Enhancement of thermoelectric properties of a poly-Si thin nanofilm by grain size engineering for energy harvesting applications

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Due to its low thermal conductivity and high values of the Seebeck coefficient, polycrystalline silicon (poly-Si) can be successfully used to create highly efficient thermoelectric energy harvesters, while the nanostructuring of thin films based on poly-Si can additionally provide flexible control of its thermoelectric properties. The dependence of the Seebeck coefficient of a poly-Si film of nanometer thickness on the grain size at a given doping concentration was analyzed, which allows determining the optimal technological parameters of its formation. Based on this analysis, a theoretical model, which correctly describes the experimental change in the thermoelectric properties of poly-Si nanofilms depending on the variation of the crystallite size, is also presented.

INTRODUCTION

Due to the rapid development of Internet of Things and wireless communication systems, modern energy-saving technologies require the development of new classes of nanomaterials for thermoelectric elements, ensuring high efficiency of converting thermal energy into an electrical signal to ensure long-term operation of devices without recharging. Poly-Si films are one of the most promising materials for energy harvesting applications due to their high thermoelectric efficiency, as well as because of their compatibility with standard silicon processing [1]. The main parameter determining the thermoelectric efficiency of nanomaterials is the so-called figure of merit $ZT = \sigma S_{eff}^2 T / \kappa_\Sigma$, where σ is the electrical conductivity, S_{eff} is the Seebeck coefficient, T is the temperature, κ_Σ is the total thermal conductivity. It is well known from [2] that the figure of merit of bulk Si, as well as thick poly-Si films (with a thickness of more than 500 nm), is a small value on the order of 0.01. It was previously shown in [3] that the nanostructuring of Si-based thermoelectric materials leads to a significant increase in figure of merit and an improvement in their thermoelectric efficiency. In our work, we analyzed the optimal parameters for the formation of p-type poly-Si nanostructured thin films with improved thermoelectric properties.

THEORETICAL MODEL

To calculate the Seebeck coefficient S_{eff} as a function of charge carrier concentration (so-called Pisarenko plot) the following analytical formula can be used: $S_{eff} = k_B / e\left[A + \ln\left\{2\left(2\pi m_{h*} k_B T\right)^{3/2} / \bar{p} h^3\right\}\right]$. As it was mentioned in [2], the average carrier concentration is expressed as $\bar{p} = f\left(N_a, d_g\right)$, where N_a is the doping (acceptor) concentration, d_g is the grain size. The following parameters were chosen in the simulation: $A = 1.93$, $N_a = 5 \cdot 10^{18}\, cm^{-3}$, $T = 300K$.

RESULTS AND DISCUSSION

Fig. 1 presents the dependence of the Seebeck coefficient and the figure of merit on the grain size. As can be seen from the figure, the values S_{eff} and ZT increase with decreasing d_g varied in the range up to 10 nm, while there is an increase in ZT with further grain growth, which reaches a value of about 0.03 at $d_g = 50nm$, which coincides with results of recent experimental studies [3].

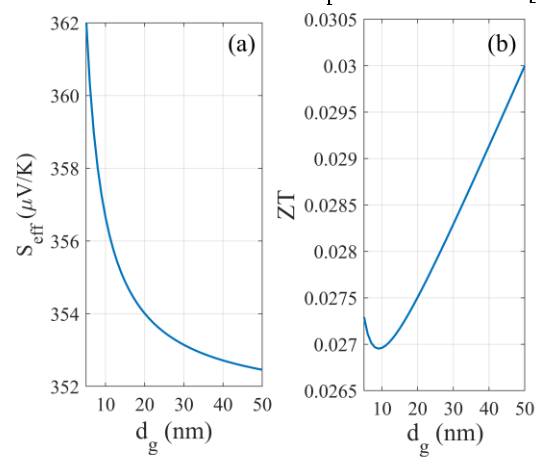

Fig. 1 (a) The Seebeck coefficient S_{eff} and (b) figure of merit ZT of poly-Si film as a function of grain size d_g.

CONCLUSION

The optimal technological parameters for the formation of poly-Si nanofilms with a thermoelectric figure of merit $ZT \approx 0.03$ and a Seebeck coefficient higher than 352.5 μV/K for d_g varied up to 50 nm are determined.

REFERENCES

1. M.T. Dunham et. al, Appl. Phys. Lett. 109, 253104 (2016)

2. N. C.-C. Lu et. al, IEEE Trans. Electron Devices, 28 (7), 818-830 (1981).

3. K. Valalaki et. al, J. Phys. D: Appl. Phys. 49, 315104 (2016)

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