Design Optimization of Large Area Si/SiGe Thermoelectric Generators

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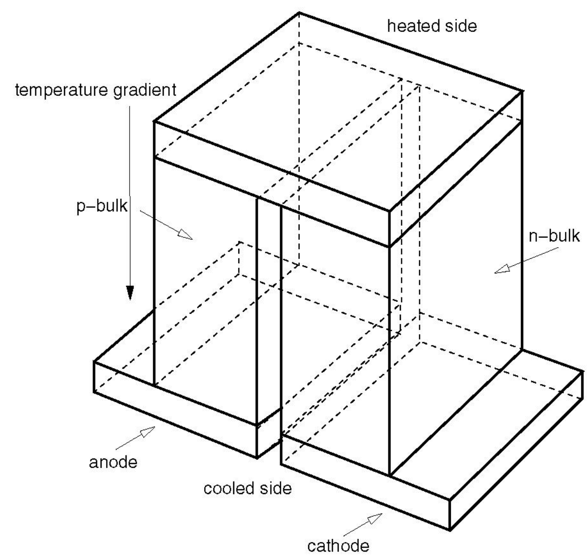
***Abstract*— We present a comparison of large area pn-junction thermoelectric generators and classical thermoelectric modules. In contrast to conventional thermocouples, the thermal generation of carriers is explicitly used within the new device structures. The gradient of the pn-junction's built-in potential causes the separation of the thermally generated carriers. For the application of waste heat recovery, the device is exposed to an external temperature gradient along the pn-junction which induces driving forces to both electrons and holes from the heated to the cooled end of the structure, where contacts are applied. The influence of device geometry and material composition on the device behavior is investigated. Simulation results obtained by our device and circuit simulator MINIMOS-NT working in conjunction with the optimization framework SIESTA are presented.**

I. INTRODUCTION

Thermoelectric power devices are an attractive possibility to directly convert heat energy to electricity. The lack of moving parts results in a long lifetime and practically no need of maintenance. Due to the relatively low efficiency and power density of today's commercially available devices, they are generally only used in environments where the advantage of using a maintance free generator outweighs the poor efficiency by now. A prominent example is the use in satellites and spacecraft systems.

In its early days, thermoelectric power conversion using semiconductors was achieved by conventional device structures as shown in Fig. 1. A p-doped and an n-doped semiconductor are electrically connected at the heated side with a metal part. The temperature gradient along the semiconductors causes a flux of the available carriers from the hot to the cold end and thus a voltage which can be measured on the electrical contacts at the cold end.

In order to meet the demand for widely usable thermoelectric elements, more efficient as well as highly reliable structures and materials are needed that are suitable for a wide range of temperatures. Recently, several approaches for improving the efficiency and power output of thermoelectric generators have been proposed. Novel materials and material alloys are investigated to benefit from their improved thermal and electric transport parameters [1–3]. The use of semiconductor nanowires is considered in [4]. The strong anisotropy of the electric and thermal material parameters within superlattices as well as their possibility to influence thermoelectric emission is presented in [5–7].



1: Principle sketch of a conventional thermoelectric generator with applied temperature gradient. A p-doped and an n-doped semiconductor are connected on the heated end of the device. Electric contacts are applied on the cold end of the device.

Until now, none of these approaches is suitable for a broad economical use because of too low efficiencies and too high costs. We present a new approach to thermoelectric power generation using large area Si/SiGe pn-junctions [8], which offers higher efficiencies at lower production costs.

We present the physical background of our approach as well as strategies to improve the efficiency and power output. A comparison to conventional thermoelectric generators is outlined. We use our device and circuit simulator MINIMOS-NT [9] to obtain predictive results. The optimization framework SIESTA [10] is applied with MINIMOS-NT to maximize the efficiency and power output for given thermal environments. A rigorous thermodynamical coupling of the heat system with the semiconductor equations is applied as proposed in [11]. Finally, we illustrate the possibilities of our devices with simulation results.

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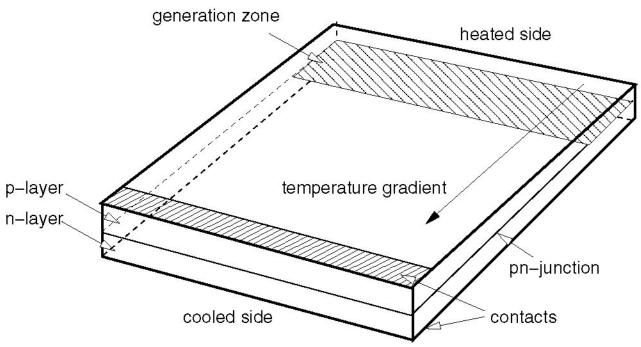
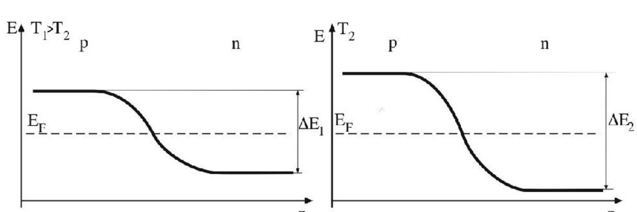


2: Principle sketch of a large area pn-junction thermoelectric generator with applied temperature gradient along the pn-junction. Electric contacts are applied on the cold end of the device.

II. New Approach

The principle design of a large area pn-junction thermoelectric generator is shown in Fig. 2. The temperature gradient is applied along the pn-junction. Contacts to the n- and the p-layer are applied on the cooled end of the structure. In contrast to conventional thermoelectric devices, the thermal generation of electron-hole pairs is explicitly used within large area pn-junction generators which allows to avoid the hot side contact.

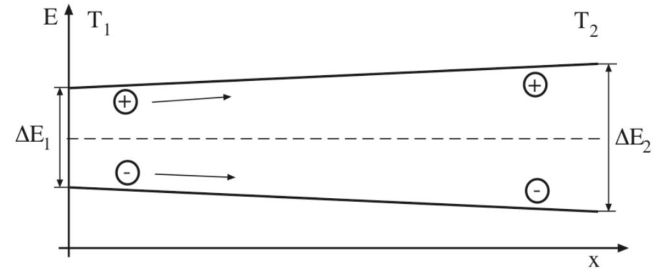
To understand why a temperature gradient within this structure leads to the generation of an electrical current, we have to consider the effect of the temperature on the electrostatic potential and carrier statistics of pn-junctions (Fig. 3). The higher temperature T_1 leads to a smaller energy step ΔE_1 from the potential of the n- to the p-layer compared to the step ΔE_2 at the lower temperature T_2.



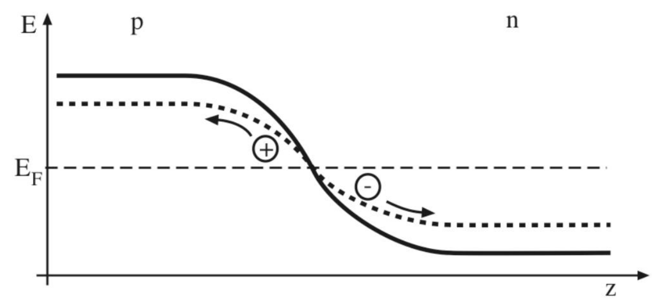
3: Temperature influence on the electrostatic potential of a pn-junction. Higher temperatures lead to smaller energy steps.

By having a temperature gradient in a large area pn-junction, both physical states occur neighboring to each other so that carriers at different potentials come into contact, resulting in a driving force to the colder region (Fig. 4).

Because both types of carriers, electrons and holes, move 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 Fig. 4, this region becomes depleted and the local thermal equilibrium distribution of carriers is disturbed.



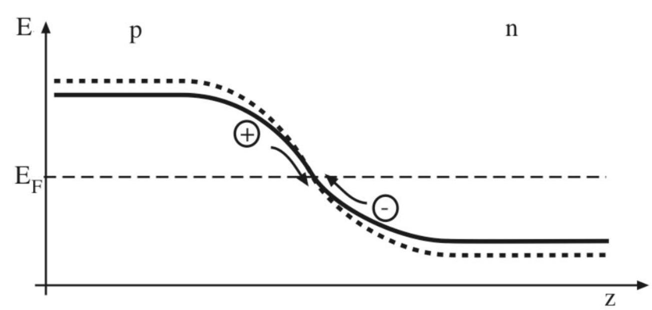
4: Driving forces to generate ambipolar drift and diffusion.



5: Higher generation because of depletion.

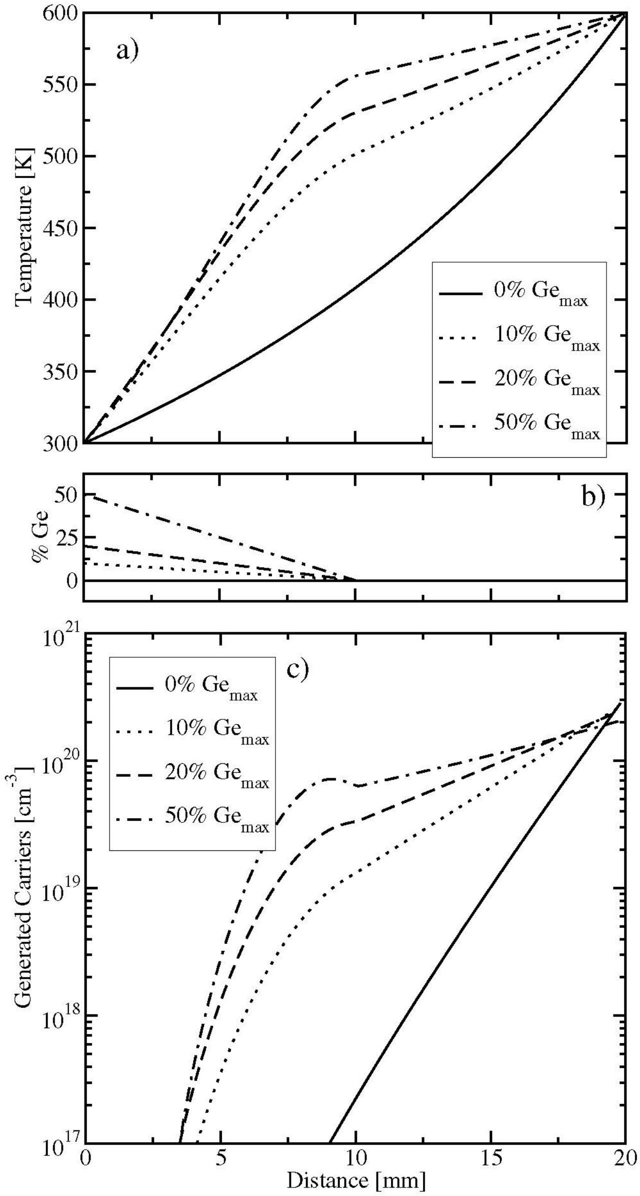
The generation-recombination balance is shifted to higher generation to compensate for the off-drifting carriers (Fig. 5).

At the part of the structure with the lower temperature T_2 on the right hand side of Fig. 4, the opposite effect takes place. The incoming carriers enhance the recombination as shown in Fig. 6. 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.

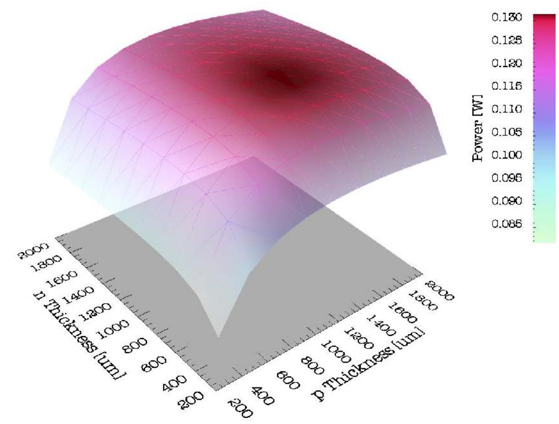


6: Recombination at the cold side.

Using selective contacts at 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. 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. This allows to utilize very high temperatures (above 1000°C) for thermoelectric power generation by choosing the right base material, e.g. wide band gap semiconductors like Carbides or Nitrides.



7: a) Temperature distribution along the pn-junction caused by the thermal conductivities of different Ge-profiles as shown in b). The generation rate depends exponentially on the temperature, thus the material composition is used to increase the generation.



8: Power output of a large area pn-junction thermoelectric generator versus p- and n-layer thicknesses. Thicknesses higher than the optimum lead to higher recombination and thus to lower power output. Too low thicknesses limit the current from the hot to the cold end of the structure.

III. Simulation Results

The generation of electron-hole pairs is a thermally activated process determined by the trap level and the band gap. Large areas of high temperature are needed to generate as much carriers as possible but at the same time a temperature gradient is necessary to remove the carriers effectively. In the following, several optimization strategies are presented.

In order to control the thermal behavior and the local band structure, graded SiGe alloy profiles are introduced as presented in Fig. 7b. The thermal conductivity drops with an increasing Ge content of up to 50%, the bandgap decreases continuosly from pure Si to pure Ge [12]. The considered Ge profile leads to a temperature distribution with a shallow slope for high temperatures and a steep slope approaching the cold part of the structure as displayed in Fig. 7a [13]. This shifted temperature distribution leads to large areas of high generation (Fig. 7c).

The p- and n-doped transport layer thicknesses are optimized for the most effective carrier transport from the high temperature generation area to the contacts (Figs. 2,8). Optimized layer thicknesses strongly increase the power output. If the layer thicknesses are too small, the according resistances are higher than in the optimized case. Both too small and too broad layer thicknesses lead to higher recombination rates and thus to lower power output.

The resulting efficiency of SiGe pn-junction thermoelectric generators is strongly influenced by the Ge content profile as shown in Fig. 9. The optimum Ge content of about 30% at the given profile results in the best generation rate at the heated end at the best transport conditions in the conducting area. The optimum efficiency is always achieved by matching the inner and the load resistances as pointed out in Fig. 10.

The performance of conventional and large area pn-junction thermoelectric generators is compared in Fig. 11. Our structures capitalize from thermal generation of electron-hole pairs especially at higher temperatures.

IV. Conclusion

The physical principles of conventional thermocouples and large area pn-junction thermoelectric generators have been presented. Their power outputs and efficiencies of large area pn-junction thermoelectric generators have been compared. The influence of the temperature gradient on the efficiency was presented. For simple step-like Ge profiles, we achieved an efficiency 6 times higher than for pure Si generators. Further increase of the output can be achieved by the adaption of the device to given thermal boundary conditions.

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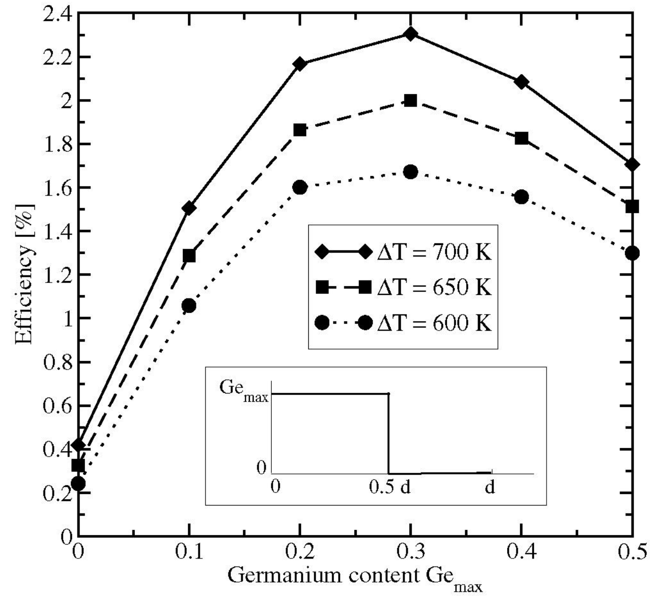
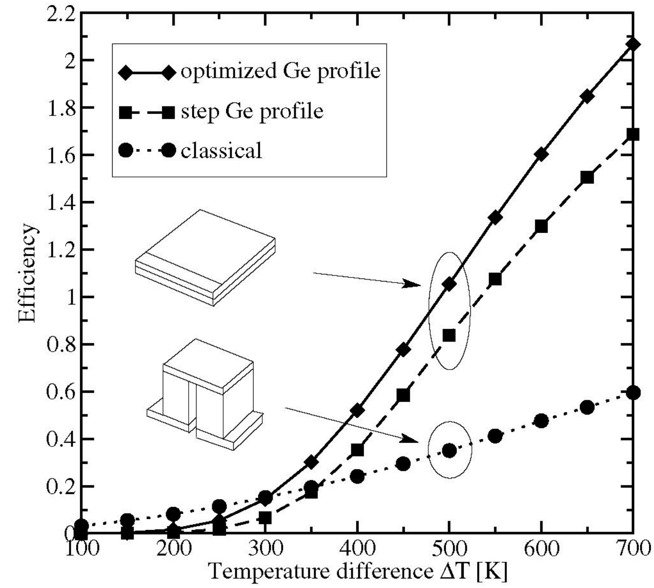
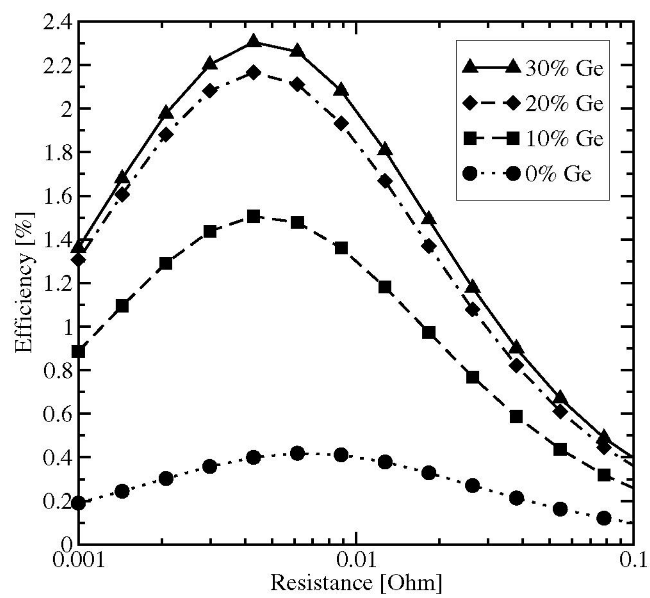


9: Resulting efficiency versus maximum Germanium content of a thermoelectric generator with a step-like Ge profile. The optimum efficiency for each thermal environment is influenced by the thermal as well as the electrical conductivity and the band gap of the considered material composition.



11: Efficiencies of conventional and large area pn-junction thermoelectric generators versus temperature difference. The influence of generated carriers at higher temperatures within pn-junction generators leads to a far better performance than conventional structures at higher temperatures with $\Delta T > 300K$.



10: Resulting efficiency versus external load resistance. The optimum efficiency is achieved by matching the inner and the load resistance $R_{\mathrm{i}} = R_{\mathrm{load}}$. The efficiency of a SiGe thermoelectric generator with $Ge_{\mathrm{max}} = 30\%$ is 6 times higher than the one of a pure silicon generator.

Acknowledgment

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