Size Dependence of the Seebeck Coefficient for Single-Material Thermocouples

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INTRODUCTION

In this paper, we present calculations which support the size-dependence of the Seebeck coefficient, observed by us in recent experiments. These findings further support the possibility of thermocouples formed by a single material using size engineering. Single-metal nanothermocouples (NTCs) are constructed by joining together two or more segments from the same metal, but with various cross sections as shown schematically in Fig. 1. These devices exploit the size-dependence of the Seebeck coefficient at the nanoscale. A narrow wire segment is placed between two wider wire segments, thus forming two junctions a few micron apart. If the temperature of one of the junctions is increased, the resulting open-circuit voltage (VOC) is proportional to the temperature difference between the hot and cold junctions and the relative Seebeck coefficient between the narrow and wide wire segments.

In order to directly measure the size-dependent relative Seebeck coefficient (RSC) of single-metal NTCs at room temperature, we fabricated a characterization platform according to the SEM image shown in Fig. 2. A nanoscale heater, energized by AC currents, is used to selectively increase the temperature of the junctions. The resulting VOC is measured with the 2ω method [1]. The four-terminal thermometer measures the temperature of the hot junction. The platform was designed by COMSOL to ensure that the temperatures are the same at the thermometer and at the hot junction. The RSCs were directly obtained using simultaneous measurement of the VOC and the temperature differences for various heater currents. Fig. 3 shows measured RSC for a constant (50-nm-wide) narrow segment cross section and wider segment widths.

MODEL

To model size dependence of single metal thermocouples, we simulate gallium arsenide (GaAs) under very high doping concentration as a proxy for the metal. Rode′s method is used to calculate the electron mobility by iteratively solving for the near-equilibrium distribution function in response to a small electric field and a small temperature gradient. We include scattering rates for acoustic deformation potential, piezoelectric scattering, polar optical, impurity, and boundary roughness scattering. The Seebeck coefficient is calculated from $S = -|\vec{E}|/|\nabla T| = L^{(2)}/L^{(1)}$ using transport integrals $L^{(j)}$ [2]. RSC shown in Fig. 4 is obtained by taking the difference between Seebeck coefficients at two different sizes.

In un-gated and highly doped nanowires, the relaxation time due to electron-boundary roughness scattering [2] is the given by

$$\tau_B\left(k\right) = \left[\frac{1-p(k)}{1+p(k)}\right]\frac{W}{\nu_\perp(k)}$$

where W is size (width or height) of the nanostructure and $\nu_\perp\left(k\right)$ is the velocity of carriers normal to the surface. The specularity parameter $p\left(k\right) = exp(-4\Delta^2k^2)$ accounts for the surface roughness (Δ) and captures the probability of the electron being reflected specularly at the surface based on the momentum of the electrons. Fig. 4 shows the variation in the relative Seebeck coefficient (RSC) as a function of the difference in width between the wide and narrow segments of the nanowire. We observe that the trend in RSC agrees well with the experimental data in Fig. 2. Finally, to justify the use of highly doped GaAs as a proxy for a metal, electrical resistivity is calculated at different temperature. For metals, the resistivity should in-

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crease linearly with temperature due to increase in phonon scattering with temperature, which is indeed observed in GaAs as shown in Fig. 5.

CONCLUSION

The increase in RSC with increasing difference between the narrow and wide wire segments is shown experimentally and numerically, and it leads to a single-metal NTC functionality.

REFERENCES

[1] H. H. Roh, J. S. Lee, D. L. Kim, J. Park, K. Kim, O. Kwon, *Novel nanoscale thermal property imaging technique: The 2ω method. I. Principle and the 2ω signal measurement*, J. Vac. Sci. Technol., B **24**, 2398 (2006).

[2] Z. Aksamija, I. Knezevic, *Thermoelectric properties of silicon nanostructures*, Journal of Computational Electronics,vol **9**, 3-4 (2010).

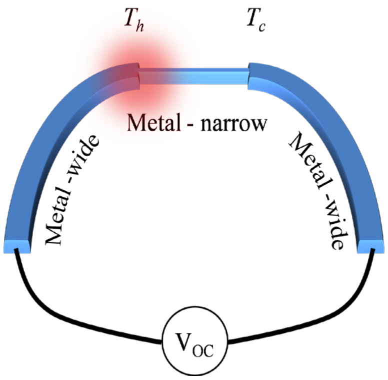

Fig. 1. Schematic of a single-metal nanothermocouple. The red shading indicates the hot junction and the T_h and T_c indicate the temperatures of the hot and cold junctions, respectively.

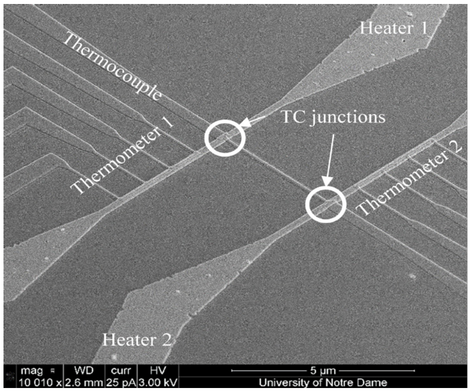

Fig. 2. SEM image of a Ni characterization platform. The hot junction is located on top of the heater separated. They are thermally connected, but electrically separated by a thin layer of alumina.

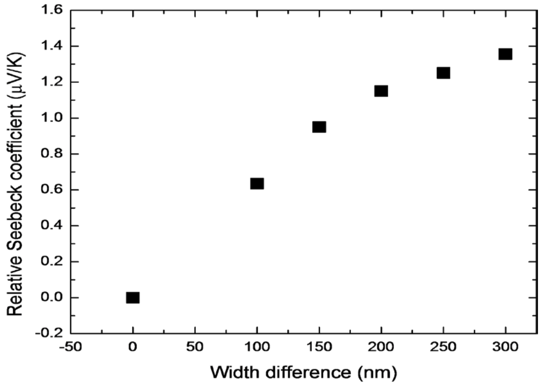

Fig. 3. Measured relative Seebeck coefficient as a function of wire width difference between the narrow and wide wires.

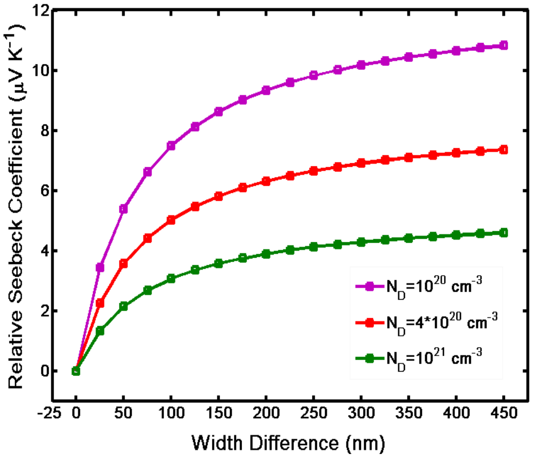

Fig. 4. Calculated relative Seebeck coefficient with wire width difference in a highly donor doped GaAs

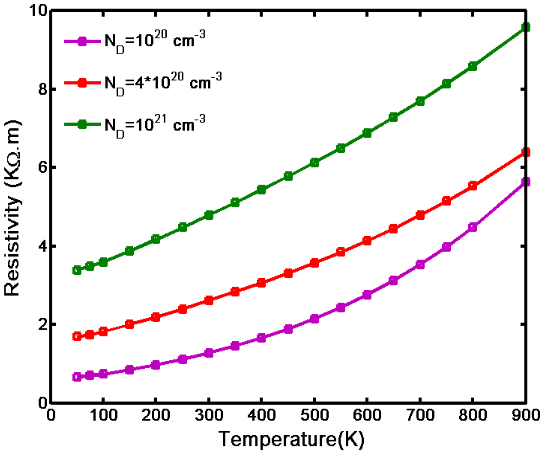

Fig. 5. Resistivity with change in temperature to demonstrate the metal-like behavior of highly doped GaAs