature influence on the electrostatic potential of a pn-junction

By having a temperature gradient in a large area pn-junction both conditions occur neighboring to each other with the result that carriers at different potentials come into contact and thus experience a driving force to the colder region (Figure 3) [2].

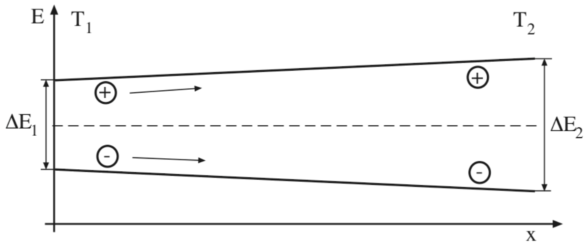

Figure 3: Driving forces to generate ambipolar drift and diffusion

Because both types of carriers, electrons and holes, are moving in the same direction (ambipolar drift and diffusion), away from the pn-junction at the higher temperature T_1 at the left hand side of Figure 3, this region becomes depleted and the local thermal equilibrium is disturbed. The generation-recombination balance is shifted to higher generation to compensate the off-drifting carriers (Figure 4).

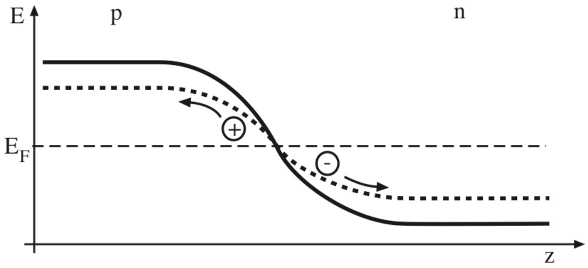

Figure 4: Higher generation because of depletion

At the part of the structure with the lower temperature T_2 on the right hand side of Figure 3 the opposite effect takes place. The incoming carriers enhance the recombination (Figure 5). So the net effect is a circular electrical current within the large area pn-junction from the hot region with enhanced generation to the cold side with increased recombination.

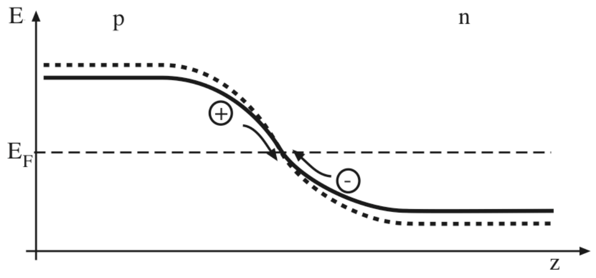

Figure 5: Recombination at the cold side

Using selective contacts to both the n- and p-type layers, this circular current can be diverted to an external load and a power source is established, a thermoelectric element (Figure 6). Because such an element only consists of one single material, mechanical tension between different materials are completely avoided and thermal cycling will not lead to fatigue. Using the right base material, a semiconducting material with high band gap energy, even very high temperatures above 1000°C can be used for thermoelectric power .

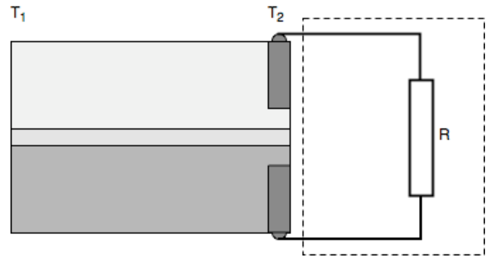

Figure 6: Principle of a thermoelectric element

An equivalent circuit of a thermoelectric element can be described as a network of diodes and ohmic resistors (Figure 7). The diodes represent the pn-junction and the ohmic resistors are the p- and n-layers.

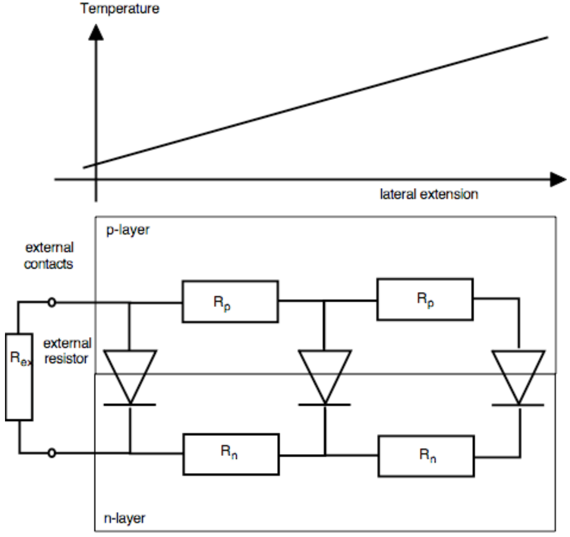

Figure 7: Equivalent circuit for a thermoelectric element

Thermoelectric modules are fabricated by stacking the thermoelectric elements in such a way that the elements are thermally in parallel and electrically connected serially (Figure 8). The elements are mechanically and electrically connected by wafer bonding similar to three-dimensional integrated circuits (3D-IC) [3].

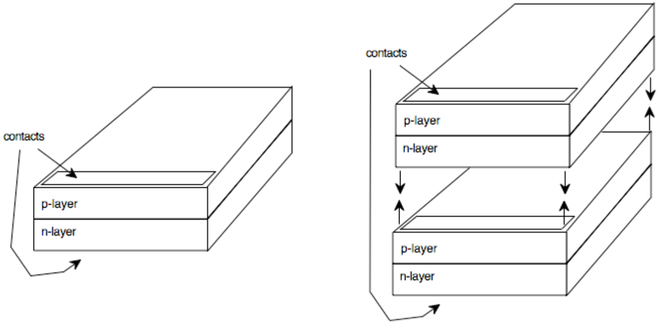

Figure 8: Fabrication of modules by stacking

Experimental Results

The first experiments were performed using Silicon based thermoelectric elements. Silicon has a very high heat conductivity which limits the achievable efficiency considerable but allows low cost solutions for prototyping. However, one advantage of the high heat conductivity would be a very high heat flux density to achieve high energy densities.

In Figure 9 the results for measurements on one thermoelectric element are presented. For the lower three temperatures it was possible to measure the output power as function of the load resistor, but for the two higher temperature ranges the high heat flux prevented constant conditions for the time of the resistance sweep, therefore only single resistance values close to the expected peak power were used. As can be expected from the activation process for the generation of electron hole pairs, the peak power shows an exponential correlation with the temperature.

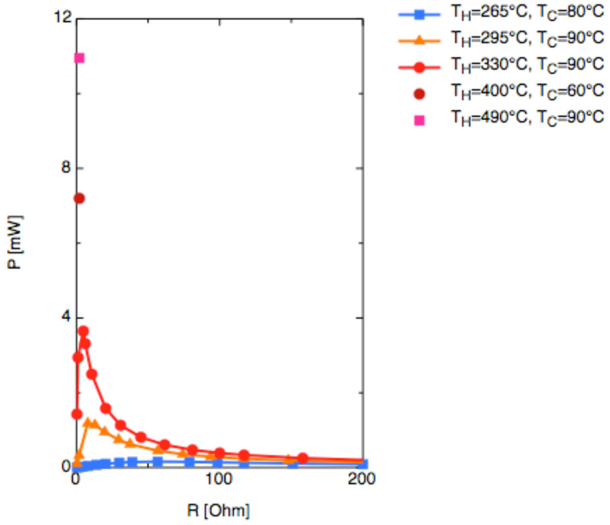

Figure 9: Experimental results for a single thermoelectric element at different temperatures

To manufacture thermoelectric modules it is necessary to stack single elements. In Figure 10 measurements of the peak power for different stacks with one, two, and four elements are shown. As expected, the peak power doubles for two elements over one element, but for four elements the peak power decreases. The thermal conductivity of four stacked elements is too high under the used heating conditions so that the temperature of the hot side remains at low values. Because of the exponential dependence of the peak power from the temperature the power output becomes very low. In future modules the thickness of the elements, especially of the substrate layer, will be reduced to minimize the heat flux.

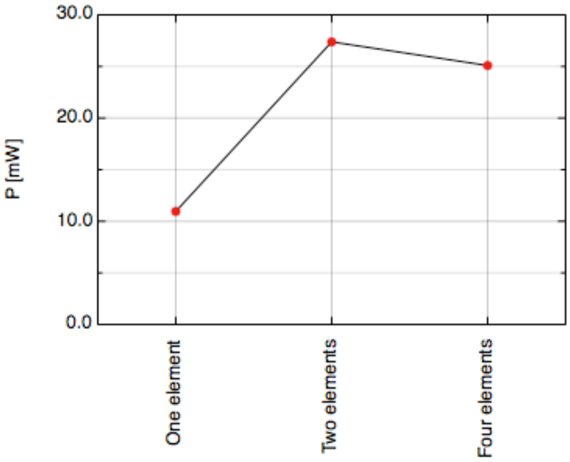

Figure 10: Results for modules with one, two, and four elements

One possibility to optimize the generation of electron hole pairs separately from the transport can be seen in Figure 11. Three different elements with the same temperature conditions generate electric currents within two orders of magnitude. Element 1 has a small density of generation centers with low effectivity (implantation with H^+ ions, which produces states all over the band-gap). Element 2 has high effective generation centers (implantation of Au in Silicon, which generates deep levels close to the center of the band gap) which increase the produced current by one order of magnitude. Because every generation center is also a recombination center, a non uniform distribution of the same generation centers used in element 2 was realized in element 3. Here, these centers are confined to the side of the element with higher temperature, thus reducing the number of recombination sites along the course to the side with lower temperature. Again, we achieve an increase of the current by one order of magnitude.

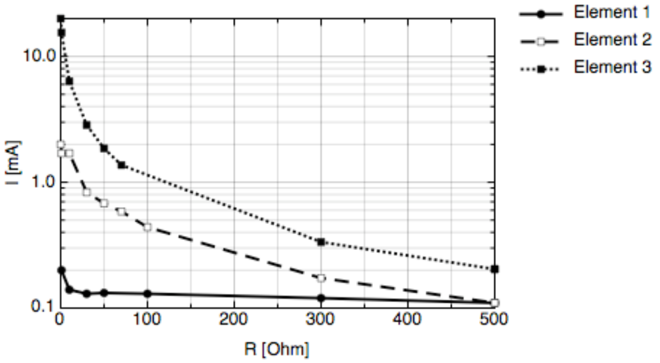

Figure 11: Generated current with different number, properties, and distribution of generation centers

Because the generation of electron hole pairs depends strongly on the temperature, the curvature of the temperature gradient has a large influence on the amount of generated current. Theoretical considerations and numerical simulations have shown that a thermoelectric element with a shallow gradient at high temperatures and a steep gradient at low temperatures have the potential for an increased power output by a tenfold, again.

Simulation Results

We use the device simulator Minimos-NT to run predictive simulations of thermoelectric devices [4]. This enables inexpensive and rapid prototype development of highly specialized devices for several application scenarios. The structure shown in Figure 12 and Figure 13 implies the idea of the separation of generation and transport zones within the device.

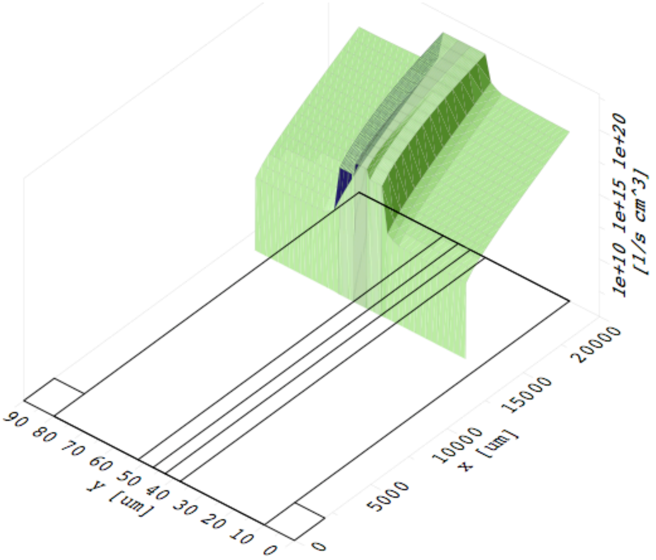

Figure 12: Generation rate of electron hole pairs

A linear temperature gradient is applied from right (hot, x = 20000 µm) to left (cold, x = 0 µm) with the electrical contacts on the cold side. Between highly doped regions, low doped and an intrinsic layer are realized. The main region of generation is the hot end of the intrinsic and the low doped layers. The doping in the low doped zones is 10^{16} cm^{-3}. The exponential dependency of the generation from the temperature can easily be verified in Figure 12. The generation rate is only plotted for values greater than 10^{10} s^{-1} cm^{-3}.

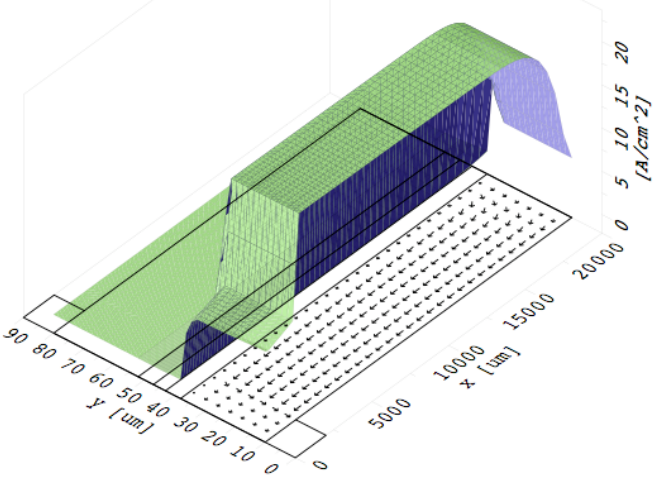

Figure 13: Current density within the p-layer

The generated carriers are transported to the contacts via the p- and n-layers. Figure 13 shows the current increase along the x axis within the generation area.

Figure 14 shows the power output of the thermoelectric generator in dependence of the external load resistance. The maximum power output is reached at $R_i = R_{ext}$. With rising temperature values T_{hot} the power output increases and the resistance of best power output decreases. The plot is very similar to the measured values shown in Figure 9 without using fitting parameters.

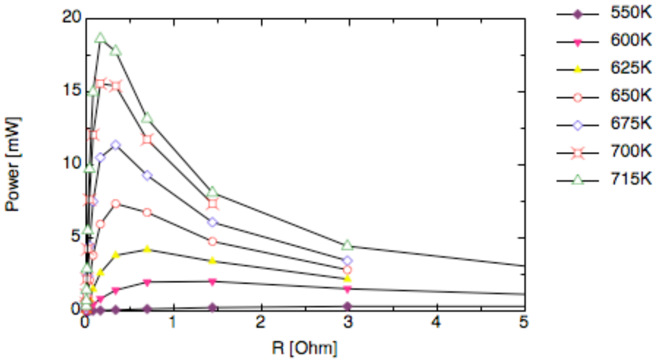

Figure 14: Simulated output power

The optimization framework SIESTA is used in combination with Minimos-NT to optimize the thermoelectric generators for maximum efficiency under given external parameters [5]. Both distributed (e.g. the distribution of generation centers) and non-distributed values (e.g. the device geometry) can be optimized.

Results and Discussion

The presented new approach to thermoelectric power generation is very promising, despite the fact that the efficiency of Silicon based thermoelectric elements and modules is very limited. By using materials like SiGe, which have similar electronic properties, but much lower thermal conductivity, much higher efficiencies are feasible.

The strong correlation of thermal and electrical properties can be overcome. The generation of electron hole pairs and the transport of the carriers are spatially separated and therefore can be optimized separately from each other. Therefore, ZT, the figure of merit is not suitable to fully describe the possibilities of our structures.

Other advantages of our technology are:

The shape of the temperature gradient within the thermoelectric element influences the amount of generated carriers and can be used to increase the power density.

Thermoelectric elements can be fabricated using only one material so the fatigue due to thermal cycling can be avoided.

The manufacturing of the elements and modules can be done in a similar way to well established processes in the semiconductor and solar cell industry.

Our goals for the next development steps are:

- Reducing the thickness of the thermoelectric elements including substrates to 100µm or below to minimize the thermal flux
- Finding the optimal type and distribution of generation centers to increase the peak power
- Using materials with lower lattice heat conductivity to increase the efficiency
- Finding the optimal temperature gradient
- Increase of power densities up to 10 W/cm^2 (100 kW/m^2)

Conclusions

The conclusion can be summarized in a table which was originally compiled by Lon E. Bell [6] and extended with the estimated values made possible by the technology of SAM.

Characteristics	Present	Needed	Technology by SAM
Thermal Power Density (W/cm^2)	6 - 12	50 - 200	up to 200
Power Output (W per module)	14 - 25	500 - 4000	up to 500
Cost/Watt Output (EUR/W)	too high	0.08 - 0.40	> 0.50
Efficiency (% Carnot)	3 - 4	16 - 25	1 - 30

Acknowledgments

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