Design of a Large Area Pn-Junction Si Thermoelectric Device via Genetic Algorithm

Ali Eftekhari, Morteza Fathi-Pour, and Abdorreza Alavi Gharahbagh

***Abstract*—A modified Genetic Algorithm (GA) have been used to obtain the optimum dimensions for a large area pn-junction thermoelectric power generator device. Optimization routine allows for obtaining maximum output thermoelectric power. The results which obtained by using computer simulations has confirmed better performance in compare to those obtained from design in a vast range of temperatures.**

***Index Terms*—Thermoelectric, device, pn-junction, large area, Genetic Algorithm.**

I. Introduction

Thermoelectric power devices provide attractive solutions for direct conversion of heat to electricity. Advantages of these devices include simplicity, low cost and lack of moving parts which results in a long lifetime and practically no need of device maintenance. Unfortunately, state of the art devices suffer from their low efficiency and thus, they normally employed in situations where low maintenance is critical such as satellites and spacecraft systems.

Fig. 1 shows schematic of a simple semiconductor thermoelectric power generator. p-doped and an n-doped semiconductor are electrically connected at the heated side using a metallic joint. The temperature gradient along the semiconductors causes a flux of the available carriers from the higher temperature end to the lower temperature end. For this reason, a voltage drop appears across width and Carrier transmission of the two lower temperature ends. Novel, efficient and highly reliable thermoelectric structures and materials suitable for operation in a wide range of temperatures are obviously needed.

Recently, several approaches such as heterostructures, nanowires and superlattices using novel complex materials for improving the efficiency and power output of thermoelectric generators have been investigated with limited success [1-4].

Wagner et al. [5] proposed use of a large area Si/SiGe pn-junctions to provide higher efficiencies at lower production costs in thermoelectric power generation.

In this paper, we employed a Si large area pn-junction thermoelectric module as shown in Fig. 2. By using this structure, the strong correlation between thermal and electrical properties can be minimized .i.e. both effects can be optimized independently from each other [6]. In this study, ATLAS Device Simulation Framework in Silvaco software has used to run simulations of this thermoelectric device [7] and a modified genetic algorithm [8] in MATLAB is applied in combination with ATLAS for dimensional optimization of this structure.

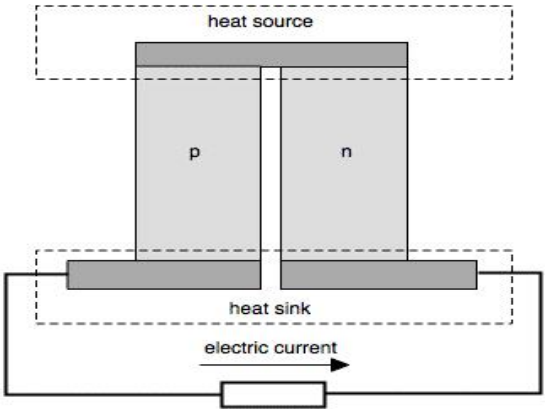


Fig. 1. Principle sketch of a conventional thermoelectric generator with applied temperature gradient. A p-doped and an n-doped semiconductor are connected on the higher temperature end of the device. Electric contacts are applied on the lower temperature end of the device.

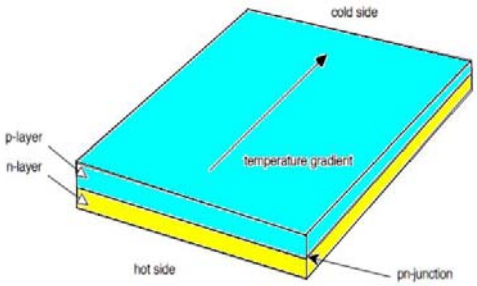


Fig. 2. Large area pn-junction with temperature gradient

II. Model

The structure of the thermoelectric device employed in this study is shown in fig. 2. First, a temperature gradient is applied along the pn-junction which causes a flux of both carrier types from the high temperature to the lower temperature regions .This is due to the fact that thermally generated electron-hole pairs are separated by the built-in potential gradient of the pn-junction. Band gap changes with the temperature as:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T+\beta} \quad (1)$$

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The effect of temperature on the energy gap as well as carrier transport is schematically depicted in Fig. 3. As the temperature decreases from T1 (higher temperature end), to T2 (lower temperature end), the band gap increases.

Because both types of carriers, electrons and holes are moving in the same direction away from the pn-junction at the higher temperature T1 (high temperature region), 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. At the cold region of the structure with the lower temperature T2 the opposite effect takes place. The incoming carriers enhance the recombination.

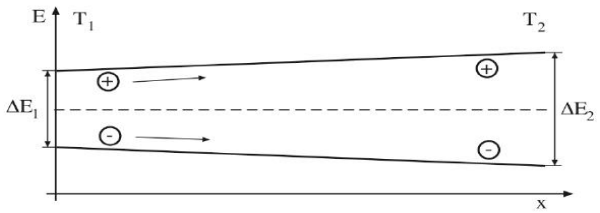


Fig. 3. Effect of temperature on energy bandwidth and Carrier transmission

Therefore, the net effect is a circular electrical current within the large area pn-junction from the high temperature region to the low temperature region. By using selective contacts for both the n- and p-type layers, this circular current can be diverted to an external load and a power source is established (See fig. 4).

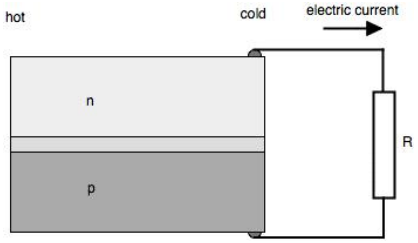


Fig. 4. Principle of a thermoelectric element

In this study, a pn-junction has been considered and assumed a single material, Si, for both n- and p-type in order to avoid mechanical stress. Mechanical tension between different materials may lead to fatigue once the device is introduced to thermal cycling .High band gap semiconductors can tolerate fabricating larger temperature gradients and are more suitable for high temperature applications.

Several parameters contribute to device thermoelectric power. These include p and n layer geometry and doping densities. As a primary estimate, doping density for both p and n layers was assumed 1019cm-3. The device length and width were assumed 20mm and 10mm respectively. The thickness of each layer was assumed 1.2mm. These parameters can be varied to obtain maximum output thermoelectric power. As mentioned above, after electrical contacts have been placed on the cold side a linear temperature gradient is applied from right (high temperature, x = 20 mm) to left (low temperature, x = 0 mm) (Fig. 5). Effect of the applied temperature gradient on the electrostatic potential of a pn-junction is shown in Fig. 6. As expected, applied temperature causes electrostatic potential drop. The potential difference between the high temperature and low temperature side causes that thermally generated carriers are transferred to the cold side and as mentioned above an electrical current will be created. After that, this current can be delivered to an external load.

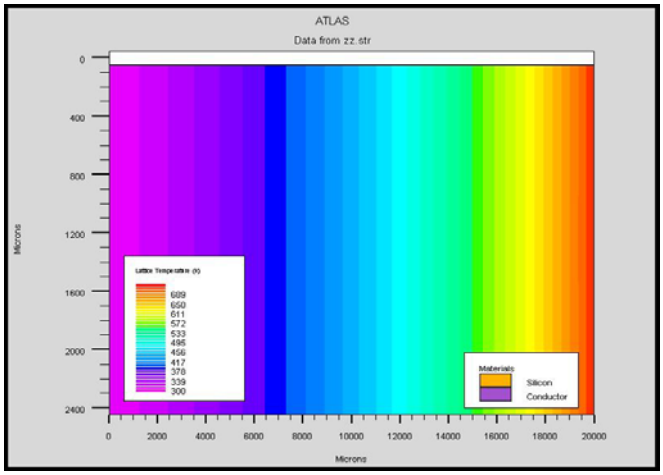


Fig. 5. Linear temperature gradient along pn- junction

The Geometry of the structure is one of the critical important parameters in output power of the thermoelectric device. If the layer thicknesses are too small, respective resistances are large. On the other hand, too small or too broad layer thicknesses lead to higher recombination rates and thus decrease output power. The length of the device directly affects the temperature gradient across the device.

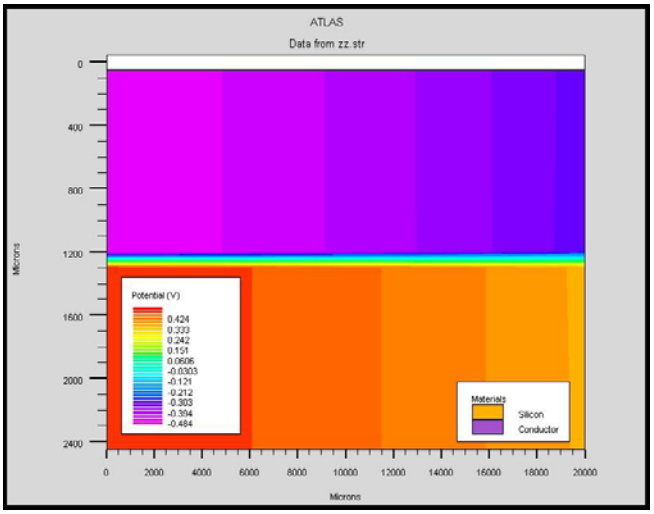


Fig. 6. Effect of the applied temperature gradient on the electrostatic potential of a pn-junction.

III. Genetic Algorithm

Since the output power of the thermoelectric device is a nonlinear function of the device geometry, Genetic Algorithm may be employed to obtain the optimum geometry of the device.

The parameters used in GA are the length and thickness of layers which are variables, width of structure, type of material, doping concentration and shape of temperature gradient, which are constant. Note that by rising T_{hot}, the output thermoelectric power considerably increases. In this optimization, T_{hot} is chosen equal to 715K.

The variable spaces are different. Length is assumed to vary between 5000 and 30000 μm and thickness is assumed between 60 and 2000 μm. The length and thickness resolution due to technical limitation are assumed to be 25 μm and 10 μm respectively. Therefore the variable length is 10 bits and the variable thickness is 8 bits in binary mode. The total length of each population is 18 bits.

The number of initial populations is assumed to be 64.

The number of cross points is assumed to be 3 according to Alavi gharahbagh [8].

Alavi gharahbagh [8] has considered the probability of mutation or Pstart to be 0.75 and DeRate to be 1.5.

Answer Error is a rational factor for breaking computation process that can be calculated from:

$$Answer\ Error = \frac{|The\ best\ answer - the\ worst\ answer|}{The\ best\ answer} \times 100 \qquad (2)$$

This value is assumed 0.01%. The cost function is the maximum thermoelectric power output of structure.

IV. Simulation Result

Once the external load resistance is connected to the thermoelectric device, Mixed Mode Circuit Simulation in Silvaco ATLAS software may be employed to estimate the generated thermoelectric power.

Generated thermoelectric power of the device is shown in Fig. 7 as a function of the external load resistance for a temperature range between 550 K to 715 K. The maximum power output is reached at $R_i = R_{ext}$. As the temperature, T_{hot} increases, output power increases and the resistance of the best output power decreases.

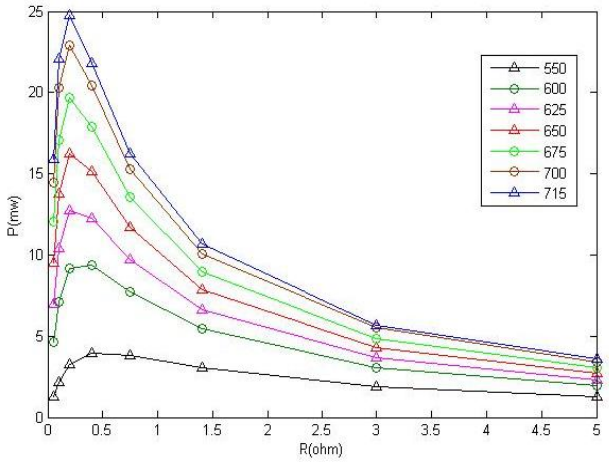


Fig. 7. Simulated thermoelectric output power

A special GA package in MATLAB 7.6 in combination with ATLAS was employed to optimize output thermoelectric power of the device. The optimized length and the thickness of each layer were found 13504 and 1840 μm respectively. Fig. 8 shows output thermoelectric power as a function of the external load resistance and should be compared with those shown in Fig. 7.

It is found that GA can be helpful in device optimization. For example, in T=715K the maximum thermoelectric power increases from 24.7 to 43.65mW i,e. Using this strategy, a 77% improvement in output power can be achieved. Similar behavior is also achieved for various temperatures.

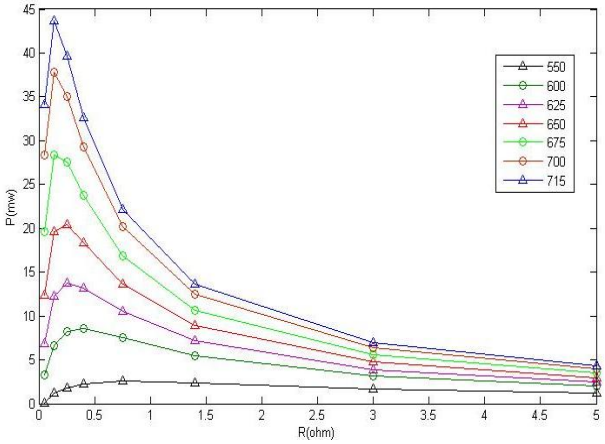


Fig. 8. Optimized thermoelectric output power

V. Conclusion

In this paper, physical principles for the operation of a large area pn-junction thermoelectric generator is described. It is shown that how performance of the device can be optimized by using device simulation software in conjunction with GA. A modified form of GA was used because of its high accuracy. The design procedure is tested for variety of temperatures. All simulation results showed a considerable improvement in output thermoelectric power.

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