Simulation of Si/Ge based thermoelectric generator

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Abstract. A thermoelectric generator based on a SiGe superlattice was simulated using the COMSOL Multiphysics software platform. Based on the created model, a prototype generator sample can be made. The output power of a single thermoelectric generator was 0.048 μW with a temperature difference ΔT=50 K. The generator area was 32 mm², and the thickness was 1 mm. This makes it possible to combine 100 or 500 single generators into one on a flexible basis. This type of a TEG can be used as an energy source for different types of autonomous devices, for example, sensors or microdevices.

1. Introduction
Thermoelectricity offers an easy way to convert waste heat into readily available electrical energy. A large number of modern electrical devices, such as miniature sensors in sensor networks, microelectronic devices [1-10], require autonomous operation, therefore thermoelectric generators (TEG) are used in areas that require low power. Modern thermoelectric materials are based on nanostructuring and the creation of fundamentally new classes of materials, unlike traditional microthermoelectric generators based on bismuth tellurides [11-12]. The usage of superlattices, nanowires, and quantum well systems has significantly increased the efficiency of thermoelectric conversion over the past 30 years. The purpose of this work is to study the possibility of developing a thermoelectric generator based on the SiGe superlattice.

2. The method of constructing a mathematical model using COMSOL Multphysics
The COMSOL Multiphysics and ANSYS Workbench software platforms [13-17] can be used to model a TEG using the finite element method. The former is used wider, this paper included, because of the built-in modules being efficient tools to model the TEG physics.

The simulation technique consists of several stages. The first stage, the creation of the project, represents the introduction of general ideas about the problem being solved, whether the problem is stationary or non-stationary, and the dimension of the system (2D / 3D) is determined. The second stage is the creation of the geometry of the future model. The third stage is the assignment of the physical properties of the materials of each part of the geometric model. The fourth stage is the selection of the physical problem (multiphysics). They represent systems of equations describing the behavior of a model at the junction of several branches of physics. The initial and boundary conditions are also specified here. The fifth stage is the creation of a grid for calculating the model. The sixth stage is the calculation and conclusion of results.
3. Object of simulation
A prototype model of a single silicon-germanium superlattice thermoelectric generator based on a silicon-germanium superlattice was taken as an object of simulation presented in [18] (figure 1).

![Figure 1. Object of simulation [18].](image)

4. Results
As a result of the simulation, a stationary temperature and potential distribution in the sample was obtained. Also, using the tool built into COMSOL, the thermoelectric figure of merit (Z) was calculated. For the simulated superlattice its maximum value was $6.16 \times 10^{-6}$ K$^{-1}$. Next, the sample behavior was simulated when the temperatures of the hot and cold surfaces vary in the range from 338 K to 388 K with a step of 10 K, and graphs of dependences for the thermopower ($E_{\text{therm}}$) and total electrical energy ($W$) on temperature were obtained.

![Figure 2. Boundary conditions.](image)
By the look of the graphs obtained, it can be said that it repeats the type of theoretical dependencies. The potential difference at the contacts increases linearly with increasing temperature difference and tends to zero at $\Delta T = 0$. The graph of the dependence of electric energy has a parabolic form, which also agrees with the theory and also tends to zero at $\Delta T = 0$.

It was also simulated the behavior of the sample when it is included in the electrical circuit. As the load was taken resistance $R_{\text{load}} = 1.5 \ \text{Ohm}$. This resistance roughly corresponds to the internal resistance of the TEG.
Figure 7. Voltage distribution through a thermoelectric generator on temperature for $R_{\text{load}}=1.5 \ \text{Ohm}$.

Figure 8. Voltage dependencies of a thermoelectric generator on temperature for $R_{\text{load}}=1.5 \ \text{Ohm}$.

5. Conclusion
TEG was simulated and results were analyzed. On the basis of the model created in the work, a real TEG can be created, and further modernization of the model in terms of introducing temperature dependences of the physical parameters of the SiGe superlattice is possible. The resulting model is physically correct and corresponds to the real TEG, which was shown in Chapter 3. In conclusion, it is also worth noting that the TEG dimensions are very small (32 mm$^2$), which makes it possible to combine 100 or 500 single generators into one. Table 1 shows the parameters of such single modules.

| Parameter            | N=1   | N=100 | N=500 |
|----------------------|-------|-------|-------|
| $T_c$ (K)            | 338   | 338   | 338   |
| $T_h$ (K)            | 389   | 389   | 389   |
| $T_m$ (K)            | 363.5 | 363.5 | 363.5 |
| $\Delta T$ (K)       | 51    | 51    | 51    |
| Thermo emf (mV)      | 0.5   | 50    | 250   |
| $U_R$ (mV)           | 0.27  | 27    | 135   |
| $Z$ (K$^{-1}$)       | 6.16*10$^{-6}$ | 6.16*10$^{-6}$ | 6.16*10$^{-6}$ |
| $ZT$                 | 2.24*10$^{-3}$ | 2.24*10$^{-3}$ | 2.24*10$^{-3}$ |
| $I$ (mA)             | 0.18  | 0.18  | 0.18  |
| $P$ (mW)             | 0.048 | 4.86  | 24.3  |

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