Power Output Improvement of SiGe Thermoelectric Generators

M. Wagner°, G. Span*, S. Holzer°, O. Triebl°, and T. Grasser°

°Institute for Microelectronics, TU Vienna, Gußhausstraße 27–29, A-1040 Wien, Austria Phone: +43-1-58801/36025, Fax: +43-1-58801/36099, *SAM - Span and Mayrhofer KEG, 6112 Wattens, Austria

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

The conversion of heat to electricity by thermoelectric devices is a promising alternative for energy production for the near future. In order to meet that role, more efficient and reliable thermoelectric devices are needed. Several approaches like heterostructures, nanowires, and superlattices using novel complex materials are currently investigated [1–4]. So far, none of these results in efficiencies high enough for economical use. To increase the conversion efficiency, we present a new approach to thermoelectric power generation using large area pn-junctions [5] and show strategies to optimize the power output for given thermal environments.

Our approach is based on the separation of thermally generated electron-hole pairs by the builtin potential gradient of a large scale pn-junction (Fig. 1). A temperature gradient applied along this pn-junction causes a flux of both carrier types from the hot to the cold region. We use MINIMOS-NT [6] for predictive simulations of our thermoelements. We apply a rigorous thermodynamical coupling of the heat system with the semiconductor equations proposed in [7]. The validity of the physical parameter models was ensured for the unusually large temperature ranges required for this application by calibrating the models with measured data and results from full band Monte-Carlo simulations. Finally the optimization framework Siesta [8] is used in conjunction with MINIMOS-NT to optimize the thermoelectric generators for a maximum power output under given external parameters.

The power output and efficiency of the investigated thermoelectric generators shown in Fig. 1 have been increased dramatically by locally adapting the band structure as well as the thermal properties by introducing graded SiGe alloys (Fig. 2). The bandgap decreases continuosly from pure Si to pure Ge. The optimized Ge content shows a strongly increased part on the hot end of the device due to the smaller bandgap of this alloy composition which results in higher generation rates. Furthermore, additional improvements have been achieved by the application of an optimized gold dopand profile as additional generation centers. The device structure and doping profile have been adapted accordingly to the amount of generated carriers. The evolution of the optimization is presented in Fig. 3. The p- and ndoped transport layer thicknesses are optimized for the most effective carrier transport from the high temperature generation area to the contacts. The optimized power output is 18 times higher than the one of a pure Si generator.

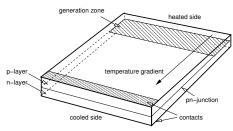


Figure 1: Large area pn-junction with applied temperature gradient. Electric contacts are applied on the cold end of the device. The heated side is the zone of strong generation.

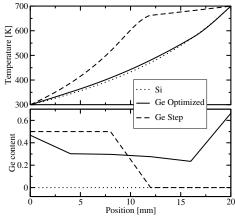


Figure 2: Temperature distributions for several Ge content profiles. The lower thermal conductivity of Ge leads to shifted temperature curves.

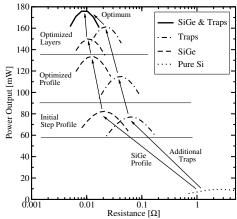


Figure 3: Power output for several structures in several development states at 700 K hot end temperature. The power output of the final optimized generator design is 18 times higher than the one of a pure Si generator.

- P. Hagelstein et al., APS Meeting Abstracts 26011 (2002).
- S. Yamaguchi et al., Appl. Phys. Lett. 87, 201902 (2005).
- [3] D. Vashaee et al., Phys. Rev. Lett. 92, 106103 (2004).
- [4] B. Yang et al., Appl. Phys. Lett. 80, 1758 (2002).
- [5] G. Span, Austrian patent AT 410 492 B; international patent application PCT/AT01/00123, granted in USA, Russia, Europe.
- 6] MINIMOS-NT 2.1 User's Guide, Institut für Mikroelektronik, Technische Universität Wien, Austria, 2004.
- [7] G. Wachutka, IEEE Trans. CAD 9, 1141 (1990).
- [8] SIESTA 1.1std, Institut für Mikroelektronik, Technische Universität Wien, Austria, 2003.