Thermoelectricity: From Atoms to Systems

Week 4: Thermoelectric Systems
Lecture 4.4: Graded materials, TE leg geometry impact

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Conventional Functionally Graded or Segmented Thermoelectric Materials

- Optimize material at each location to have highest $ZT_{\text{local}}$ at that location.
- Typically for power generation applications (large $\Delta T$)
Thermoelectric properties of a composite medium

David J. Bergman and Ohad Levy

We study the thermoelectric properties of a composite medium. … We prove that $Z_{\text{effective}}$ of the composite can never exceed the largest value of $Z$ in any component.

*(rigorous proof for two-component system)*

\[
Q_{11} = \frac{1}{V} \int dV (Q_{11} E_1^{(1)2} + 2 Q_{12} E_1^{(1)} \cdot E_2^{(1)} + Q_{22} E_2^{(1)2})
\]

A new materials property $s = (\sqrt{1 + zT} - 1)/(\alpha T)$, which we call the compatibility factor. Materials with dissimilar compatibility factors cannot be combined by segmentation into an efficient thermoelectric generator. Thus, control of the compatibility factor $s$ is, in addition to $z$, essential for efficient operation of a thermoelectric device.

**Application of the compatibility factor to the design of segmented and cascaded thermoelectric generators**


... Cascaded generators avoid the compatibility problem.
Maximum cooling of uniform thermoelectrics

- Maximum cooling is only a function of $ZT$
- It is geometry independent
- At maximum current, half of the cooling power is cancelled by the Joule heating

Can we beat the $\frac{1}{2} ZT_c^2$ limit by redistributing the Joule heating in the material?

\[ Q = IST_c - \frac{1}{2} I^2 R - K\Delta T \]

\[ I_{\text{max}} = \frac{ST_c}{R} \]

\[ \Delta T_{\text{max}} = \frac{ZT_c^2}{2} \]
In analyzing multiple-section thermoelectric materials, we can convert distributed Joule heating in each section to two local heat sources.
An intuition to improve maximum cooling in graded thermoelectric materials (Zhixi Bian)

Assumption: power factor and thermal conductivity are constant through the materials, small ZT

\[ S^2 \sigma = \text{constant} \]

- If \( I = ST/R \), Joule heating and Peltier cooling are cancelled inside material

\[
\Delta T_{\text{max}} = \frac{1}{2} ZT_C^2 \sum_{n=1}^{\infty} \frac{1}{n^2}
\]

\( n = \text{number of sections} \)

Maximum cooling can be **33-78% times** larger for 2-5 sections (\( S_{\text{max}}/S_{\text{min}} \sim 10 \)).


Zhixi Bian
Assumption: power factor and thermal conductivity are constant through the materials, small $ZT$

\[
\frac{d}{dx} \left( K(x) \frac{dT(x)}{dx} \right) = - \frac{J^2}{\sigma(x)} + JT \frac{dS(x)}{dx}
\]

\[
S(x)^2 \sigma(x) = A
\]

\[
\Delta T_{\text{max}} = \frac{1}{2} ZT^2 \frac{1}{2} \left( \int_0^L S(x) dx \right)^2 \frac{1}{L} \int_0^L dx \int_0^x S^2(x') dx'
\]

\[
\geq \frac{1}{2} ZT^2
\]

- If $S$ increases with $x$ monotonically, $\Delta T_{\text{max}}$ beats uniform materials

Analytical solution: Optimum Seebeck Profile

\[ S(x) = \begin{cases} 
S_0, & 0 < x < L/2 \\
\frac{S_0}{2}, & L/2 < x < (1 - S_0 / 2S_L)L \\
\frac{1 - x/L}{S_L}, & (1 - S_0 / 2S_L)L < x < L 
\end{cases} \]

\[ \Delta T_{\text{max}} = \left( 1 + \frac{1}{2} \ln \left( \frac{S_L}{S_0} \right) \right) \left( \frac{1}{2} ZT^2 \right) \]

For the case \( S^2\sigma = \text{constant}, \ ZT = \text{small}, \) the optimum Seebeck profile and \( \Delta T_{\text{max}} \) can be calculated.


Intuition: Uniform Efficiency Criterion
Conventional functionally graded TE materials try to optimize material at each location to have highest $ZT_{local}$ at that location.

New analysis points to uniform efficiency criterion. This can increase maximum cooling of thermoelectric materials significantly.

Graded $\text{Bi}_2\text{Te}_3$ can increase maximum cooling of TE refrigerators from 240K to 210K (without changing max ZT).

Zhixi Bian et al. PRB 2007
Lecture 4.4 Part I Summary

• Inhomogeneous thermoelectric materials can break the maximum cooling $\frac{1}{2} ZT_{c}^{2}$ (by ~30%)
• The cooling efficiency at large $\Delta T$ can also be improved.
• Analytical solution is given for constant power factor approximation.
• Uniform efficiency criterion provides physical insight into the mathematical solution
• Cooling enhancement is independent of material dimensions.

Acknowledgement: ONR-MURI Thermionic Energy Conversion Center
Can Thermoelectric Leg Geometry Improve the Performance?

Yan Zhang, and Ali Shakouri, "Three-dimensional high cooling power density thermoelectric coolers", 23rd International conference on Thermoelectrics, Adelaide, Australia, 2004
Device Geometries

1D geometry

410x410µm²

Contacting area ranging
50x50 ~ 200x200 µm²

3D geometry

Leg length
$T_h$ (0.2mm)

Heat and current flow

BiTe material Properties:

- $\alpha$, Seebeck Coefficient, 205µV/K
- $\sigma$, electrical conductivity, $1.010 \cdot (\Omega \text{cm})^{-1}$
- $\kappa$, thermal conductivity, 1.405 K/W
- $Z$, figure of merit, $3.02 \cdot 10^{-3} \text{ K}^{-1}$
Cooling for various device sizes

3D geometry device cools over 100°C

Theoretical limit, 76°C predicted by 0.5ZT_c^2

Yan Zhang, and Ali Shakouri, "Three-dimensional high cooling power density thermoelectric coolers", 23rd International conference on Thermoelectrics, Adelaide, Australia, 2004
Device cooling distribution

Solid brick meshing

1D device, contact area 410x410µm²
Max. Cooling, 76.5°C
with supplied current 4A

3D device, contact area 50x50µm²
Max. Cooling, 108.8°C
with supplied current 0.8A
Seemed too good to be true???

• Different opinion

Poisson Equation

\[ \nabla^2 \varphi = -\frac{i^2}{\lambda \sigma} \]

Two assumptions:
1. No current, heat flux due to \( T_1 - T_0 \)
2. With current but uniform contact \( T_0 \)

Conclusion: The maximum energy efficiency in the most general case is independent of the shape of the conductor

Assumption: Uniform temperature at contact area
What it really matters?

Different Boundary Conditions at contact region:
1. Uniform Potential;
2. Uniform Current Density;

Yan Zhang, Zhixi Bian and Ali Shakouri, "Improved energy conversion efficiency by optimizing the geometry of thermoelectric leg elements", Proceedings of the 24th International conference on Thermoelectrics, pp.233-236, June, 2005, Clemson, SC

Yan Zhang, Gehong Zeng, Avram Bar-Cohen and Ali Shakouri, "Is ZT the main main performance factor for hot spot cooling using 3D microrefrigerators?", IMAPS on Thermal Management, 2005, Palo Alto, CA (Student Competition Award)
Boundary Condition 1: Uniform Potential

Potential Distribution  Temperature Distribution

Supplied I=0.6A
Boundary Condition 2: Uniform Current

Potential Distribution

Supplied $I=0.6\, \text{A}$

Current Distribution
Temperature Cross-section under different Boundary Conditions

Contact area

1D theoretical limit

\[ \Delta T_{\text{max}} = 0.5ZTc^2 \]
Benefit of 3D device with uniform current

Center Peak Cooling Region 20x20µm²

High Cooling Power Density
@ center region 655 W/cm²
How to Achieve the uniform current injection?

**Array Device Solution:**
Send different potential to each device to achieve the uniform current profile

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**Diagonal Potential Distribution @ supplied 0.5A**

![Potential Distribution Graph](image_url)
Lecture 4.4 Part II Summary

• The 3D device can cool better than 1D under the condition of uniform current distribution;
  – The temperature distribution is non-uniform at contact area;
  – The center peak region, 20x20µm², could cool over 85°C, or cooling power density of 650 W/cm²;

• It is possible to create an array structure and manipulating the potential of each device to achieve the maximum cooling in the center;

Yan Zhang, Zhixi Bian and Ali Shakouri, "Improved energy conversion efficiency by optimizing the geometry of thermoelectric leg elements", Proceedings of the 24th International conference on Thermoelectrics, pp.233-236, June, 2005, Clemson, SC