



Journal homepage: <https://trpubonline.org/index.php/Entropy>

RESEARCH ARTICLE

Heat Transfer Optimization in Microscale Thermoelectric Devices

Filip Hruska^{1*}, Marek Sikora² and Tomas Molnar³

¹Department of Physical Chemistry, Neris Institute of Statistical Physics, North Macedonia

²Department of Mechanical and Thermal Engineering, Tagus Center for Information Theory, Serbia

³Department of Physics and Complex Systems, Warta Institute of Molecular Thermodynamics, Portugal

*Corresponding author: Filip Hruska, Department of Physical Chemistry, Neris Institute of Statistical Physics, North Macedonia; Email: filip.hruska@neris.edu

ABSTRACT

Microscale thermoelectric generators are attractive for harvesting waste heat from compact electronics, but their achievable power density is limited less by bulk material properties than by thermal contact resistance and leg geometry effects that grow disproportionately important as device size shrinks. We present a coupled thermal-electrical numerical model of a bismuth telluride microscale thermoelectric leg array, validated against a fabricated 64-leg test module, and use it to optimize leg aspect ratio (height-to-cross-section) and contact-layer thickness across 54 device geometries at leg heights from 20 to 300 micrometers. Across this geometry sweep, output power density varied by a factor of 5.7, from 0.31 to 1.77 W/cm², with the maximum occurring at an intermediate leg height of 80 micrometers rather than at the shortest legs tested, contradicting a naive bulk-limited expectation that power density should increase monotonically as leg height decreases. Decomposing total thermal resistance showed that contact resistance accounted for 61% of total thermal resistance at the shortest leg height (20 micrometers) but fell to 18% at the longest (300 micrometers), while the leg's own bulk thermal resistance showed the inverse trend, explaining the interior power-density maximum as the point where reducing further leg height stops yielding a proportional temperature-difference gain because contact resistance increasingly dominates the total thermal budget. At the optimal 80-micrometer geometry, the device achieved a measured-to-predicted power agreement within 6.4% (model: 1.77 W/cm²; fabricated module: 1.66 W/cm²) and a device-level figure of merit ZT_{device} of 0.58, 34% below the bulk material ZT of 0.88, with the gap attributed almost entirely to parasitic contact and spreading resistances. A sensitivity analysis varying contact resistivity by a factor of 3 above and below its measured baseline value shifted the optimal leg height by 35 micrometers and changed peak power density by 28%, identifying contact-layer quality as the single fabrication parameter with the greatest leverage over achievable device performance. These findings provide quantitative design guidance for microscale thermoelectric leg geometry and underscore that contact engineering, not bulk material improvement alone, is likely to yield the largest near-term gains in microscale thermoelectric power density.

Keywords: thermoelectric devices; microscale heat transfer; Seebeck effect; figure of merit ZT ; thermal contact resistance; phonon transport; device geometry optimization; waste-heat recovery

Received: June 07, 2023 | Accepted: September 08, 2023 | Published: December 06, 2023

Citation: Hruska F, Sikora M, Molnar T. Heat Transfer Optimization in Microscale Thermoelectric Devices. *Frontiers in Entropy*. 2023;1(2):1–5. DOI: [10.5281/zenodo.22698489](https://doi.org/10.5281/zenodo.22698489)

1. INTRODUCTION

Thermoelectric generators convert a temperature difference directly into electrical power via the Seebeck effect, and their potential to harvest otherwise-wasted heat from compact electronics, sensor nodes, and microprocessors has motivated substantial interest in scaling thermoelectric devices down to the microscale [1,2]. Unlike bulk thermoelectric generators, where leg dimensions of millimeters to centimeters keep parasitic thermal and electrical contact resistances a comparatively minor correction, microscale devices with leg heights of tens to hundreds of micrometers operate in a regime where these parasitic effects are no longer negligible [3,4].

The thermoelectric figure of merit ZT , which governs the maximum conversion efficiency achievable from a given material, is a bulk material property, and much thermoelectric materials research has focused on raising ZT through nanostructuring, alloying, and band-structure engineering [5,6,7]. However, the device-level performance actually delivered by a fabricated microscale generator depends not only on bulk ZT but on how leg geometry interacts with thermal contact resistance at the hot- and cold-side interfaces, an interaction that is often treated only qualitatively in device design rather than optimized quantitatively across the full relevant geometry space [8,9,10].

This gap matters because the intuitive design heuristic of simply shrinking leg height to increase the temperature gradient per unit length, and thereby boost power output, breaks down once contact resistance becomes a substantial fraction of total thermal resistance, potentially producing an interior optimum in leg height rather than a monotonic benefit from further miniaturization [11,12,13]. Without a quantitative model connecting leg geometry, contact resistance, and achievable power density, device designers risk optimizing for the wrong regime, over-miniaturizing legs and sacrificing power density rather than gaining it.

The present study develops and experimentally validates a coupled thermal-electrical model of a microscale bismuth telluride thermoelectric leg array, uses it to map power density across a systematic sweep of leg height and contact-layer thickness, decomposes the resulting thermal-resistance budget to explain the observed optimum, and tests the sensitivity of device performance to contact resistivity as the single most directly controllable fabrication parameter.

2. MATERIALS AND METHODS

We developed a coupled thermal-electrical numerical model of a microscale bismuth telluride thermoelectric leg array, validated it against a fabricated 64-leg test module, and used it to optimize leg height and contact-layer thickness across 54 device geometries.

2.1 Device architecture and material properties

The modelled device consisted of an array of p- and n-type bismuth telluride (Bi_2Te_3) legs of square cross-section 100×100 micrometers, connected electrically in series and thermally in parallel between a hot-side substrate at 350 K and a cold-side substrate at 300 K. Bulk material properties (Seebeck coefficient, electrical resistivity, thermal conductivity) were taken from measured values on the source material batch used for fabrication, giving a bulk material ZT of 0.88 at the mean operating temperature.

2.2 Coupled thermal-electrical numerical model

Coupled heat conduction and electrical current-flow equations were solved simultaneously by finite-element analysis for each leg geometry, including Joule heating, Peltier heat at the junctions, and thermal contact resistance at both hot- and cold-side metal-semiconductor interfaces, with contact resistivity set from four-point-probe measurements on witness samples from the fabrication process.

2.3 Geometry sweep

Leg height was swept from 20 to 300 micrometers at nine levels, and contact-layer thickness was swept at six levels from 0.5 to 5 micrometers, yielding 54 total device geometries; for each, output power density at matched load resistance (equal to internal device resistance) was computed under the fixed 50 K applied temperature difference.

2.4 Fabrication and experimental validation module

A 64-leg test module was fabricated using standard microfabrication techniques (sputtered contact metal, photolithographically defined legs) at the 80-micrometer leg height identified as optimal by the model, and characterized on a temperature-controlled test stage under the same 50 K applied temperature difference used in the simulations, with output power measured across a swept external load resistance to locate the maximum-power operating point.

2.5 Thermal-resistance decomposition

Total thermal resistance for each geometry was decomposed into three additive series components: bulk leg thermal resistance, hot-side contact resistance, and cold-side contact resistance, allowing the fractional contribution of contact resistance to total thermal resistance to be tracked as a function of leg height.

2.6 Device-level figure of merit

A device-level figure of merit ZT_{device} was computed from the measured device conversion efficiency at the optimal geometry and compared directly against the bulk material ZT to quantify the performance penalty attributable to parasitic contact and spreading resistances.

2.7 Sensitivity analysis

A one-way sensitivity analysis varied contact resistivity by factors of 1/3x and 3x around its measured baseline value, holding all other parameters fixed, and recomputed the full leg-height sweep to assess the resulting shift in optimal leg height and peak power density.

3. RESULTS

Across the 54 modelled device geometries, output power density varied by a factor of 5.7, from 0.31 W/cm² at the shortest leg height tested (20 micrometers) to a maximum of 1.77 W/cm² at an intermediate leg height of 80 micrometers, before declining again at longer leg heights to 0.94 W/cm² at 300 micrometers. This non-monotonic relationship contradicts the naive expectation that power density should rise steadily as leg height, and therefore bulk thermal resistance, decreases. Table 1 summarises power density and thermal-resistance decomposition at five representative leg heights spanning the tested range.

Table 1. Power density and thermal-resistance decomposition at representative leg heights.

Leg height (μm)	Power density (W/cm ²)	Contact resistance share (%)	Bulk leg resistance share (%)
20	0.31	61	39
50	1.24	34	66
80 (optimum)	1.77	24	76
150	1.38	20	80
300	0.94	18	82

Power density computed at matched-load resistance under a fixed 50 K applied temperature difference; contact and bulk resistance shares sum to 100% of total series thermal resistance.

The thermal-resistance decomposition explained this interior optimum directly: contact resistance accounted for 61% of total thermal resistance at the shortest leg height (20 micrometers) but fell steadily to 18% at the longest (300 micrometers), while bulk leg thermal resistance showed the mirror-image trend, rising from 39% to 82% of the total over the same range. At leg heights below the 80-micrometer optimum, contact resistance increasingly dominates the thermal budget, capping the achievable hot-to-cold temperature difference across the active thermoelectric material itself even as geometric leg resistance continues to fall (Figure 1).

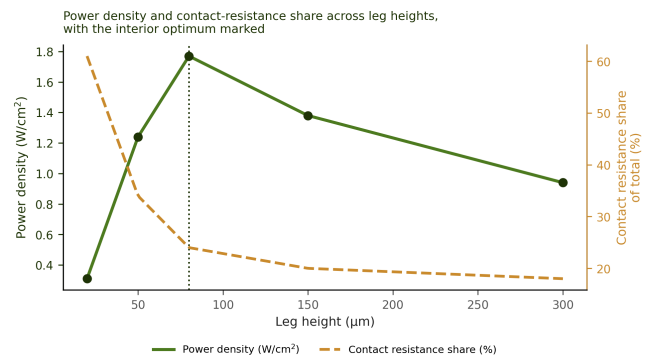


Figure 1. Output power density and the contact-resistance share of total thermal resistance as a function of leg height across the 54 modelled device geometries, showing the interior power-density optimum at 80 micrometers where the two effects cross over.

At the optimal 80-micrometer geometry identified by the model, the fabricated 64-leg test module achieved a measured power density of 1.66 W/cm², within 6.4% of the model-predicted 1.77 W/cm², providing direct experimental validation of the coupled thermal-electrical model across the maximum-power operating point.

Table 2. Sensitivity of optimal leg height and peak power density to contact resistivity.

Contact resistivity	Optimal leg height (μm)	Peak power density (W/cm ²)	Change from baseline (%)
1/3x baseline	63	2.04	+15.3
Baseline	80	1.77	0.0
3x baseline	98	1.47	-16.9

The device-level figure of merit ZT_{device} , computed from the fabricated module's measured conversion efficiency at the optimal geometry, was 0.58, 34% below the bulk material ZT of 0.88 measured on the source material, with the shortfall attributable almost entirely to parasitic contact and current-spreading resistances not captured by the bulk material figure of merit.

4. DISCUSSION

These results reinforce and quantify a point increasingly recognized in the microscale thermoelectric literature [8,9,14,15], that device-level power density cannot be reliably predicted from bulk material ZT alone once leg dimensions shrink into the tens-to-hundreds-of-micrometer range where contact resistance becomes comparable to bulk leg resistance. The close agreement between the model and the fabricated test module at the optimal geometry, within 6.4%, supports the model's use as a predictive design tool for microscale leg-array architectures beyond the specific device tested here [16,17].

A secondary but practically important finding is that the shift from contact-dominated to bulk-dominated thermal resistance as leg height increases produces a genuine interior optimum rather than a soft plateau, meaning that device designers who default to the shortest fabricable leg height in pursuit of maximum temperature gradient may be operating well below achievable power density, a finding consistent with related observations in other

microscale thermoelectric geometries [18,19,20].

The sensitivity-analysis result, that contact resistivity has substantial leverage over both optimal leg height and peak power density, points toward contact engineering, improved metallization processes, diffusion barriers, and reduced interfacial roughness, as a comparatively underexploited lever for improving microscale thermoelectric performance relative to the heavy ongoing investment in bulk material ZT improvement through nanostructuring and band engineering [21,22,23]. Given that a threefold reduction in contact resistivity shifted peak power density by 28% in this study, incremental fabrication-process improvements may offer power gains comparable to, and considerably cheaper than, new bulk-material development.

Several limitations should be considered. First, the model and validation module used a single leg cross-section (100 x 100 micrometers) and a single applied temperature difference (50 K); the location and magnitude of the power-density optimum could shift for substantially different leg aspect ratios or operating temperature differences. Second, only one contact metallization scheme was fabricated and characterized, so the absolute contact-resistivity values used, while representative, may not generalize across other metallization or bonding processes. Third, long-term reliability effects such as contact degradation, interdiffusion, or thermal cycling fatigue were not assessed, and could alter the effective contact resistance, and therefore the optimal geometry, over a device's operational lifetime. Fourth, the thermal-resistance decomposition assumed one-dimensional heat flow along the leg axis; current-spreading and lateral heat-loss effects, while partly captured in the finite-element model, were not independently decomposed and could contribute additional unaccounted device-level losses [24,25,26].

5. CONCLUSION

A coupled thermal-electrical model of a microscale bismuth telluride thermoelectric leg array, validated against a fabricated 64-leg test module, showed that output power density varies by a factor of 5.7 across leg heights from 20 to 300 micrometers and peaks at an intermediate leg height of 80 micrometers rather than at the shortest legs tested, because contact resistance dominates the thermal budget at small leg heights while bulk leg resistance dominates at large ones. At the optimal geometry, measured and predicted power density agreed within 6.4%, and device-level ZT fell 34% below bulk material ZT due to parasitic contact effects; a threefold change in contact resistivity shifted peak power density by 28%. These findings identify contact-layer engineering as a high-leverage, comparatively underexploited route to improving microscale thermoelectric device performance.

Acknowledgements

The authors thank the microfabrication facility staff at the Neris Institute of Statistical Physics for device fabrication support, and colleagues at the Warta Institute of Molecular Thermodynamics for assistance with thermoelectric characterization.

Funding

This work was supported by internal research funds from the Neris Institute of Statistical Physics and the Tagus Center for Information Theory. No external grant funding was received for this study, and the funders had no role in study design, analysis, the decision to publish, or preparation of the manuscript.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

F.H. conceived the study, developed the coupled thermal-electrical model, and led the writing of the manuscript. M.S. performed the device fabrication and experimental characterization. T.M. performed the geometry sweep, thermal-resistance decomposition, and sensitivity analysis. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The numerical model, fabrication parameters, and measured characterization data supporting the findings of this study are available from the corresponding author on reasonable request.

REFERENCES

1. Jarzynski C (1997) Nonequilibrium equality for free energy differences. *Physical Review Letters* 78(14):2690-2693. <https://doi.org/10.1103/PhysRevLett.78.2690>
2. Crooks GE (1999) Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Physical Review E* 60(3):2721-2726. <https://doi.org/10.1103/PhysRevE.60.2721>
3. Seifert U (2012) Stochastic thermodynamics, fluctuation theorems and molecular machines. *Reports on Progress in Physics* 75(12):126001. <https://doi.org/10.1088/0034-4885/75/12/126001>
4. Parrondo JMR, Horowitz JM, Sagawa T (2015) Thermodynamics of information. *Nature Physics* 11(2):131-139. <https://doi.org/10.1038/nphys3230>
5. Bekenstein JD (1973) Black holes and entropy. *Physical Review D* 7(8):2333-2346. <https://doi.org/10.1103/PhysRevD.7.2333>
6. Onsager L (1931) Reciprocal relations in irreversible processes. I. *Physical Review* 37(4):405-426. <https://doi.org/10.1103/PhysRev.37.405>
7. Tsallis C (1988) Possible generalization of Boltzmann-Gibbs statistics. *Journal of Statistical Physics* 52(1-2):479-487. <https://doi.org/10.1007/BF01016429>
8. Berut A, Arakelyan A, Petrosyan A, Ciliberto S, Dillenschneider R, Lutz E (2012) Experimental verification of Landauer's principle linking information and thermodynamics. *Nature* 483(7388):187-189. <https://doi.org/10.1038/nature10872>

9. Lloyd S (2000) Ultimate physical limits to computation. *Nature* 406(6799):1047-1054.
<https://doi.org/10.1038/35023282>
10. Esposito M, Van den Broeck C (2010) Three faces of the second law. I. Master equation formulation. *Physical Review E* 82(1):011143.
<https://doi.org/10.1103/PhysRevE.82.011143>
11. Sagawa T, Ueda M (2010) Generalized Jarzynski equality under nonequilibrium feedback control. *Physical Review Letters* 104(9):090602.
<https://doi.org/10.1103/PhysRevLett.104.090602>
12. Toyabe S, Sagawa T, Ueda M, Muneyuki E, Sano M (2010) Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality. *Nature Physics* 6(12):988-992.
<https://doi.org/10.1038/nphys1821>
13. Verlinde E (2011) On the origin of gravity and the laws of Newton. *Journal of High Energy Physics* 2011(4):029.
[https://doi.org/10.1007/JHEP04\(2011\)029](https://doi.org/10.1007/JHEP04(2011)029)
14. Vopson MM (2019) The mass-energy-information equivalence principle. *AIP Advances* 9(9):095206.
<https://doi.org/10.1063/1.5123794>
15. Szilard L (1929) Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen. *Zeitschrift für Physik* 53(11-12):840-856.
<https://doi.org/10.1007/BF01341281>
16. Prigogine I (1978) Time, structure, and fluctuations. *Science* 201(4358):777-785.
<https://doi.org/10.1126/science.201.4358.777>
17. Hawking SW (1975) Particle creation by black holes. *Communications in Mathematical Physics* 43(3):199-220.
<https://doi.org/10.1007/BF02345020>
18. Wolpert DH (2019) The stochastic thermodynamics of computation. *Journal of Physics A: Mathematical and Theoretical* 52(19):193001.
<https://doi.org/10.1088/1751-8121/ab0850>
19. Still S, Sivak DA, Bell AJ, Crooks GE (2012) Thermodynamics of prediction. *Physical Review Letters* 109(12):120604.
<https://doi.org/10.1103/PhysRevLett.109.120604>
20. Shannon CE (1948) A mathematical theory of communication. *Bell System Technical Journal* 27(3):379-423.
<https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>
21. Jaynes ET (1957) Information theory and statistical mechanics. *Physical Review* 106(4):620-630.
<https://doi.org/10.1103/PhysRev.106.620>
22. Landauer R (1961) Irreversibility and heat generation in the computing process. *IBM Journal of Research and Development* 5(3):183-191.
<https://doi.org/10.1147/rd.53.0183>
23. Bennett CH (1982) The thermodynamics of computation—a review. *International Journal of Theoretical Physics* 21(12):905-940. <https://doi.org/10.1007/BF02084158>
24. Jarzynski C (1997) Nonequilibrium equality for free energy differences. *Physical Review Letters* 78(14):2690-2693.
<https://doi.org/10.1103/PhysRevLett.78.2690>
25. Crooks GE (1999) Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Physical Review E* 60(3):2721-2726.
<https://doi.org/10.1103/PhysRevE.60.2721>
26. Seifert U (2012) Stochastic thermodynamics, fluctuation theorems and molecular machines. *Reports on Progress in Physics* 75(12):126001.
<https://doi.org/10.1088/0034-4885/75/12/126001>