Semicond. Sci. Technol. **22** (2007) S173–S176 doi:10.1088/0268-1242/22/1/S41

Thermoelectric power generation using large-area Si/SiGe pn-junctions with varying Ge content

M Wagner[1], G Span[2], S Holzer[1] and T Grasser[3]

[1] Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria
[2] SAM—Span and Mayrhofer KEG, 6112 Wattens, Austria
[3] Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics, TU Wien, Wien, Austria

E-mail: martin.wagner@iue.tuwien.ac.at

Received 3 August 2006, in final form 26 September 2006
Published 7 December 2006
Online at stacks.iop.org/SST/22/S173

Abstract
We present strategies for improving the power output of large-area pn-junctions for thermoelectric power conversion. The gradient of the pn-junction's built-in potential is used to separate thermally generated electron–hole pairs. An externally applied temperature gradient along the pn-junction induces a driving force to both electrons and holes which results in currents from the hot end to the contacts. Due to the exponential dependence of the thermal generation rate on the local temperature, the temperature distribution within the device strongly influences the device behaviour. We present simulation results describing the possible application of graded SiGe alloys in order to control the temperature distribution and thus improve the power output and efficiency of thermoelectric generators using large-area pn-junctions.

1. Introduction

The conversion of heat to electricity by thermoelectric devices is a promising option to raise the total efficiency of many combustion processes in the near future. However, in order to meet that role, more efficient thermoelectric devices and materials are needed that are suitable for a wide range of temperatures. Several ideas and approaches such as heterostructures, nanowires and superlattices using novel complex materials are currently under investigation [1–5]. So far, none of these results in efficiencies high enough to allow economical use. To increase the efficiency of the conversion process, we present a new approach to thermoelectric power generation using large-area pn-junctions [6].

2. New approach

Our approach is based on the separation of thermally generated electron–hole pairs by the built-in potential gradient of the pn-junction. A temperature gradient applied along this pn-junction then causes a flux of both carrier types from the hot to the cold region [7]. Figure 1(*a*) shows a principal sketch of the device. This principle allows us to use layer structures similar to solar cells as thermoelectric elements.

To improve the power output of our thermoelectric generators, material parameters, namely the thermal and electrical conductivities as well as the bandgap, are locally modified by changing the material composition. SiGe alloys show decreasing thermal conductivity for Ge contents of up to 50% as well as a decreasing bandgap with rising Ge content. The use of SiGe with varying Ge content makes it possible to introduce a nonlinear temperature distribution which enhances the amount of generated carriers while reducing the thermal conductivity of the overall structure.

3. Thermal generation and Seebeck effect

Electron–hole pairs are thermally generated within a pn-junction and separated by the built-in potential gradient. In thermal equilibrium, the generation is exactly compensated by recombination and no net current occurs. The built-in potential becomes smaller with increasing temperature, which

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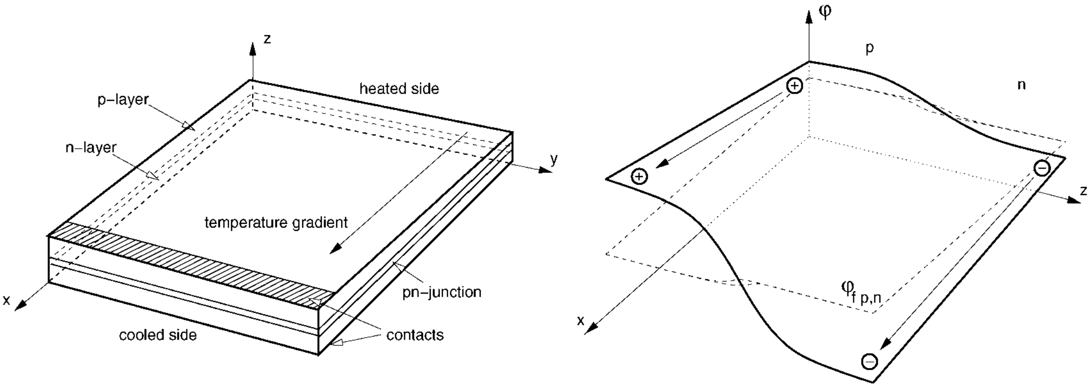
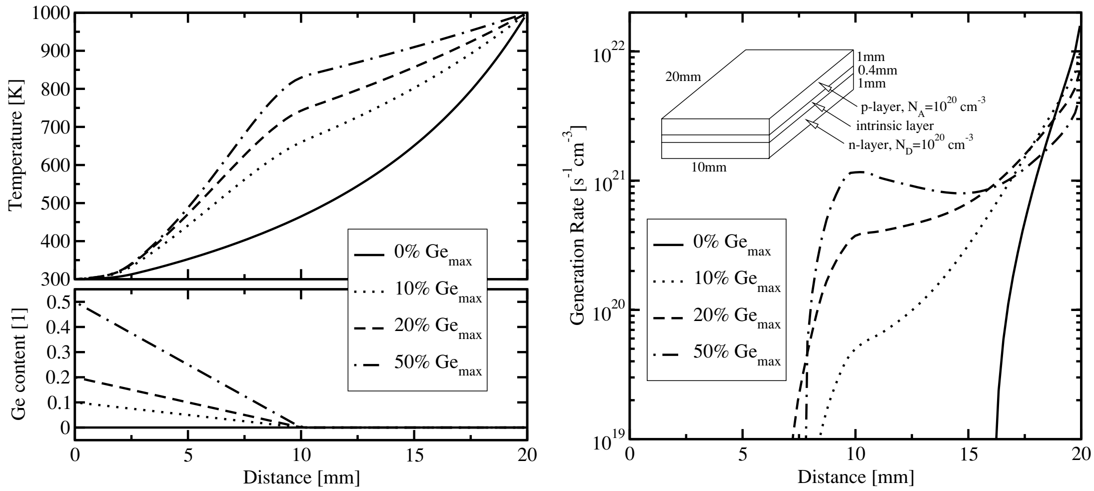


(*a*) (*b*)

Figure 1. (*a*) A large-area pn-junction with applied temperature gradient. Thermal generation takes place on the heated side of the structure, both electric contacts are mounted on the cooled side. (*b*) The electrostatic potential is affected by the local temperature. Higher temperatures lead to smaller energy differences across the pn-junction. The potential change along the *x*-axis causes a driving force to both carrier types from the zone of strong thermal generation at the hot end to the contacts at the cold end.



(*a*) (*b*)

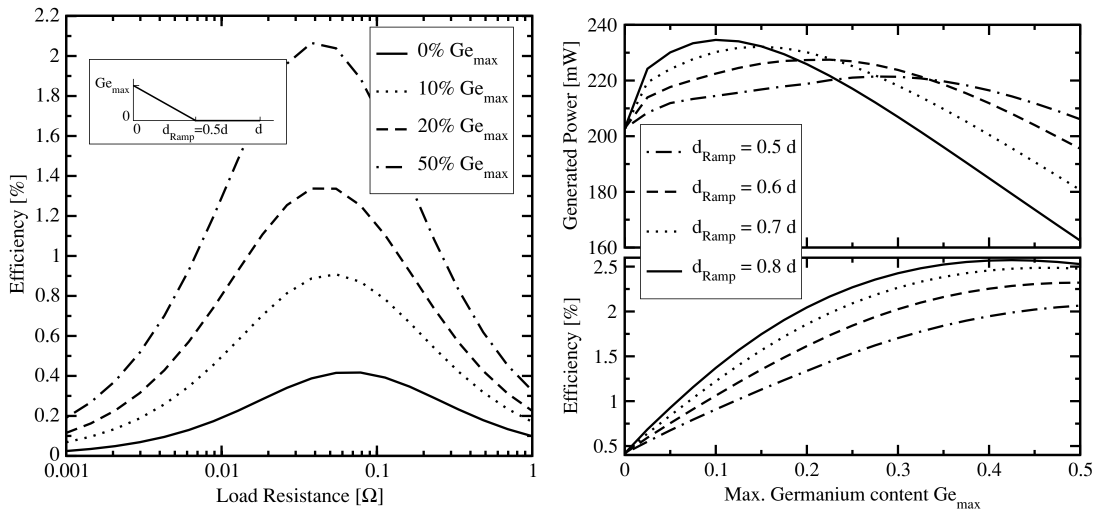
Figure 2. (*a*) Material composition and corresponding temperature distribution within the device. Higher Ge concentrations on the cold end of the device result in lower thermal conductivity and thus larger area of high temperature. (*b*) Generated carriers for different Ge contents. The inset shows the geometry and the dopings of the simulated device.

leads to the Seebeck effect. By having a temperature gradient along a large-area pn-junction, the free carriers experience a driving force from the hot to the cold part of the structure. This carrier movement alters the local carrier balance between generation and recombination and leads to enhanced generation of electron–hole pairs at the hot part and to increased recombination at the cold part of the structure. By installing contacts to the cold side, the generated current can be used and the whole structure works as a source of electricity, a thermoelectric power generator. This principle is illustrated in figure 1(*b*). Thermoelectric modules can be manufactured by stacking these elements, similarly to [8].

4. Advantages of this technique

The assembly of elements as illustrated in figure 1(*a*) and stacked modules has several advantages compared to conventional thermocouples. Among them are the following.

- 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 for each carrier type separately to achieve high electrical conductivity.
- The shape of the temperature gradient within the thermoelectric element influences the amount of generated carriers and thus the power density can be optimized by geometrical engineering and by using distributed material compositions.
- Thermoelectric elements can be fabricated using only one main material so fatigue due to thermal cycling can be avoided.
- The elements can be manufactured in a similar way to well-established processes in the semiconductor and solar cell industry.



(*a*) (*b*)

Figure 3. (*a*) Conversion efficiency for different Ge concentrations versus electrical load resistance. The optimum efficiency is reached at a matching load resistance of $R_{ext} = R_i$. (*b*) Electrical power output and efficiency versus Ge content for $Ge_{max} = 0.5$ and different Ge lengths. The alloy length influences the centroid over the Ge content.

5. Simulation environment

We use the device and circuit simulator MINIMOS-NT [9] for predictive simulation of our thermoelements. A non-isothermal drift diffusion model with a rigorous coupling of the electrical and the thermal system as proposed in [10] is applied. Dirichlet boundary conditions are assumed for the heat flux equation at the heated and the cooled side. Carrier generation and recombination is modelled using the Shockley–Read–Hall equation. Measurement data for carrier mobilities are typically available for temperatures up to 500 K [11]. Therefore, we apply calibrated full band Monte Carlo simulations to extract mobility data for the entire temperature range. Measurement data for both thermal conductivity and specific heat are available over the entire temperature range [12, 13]. The efficiency is extracted as the ratio of generated electrical power and incoming heat flux at the hot end of the device.

6. Influence of the temperature distribution

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. The generation will be a maximum for a temperature distribution with a shallow slope for high temperatures and a steep slope approaching the cold part of the structure (figure 2). The temperature distribution is controlled by the device geometry and the local thermal conductivity distribution, which is a function of the Ge content. Using pure Si on the hot side in combination with SiGe on the cold side, the temperature distribution along the element can be tailored accordingly as shown in figure 2(*a*). The thermoelectric element consists of a SiGe part with a Ge content of 0–50% on the cold end and pure Si on the hot end of the structure. The corresponding amounts of generated carriers are shown in figure 2(*b*). In figure 3(*a*), the corresponding efficiencies with respect to an external load resistance are displayed. The optimum efficiency is achieved with a matching load resistance. Figure 3(*b*) shows the influence of the alloy profile along the device on the output. For short Ge profiles, the influence on the thermal conductivity and thus on the temperature distribution dominates. In this regime, the power output and efficiency increase with the maximum Ge content in a wide range. For longer profiles, another mechanism becomes important. The mobility decreases with increasing Ge contents up to 50% which leads to worse transport conditions and thus to higher recombination rates. Fewer carriers can be transported to the device contacts which means lower power output. The efficiency still goes up because of the also decreasing thermal conductivity and therefore reduced heat flux through the device.

7. Conclusions and outlook

By using the low thermal conductivity of SiGe to increase the average temperature along the pn-junction of the structure, the efficiency and power output of our thermoelectric elements can be increased dramatically. Further improvement can be achieved by using optimized graded Ge content to fully adapt the temperature distribution to our needs.

Acknowledgments

We acknowledge financial support through the FFG, the Austrian Research Promotion Agency (Österreichische Forschungsförderungsgesellschaft mbH) for SAM (project no 809975) and project no 810128 and the local government (Impulspaket Tirol).

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