

Thermoelectricity: From Atoms to Systems

Week 4: Thermoelectric Systems

Tutorial 4.1 [Homework solutions, problems 1-6](#)

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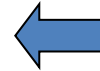
Prob. 1. Heat balance equation

1-1. Second derivative of temperature

The heat generation rate per unit volume

Coupled charge and heat current eq.

$$\dot{q} = -\frac{dJ_Q}{dx} + J_e E$$



$$J_Q = STJ_e - \kappa \frac{dT}{dx}$$

$$E = \frac{J_e}{\sigma} + S \frac{dT}{dx}$$

For one-dimensional problem, and assuming temperature- and position-independent properties,

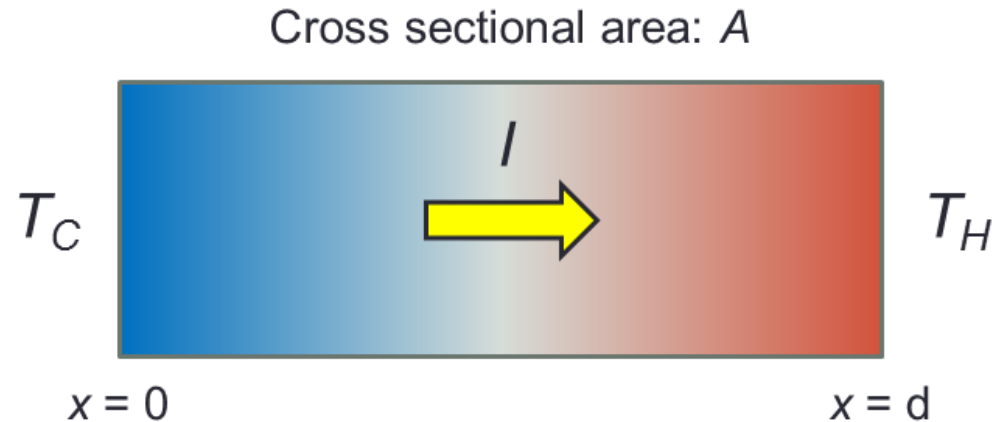
$$\begin{aligned}\dot{q} &= -\left[S \frac{dT}{dx} J_e - \kappa \frac{d^2 T}{dx^2} \right] + \frac{J_e^2}{\sigma} + SJ_e \frac{dT}{dx} \\ &= \kappa \frac{d^2 T}{dx^2} + \frac{J_e^2}{\sigma}\end{aligned}$$

At steady-state, $\dot{q} = 0$

$$\therefore \frac{d^2 T}{dx^2} = -\frac{1}{\kappa \sigma} J_e^2$$

Prob. 1. Heat balance equation

1-2. Temperature profile with current



$$\frac{d^2 T}{dx^2} = -\frac{1}{\kappa \sigma} J_e^2$$

➔

$$T(x) = -\frac{J_e^2}{2\kappa\sigma} x^2 + C_1 x + C_2$$

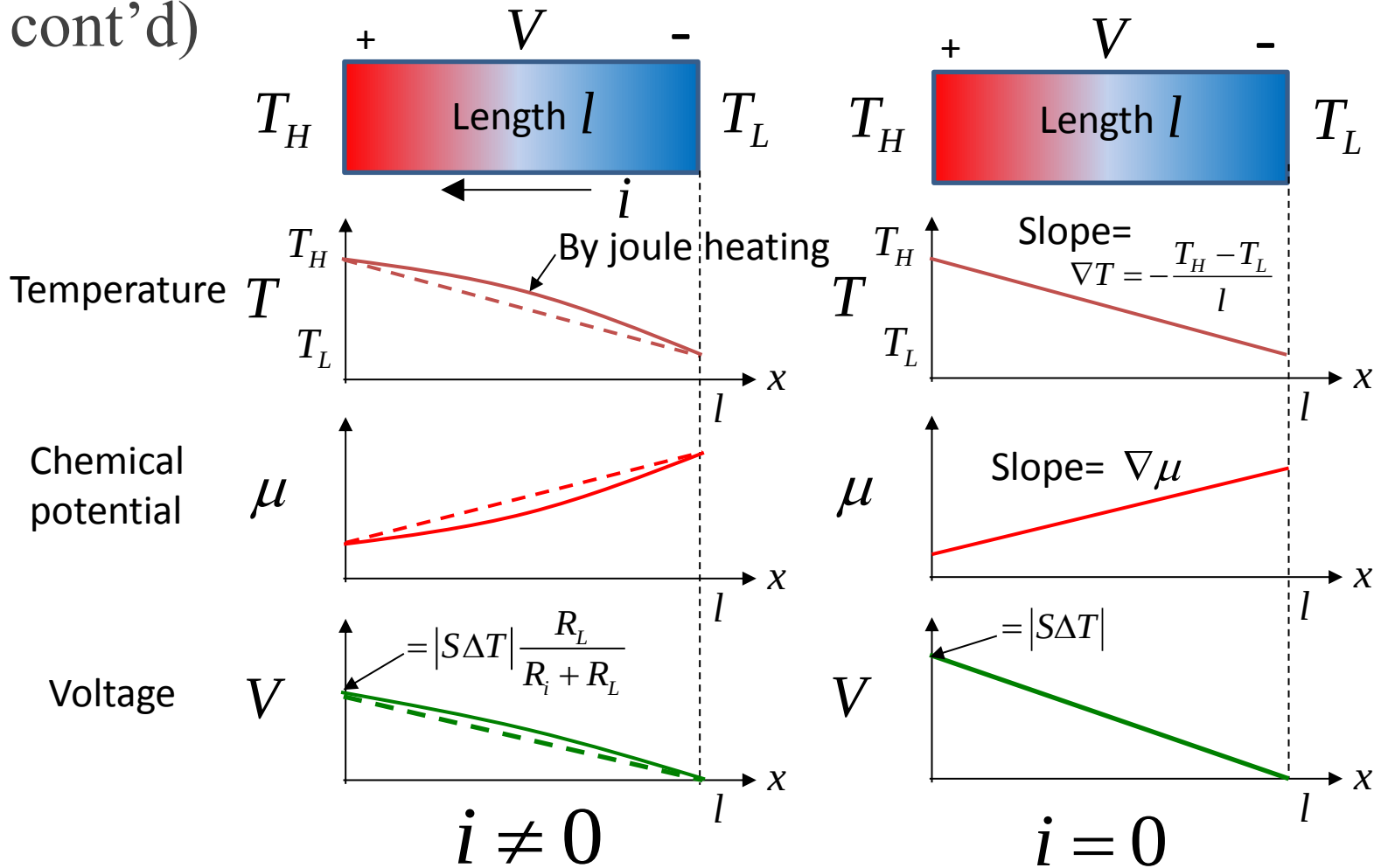
Boundary conditions:

$$\begin{cases} T(x=0) = T_C \\ T(x=d) = T_H \end{cases}$$

$$\therefore T(x) = -\frac{RI^2}{2Kd^2} x^2 + \left(\frac{\Delta T}{d} + \frac{RI^2}{2Kd} \right) x + T_C$$

Prob. 1. Heat balance equation

1-2. Comparison between with and without current flow
cont'd)



Prob. 1. Heat balance equation

1-3. Heat balance equation at cold side

$$Q_{\text{out}} = \kappa A \left. \frac{dT}{dx} \right|_{x=0} \quad \leftarrow \text{From 1-2. } T(x) = -\frac{RI^2}{2Kd^2} x^2 + \left(\frac{\Delta T}{d} + \frac{RI^2}{2Kd} \right) x + T_C$$

$$Q_{\text{out}} = \kappa A \left[-\frac{RI^2}{Kd^2} x + \left(\frac{\Delta T}{d} + \frac{RI^2}{2Kd} \right) \right] \bigg|_{x=0}$$

$$Q_{\text{out}} = \kappa A \left(\frac{\Delta T}{d} + \frac{RI^2}{2Kd} \right) = K\Delta T + \frac{1}{2} RI^2$$

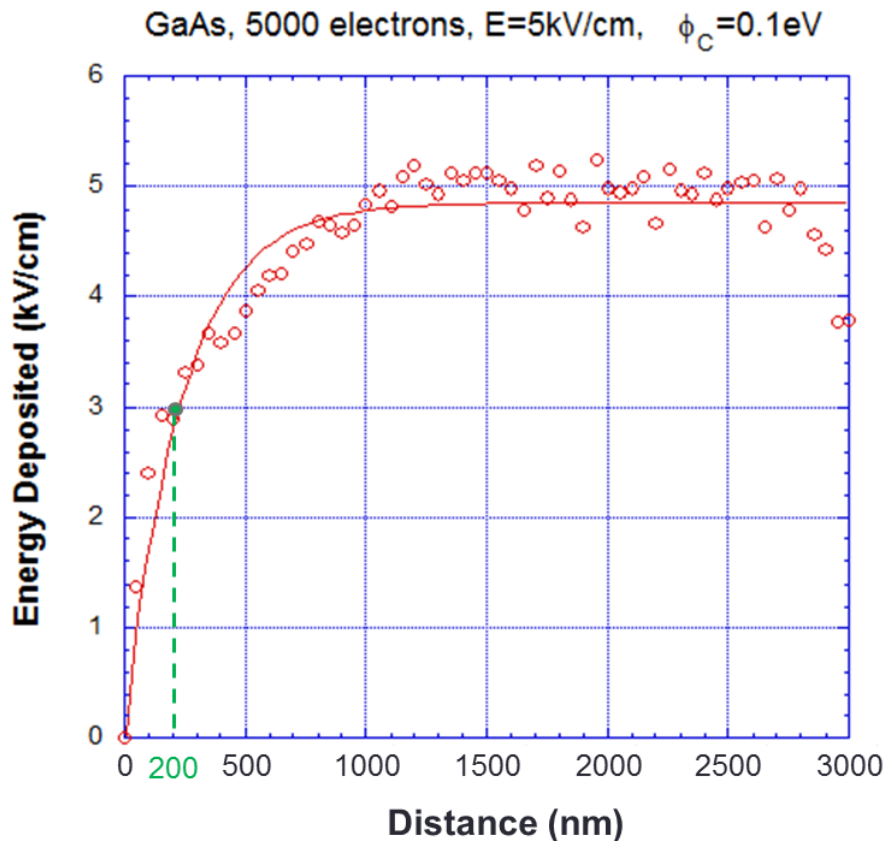
$$\therefore Q_C = ST_C I - Q_{\text{out}} = ST_C I - \frac{1}{2} RI^2 - K\Delta T$$

Prob. 2. Quasi-ballistic TE cooler

2-1. Temperature profile for quasi-ballistic TE cooler

$$\frac{dq_{\text{Joule}}}{dx} = \frac{1}{\sigma} J_e^2 \left[1 - \exp\left(-\frac{x}{\lambda_E}\right) \right]$$

$$-\kappa \frac{d^2 T}{dx^2} = \frac{dq_{\text{Joule}}}{dx}$$



$$\frac{d^2 T}{dx^2} = -\frac{1}{\kappa \sigma} J_e^2 \left[1 - \exp\left(-\frac{x}{\lambda_E}\right) \right]$$

Boundary conditions:

$$\left\{ \begin{array}{l} T(x=0) = T_C \\ T(x=d) = T_H \end{array} \right.$$

Prob. 2. Quasi-ballistic TE cooler

2-1. (cont'd)
$$\frac{d^2 T}{dx^2} = -\frac{1}{\kappa \sigma} J_e^2 \left[1 - \exp\left(-\frac{x}{\lambda_E}\right) \right]$$

$$T'' = -B \left[1 - \exp\left(-\frac{x}{\lambda_E}\right) \right] \quad \text{where} \quad B = \frac{1}{\kappa \sigma} J_e^2 = \frac{RI^2}{Kd^2}$$

$$T' = -B\lambda_E \exp\left(-\frac{x}{\lambda_E}\right) - Bx + C_1$$

 $T(x=0) = T_C$

$$T = B\lambda_E^2 \exp\left(-\frac{x}{\lambda_E}\right) - \frac{B}{2} x^2 + C_1 x + T_C - B\lambda_E^2$$

 $T(x=d) = T_H$

$$T(x=d) = B\lambda_E^2 \exp\left(-\frac{d}{\lambda_E}\right) - \frac{B}{2} d^2 + C_1 d + T_C - B\lambda_E^2 = T_H$$

Prob. 2. Quasi-ballistic TE cooler

2-1. (cont'd)

$$B\lambda_E^2 \exp\left(-\frac{d}{\lambda_E}\right) - \frac{B}{2}d^2 + C_1d + T_C - B\lambda_E^2 = T_H$$

$$C_1 = -\frac{B\lambda_E^2}{d} \exp\left(-\frac{d}{\lambda_E}\right) + \frac{B}{2}d + \frac{T_H - T_C}{d} + \frac{B\lambda_E^2}{d}$$

$$C_1 = \frac{B\lambda_E^2}{d} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] + \frac{B}{2}d + \frac{\Delta T}{d}$$

$$\therefore T = B\lambda_E^2 \exp\left(-\frac{x}{\lambda_E}\right) - \frac{B}{2}x^2 + \left\{ \frac{B\lambda_E^2}{d} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] + \frac{B}{2}d + \frac{\Delta T}{d} \right\} x + T_C - B\lambda_E^2$$

 $B = \frac{RI^2}{Kd^2}$

$$\therefore T(x) = -\frac{RI^2}{2Kd^2}x^2 + \left\{ \frac{\Delta T}{d} + \frac{RI^2}{2Kd} + \frac{RI^2\lambda_E^2}{Kd^3} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] \right\} x + T_C - \frac{RI^2\lambda_E^2}{Kd^2} \left[1 - \exp\left(-\frac{x}{\lambda_E}\right) \right]$$

Prob. 2. Quasi-ballistic TE cooler

2-2. Heat dissipation at cold side

$$Q_{\text{out}} = \kappa A \left. \frac{dT}{dx} \right|_{x=0}$$

$$\frac{dT(x)}{dx} = -\frac{RI^2}{Kd^2}x + \left\{ \frac{\Delta T}{d} + \frac{RI^2}{2Kd} + \frac{RI^2\lambda_E^2}{Kd^3} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] \right\} - \frac{RI^2\lambda_E}{Kd^2} \exp\left(-\frac{x}{\lambda_E}\right)$$

$$\left. \frac{dT(x)}{dx} \right|_{x=0} = \left\{ \frac{\Delta T}{d} + \frac{RI^2}{2Kd} + \frac{RI^2\lambda_E^2}{Kd^3} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] \right\} - \frac{RI^2\lambda_E}{Kd^2}$$

$$\kappa A \left. \frac{dT(x)}{dx} \right|_{x=0} = \left\{ K\Delta T + \frac{RI^2}{2} + \frac{RI^2\lambda_E^2}{d^2} \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] \right\} - \frac{RI^2\lambda_E}{d}$$



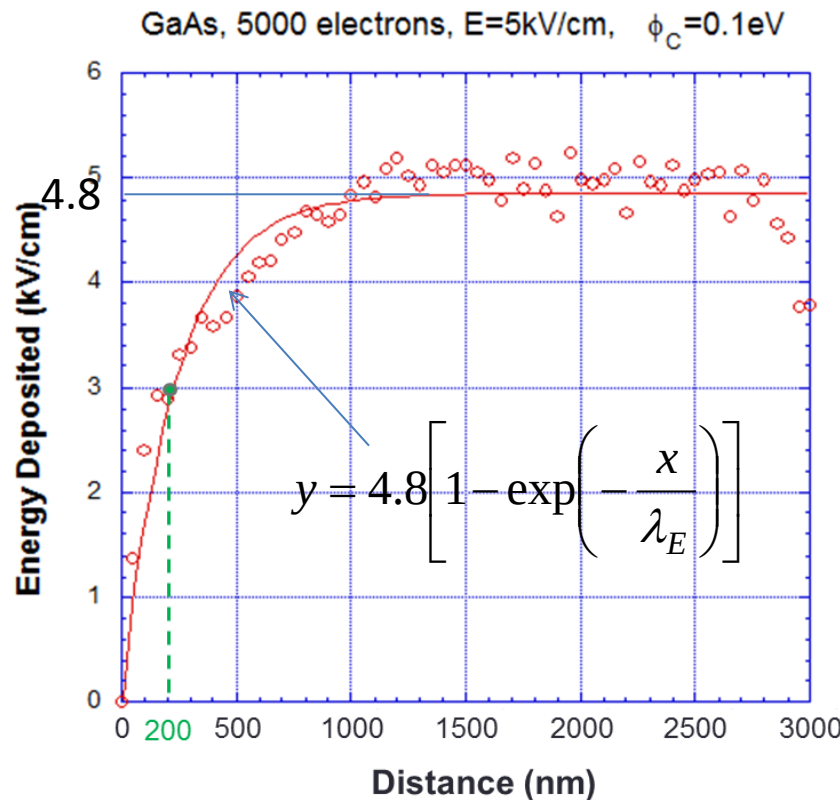
$$\therefore Q_{\text{out}} = RI^2 \left\{ \frac{1}{2} - \frac{\lambda_E}{d} + \left(\frac{\lambda_E}{d} \right)^2 \left[1 - \exp\left(-\frac{d}{\lambda_E}\right) \right] \right\} + K\Delta T$$

Prob. 2. Quasi-ballistic TE cooler

2-3. Fraction of Joule heating dissipated to cathode

$$Q_{\text{out}} = RI^2 \left\{ \frac{1}{2} - \frac{\lambda_E}{d} + \left(\frac{\lambda_E}{d} \right)^2 \left[1 - \exp\left(-\frac{d}{\lambda_E} \right) \right] \right\} + K\Delta T$$

Fraction of RI^2



$$d = 3000 \text{ nm}$$

From the left figure, at $x = \lambda_E$

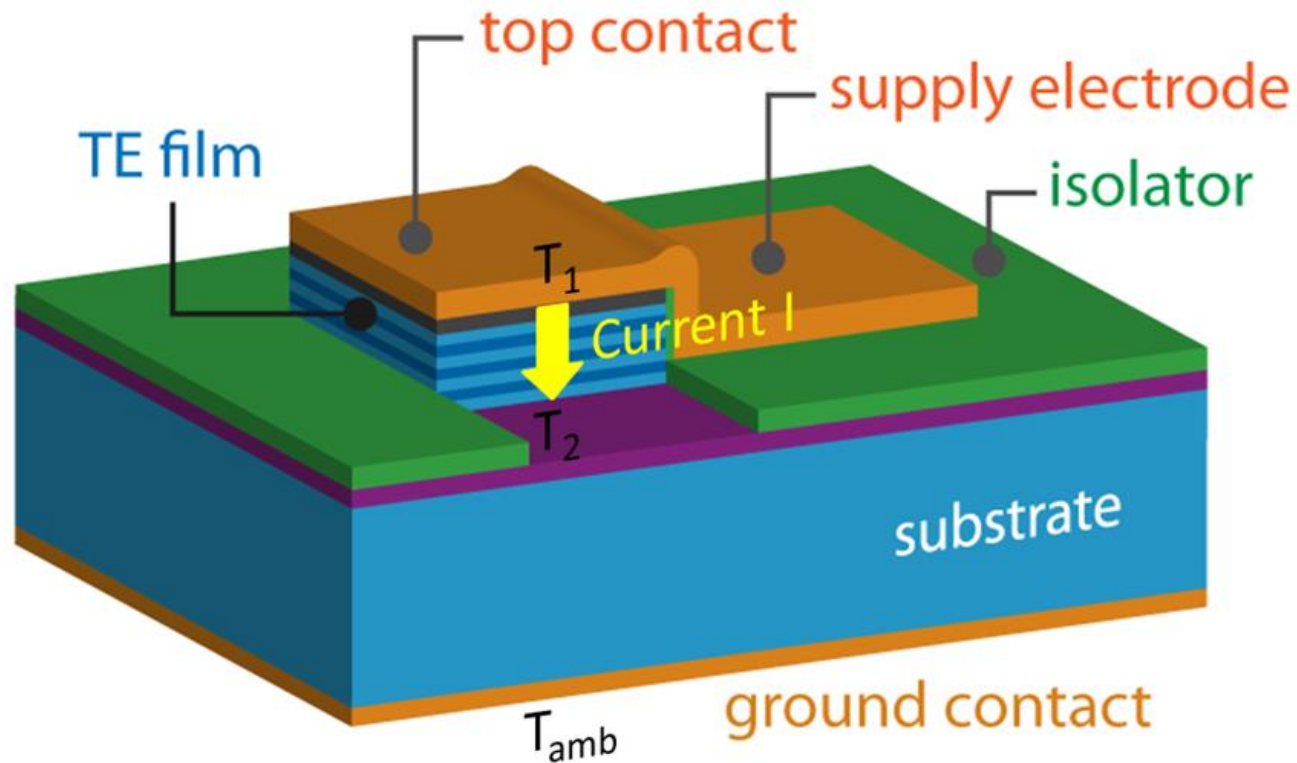
$$y = 4.8[1 - \exp(-1)] = 3.0$$

$$\therefore \lambda_E = 200 \text{ nm}$$

$$\frac{\lambda_E}{d} = \frac{1}{15}$$

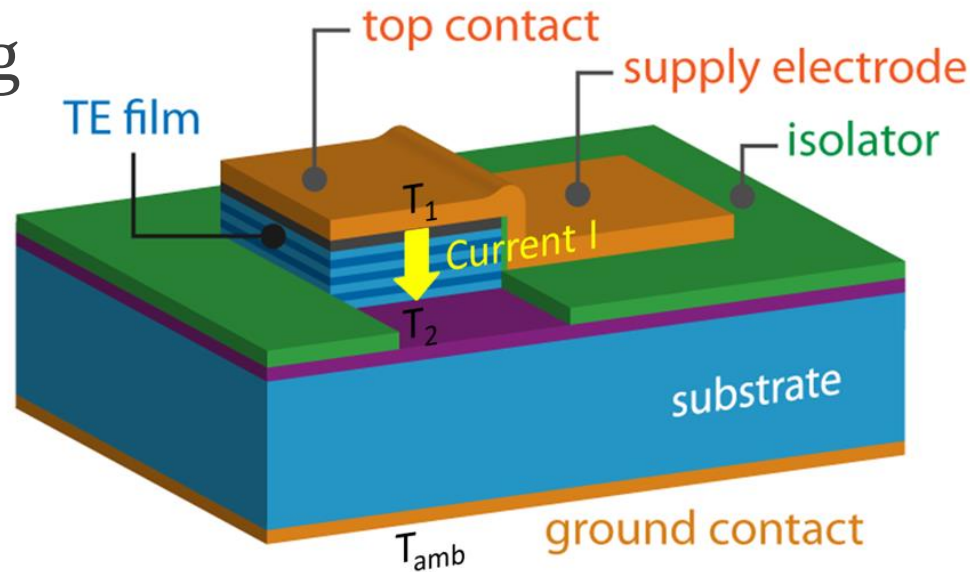
$$\therefore \frac{1}{2} - \frac{\lambda_E}{d} + \left(\frac{\lambda_E}{d} \right)^2 \left[1 - \exp\left(-\frac{d}{\lambda_E} \right) \right] = \underline{0.44}$$

Prob. 3. Thermoelectric cooler



Prob. 3. Thermoelectric cooler

3-1. Max cooling



$$0 = ST_C I - \frac{1}{2} R I^2 - K \Delta T \quad \Rightarrow \quad \Delta T = -\frac{R}{2K} I^2 + \frac{ST_C}{K} I$$

$$\Delta T = -\frac{R}{2K} \left(I - \frac{ST_C}{R} \right)^2 + \frac{1}{2} Z T_C^2$$
$$\therefore \Delta T_{\max} = \frac{1}{2} Z T_C^2 \quad \text{when} \quad I = \frac{ST_C}{R}$$

Prob. 3. Thermoelectric cooler

3-2. Simulation (<https://nanohub.org/tools/thermo>)

(1)

Click here

1 Intro → 2 Mode Selection and Conditions → 3 Material Properties and Dimensions → 4 Simulate

Thermoelectric Device Simulator

Welcome! This simulation tool is intended to simulate thermoelectric (TE) devices under various conditions and designs. Both micro-scale thin-film TE devices fabricated on a substrate (Fig. 1) and large-scale multi-element TE modules (Fig. 2) can be simulated.

There are currently six modes that user can choose from in the next page. Please select one mode depending on what type of TE device (Thin film or module), what operation mode (cooling or power generation), and what boundary conditions (Heat input or top temperature) to simulate. Then, enter the material properties and dimensions of the TE device, specify the simulation conditions, and then press 'simulate' button.

Users can choose an independent variable such as material parameters and dimensions of the TE device, and simulation conditions. The device performances are simulated as a function of the independent variable.

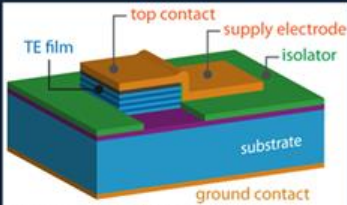


Figure courtesy of Bjorn Vermeersch

Fig. 1 Thin film thermoelectric device

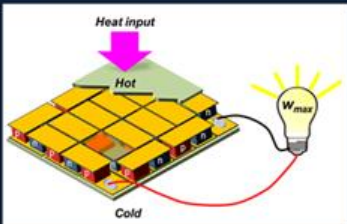


Fig. 2 Multi-element thermoelectric module

Click [here](#) for more information about the modeling of thermoelectric devices.

Or click this button to proceed to the second phase

Mode Selection and Conditions >

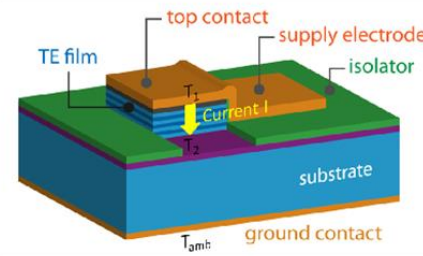
(2)

1 Intro → 2 Mode Selection and Conditions → 3 Material Properties and Dimensions → 4 Simulate

Select a mode: Mode 1: Thermoelectric Thin Film Cooler: Cooling power is known

Select Mode 1 Thin Film Thermoelectric Cooler (Q_{in} is known)

In this mode, the cooling power density (Q_{in}) is known. The model solves for the temperatures (T_1, T_2) with a given current (I) applied. The model can also solve for the adiabatic condition at the top surface by $Q_{in} = 0$. The total electrical power consumed (W) and the coefficient of performance ($COP = Q_{in}/W$) are also obtained. In the substrate, both electrical current and heat spreading effects are taken into account.



Enter the values here

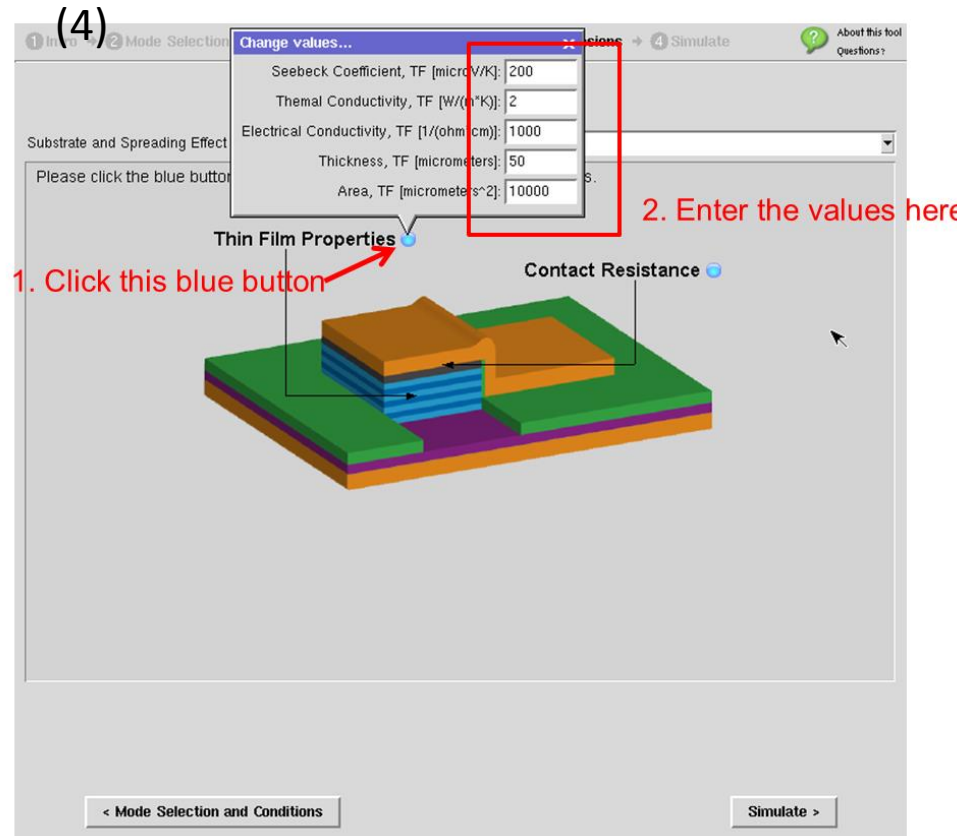
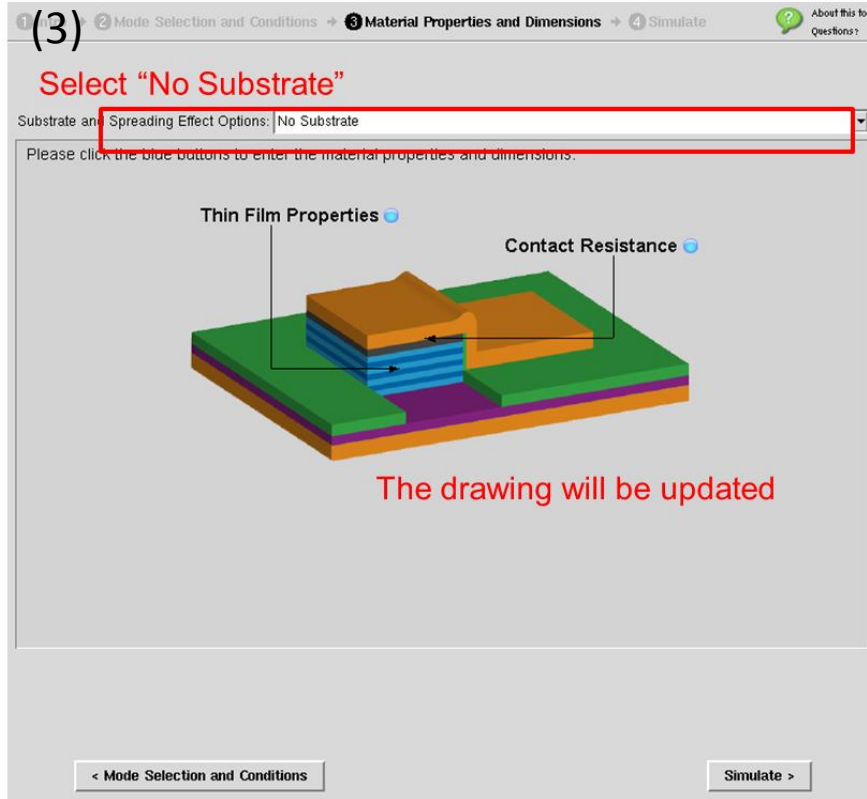
Boundary Condition	Independent Variable
Cooling Power Density [W/cm^2]: 0	Independent Variable: Current [Amp]
Other Conditions	Minimum Value: 0
T ambient [K]: 300	Step Value: 0.01
Current [Amp]: .5	Maximum Value: 2

< Intro

Material Properties and Dimensions >

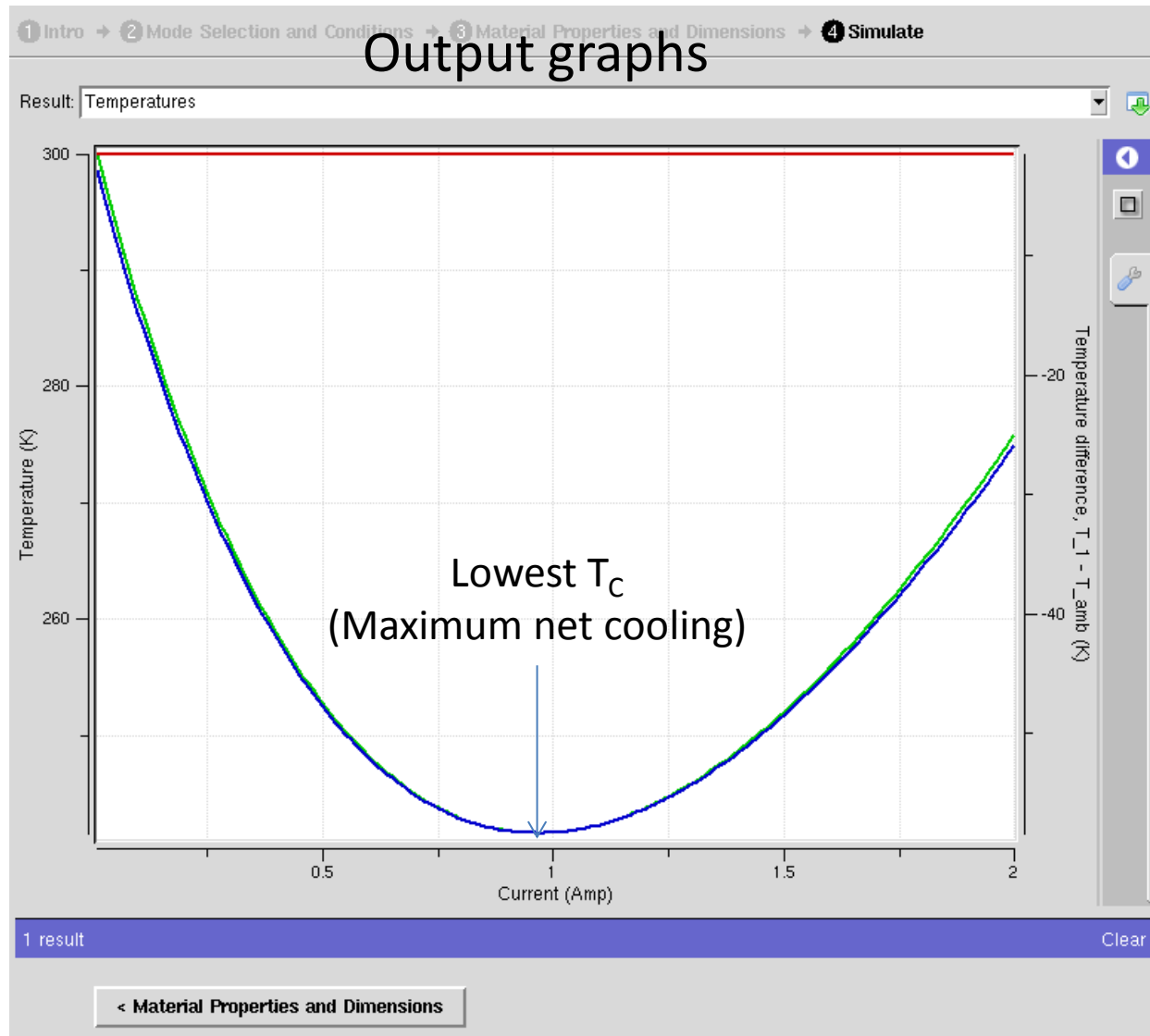
Prob. 3. Thermoelectric cooler

3-2. Simulation for maximum net cooling (cont'd)



Prob. 3. Thermoelectric cooler

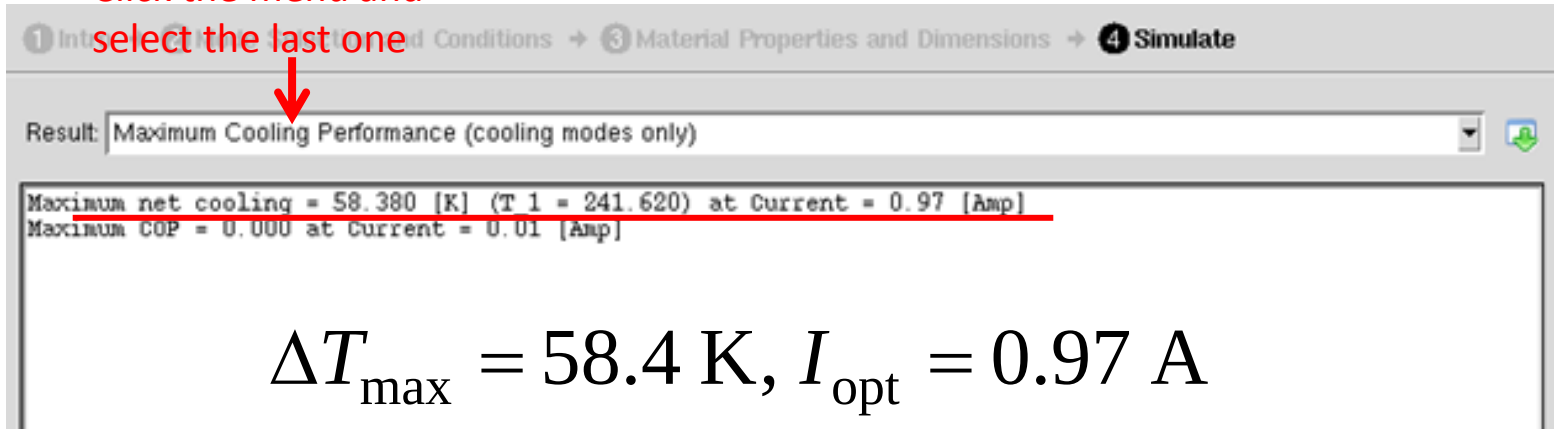
3-2.
(cont'd)



Prob. 3. Thermoelectric cooler

3-2.
(cont'd)

Click the menu and select the last one



Result: Maximum Cooling Performance (cooling modes only)

Maximum net cooling = 58.380 [K] (T 1 = 241.620) at Current = 0.97 [Amp]
Maximum COP = 0.000 at Current = 0.01 [Amp]

$$\Delta T_{\max} = 58.4 \text{ K}, I_{\text{opt}} = 0.97 \text{ A}$$

Check: $T_C = 241.6 \text{ K}$

$$Z = \frac{(200 \times 10^{-6} \text{ V/K})^2 (1000 \times 10^2 \text{ } \Omega^{-1} \text{ m}^{-1})}{(2 \text{ W/mK})} = 0.002 \text{ K}^{-1}$$

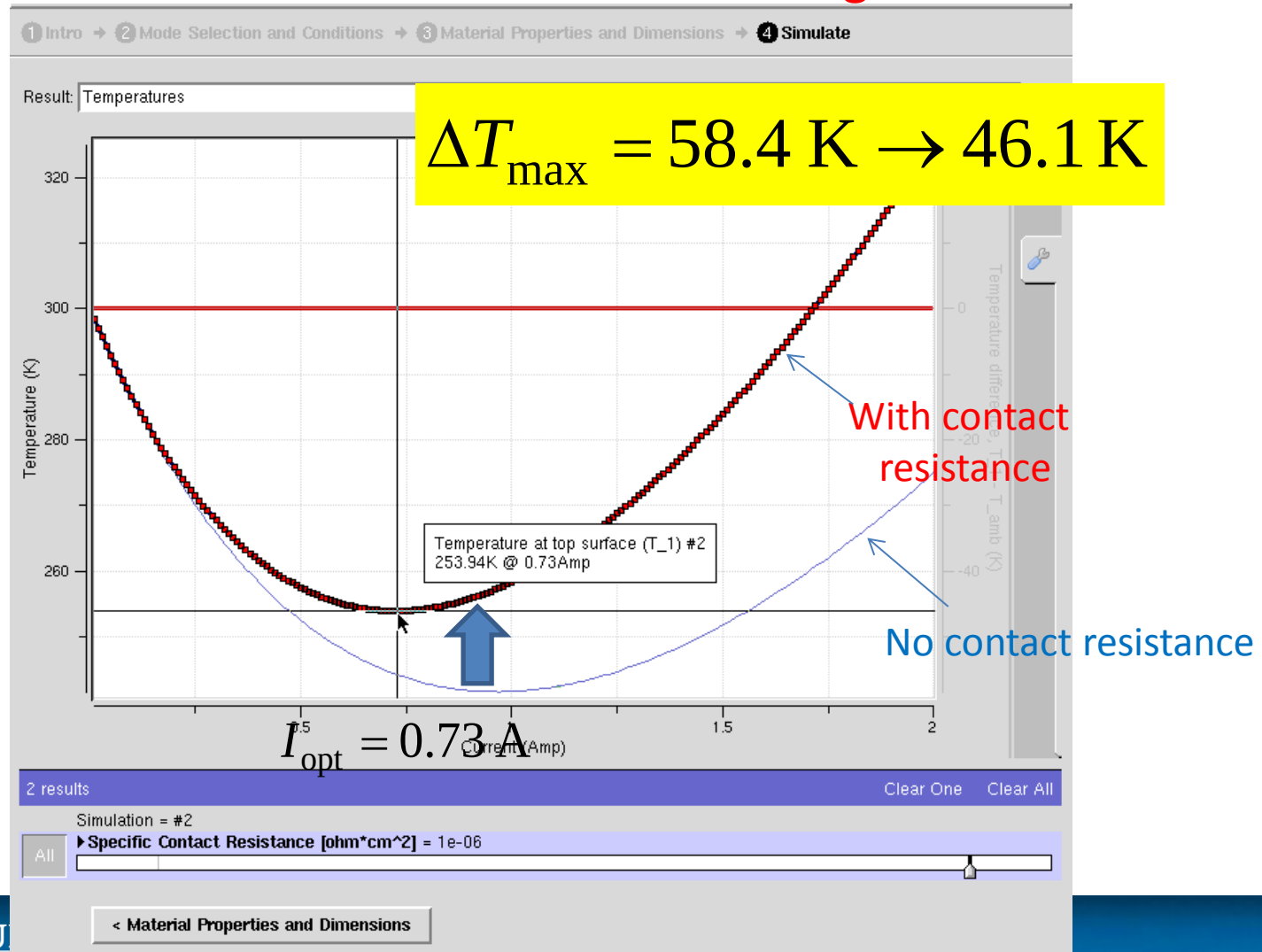
$$\begin{aligned} \therefore \frac{1}{2} Z T_C^2 &= \frac{1}{2} (0.002 \text{ K}^{-1}) (241.6 \text{ K})^2 = 58.4 \text{ K} \\ &= \Delta T_{\max} \quad (\text{match!}) \end{aligned}$$

Prob. 3. Thermoelectric cooler

3-3.

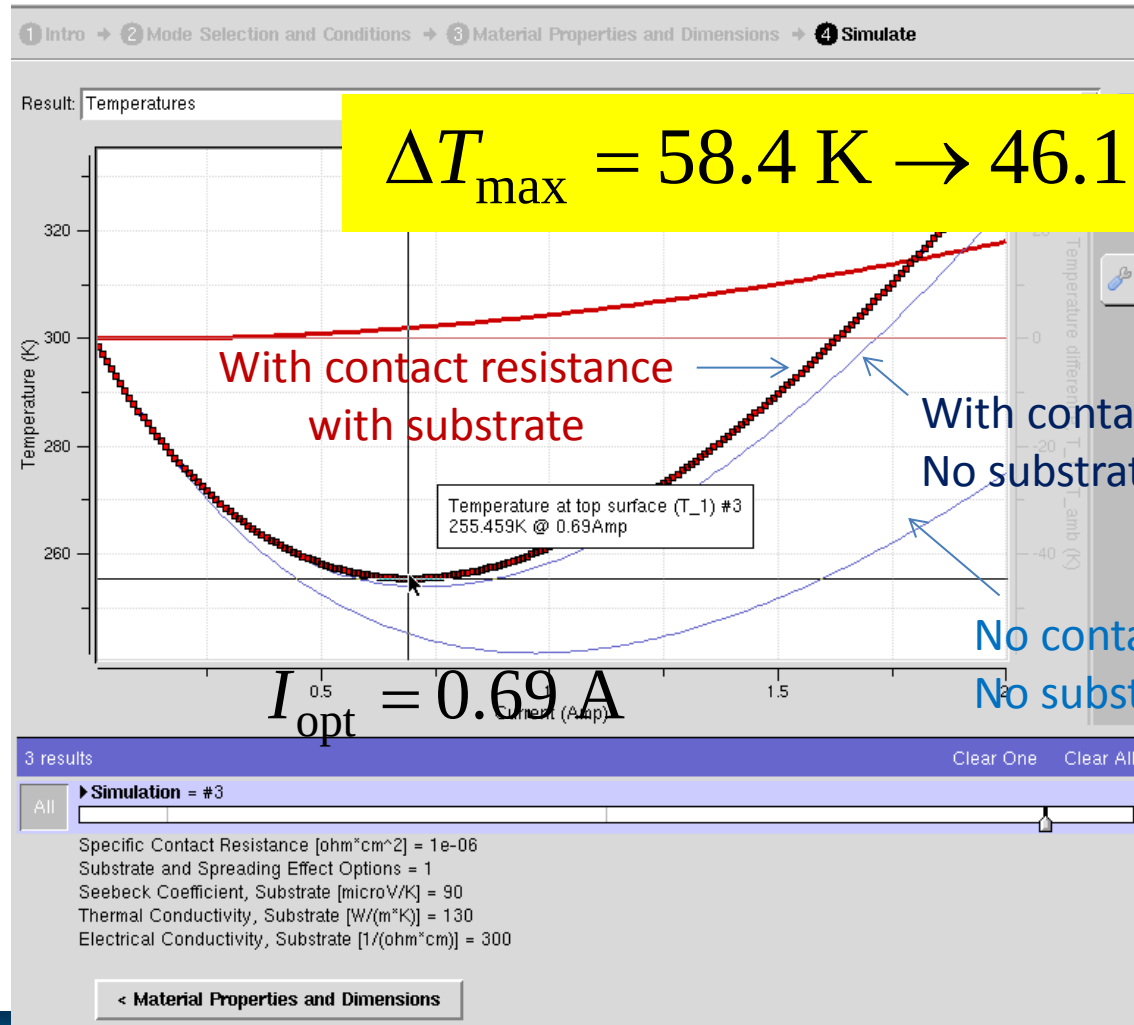
With specific contact resistance= $1\text{e-}6 \Omega \text{ cm}^2$

-> Additional Joule heating



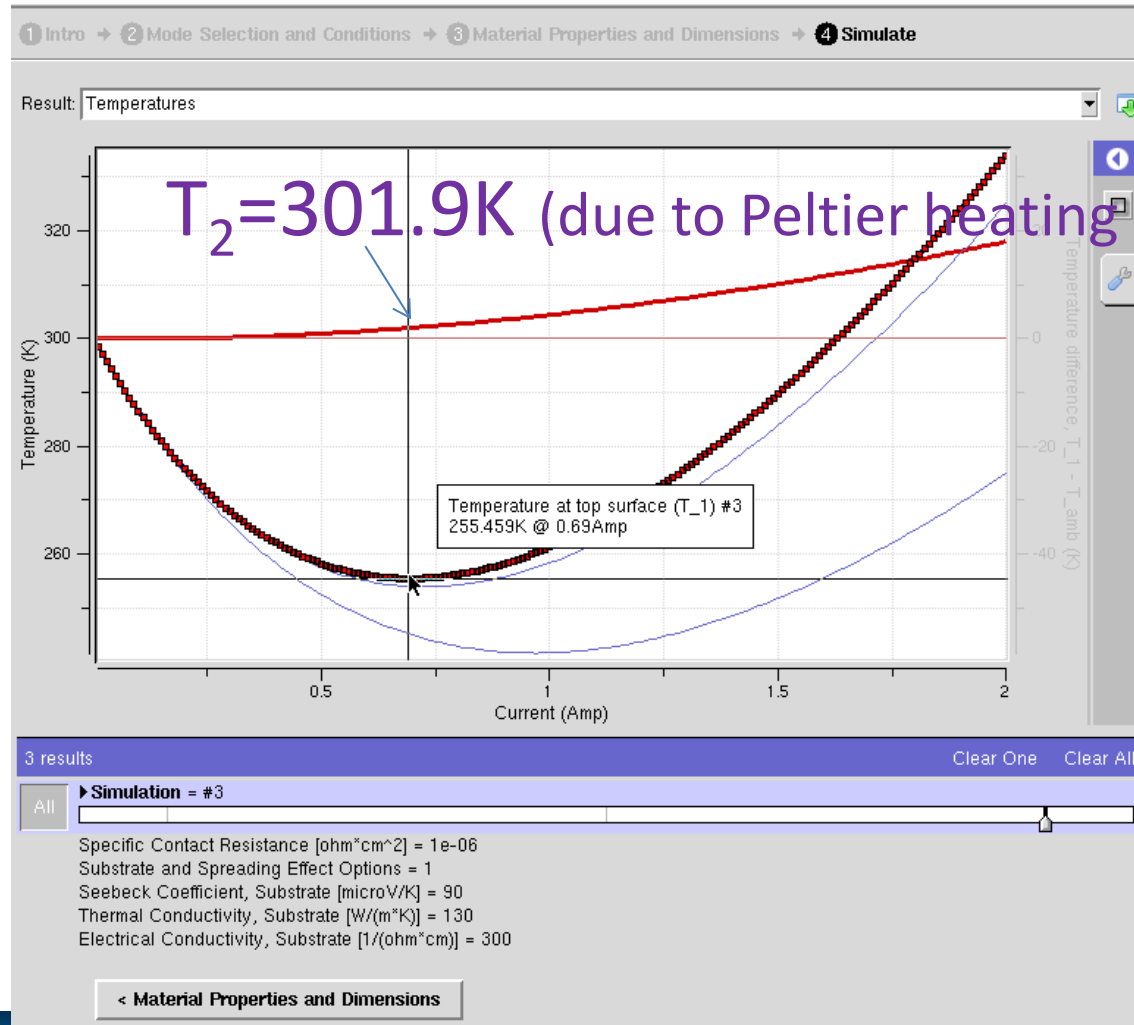
Prob. 3. Thermoelectric cooler

3-4. With substrate with spreading effect



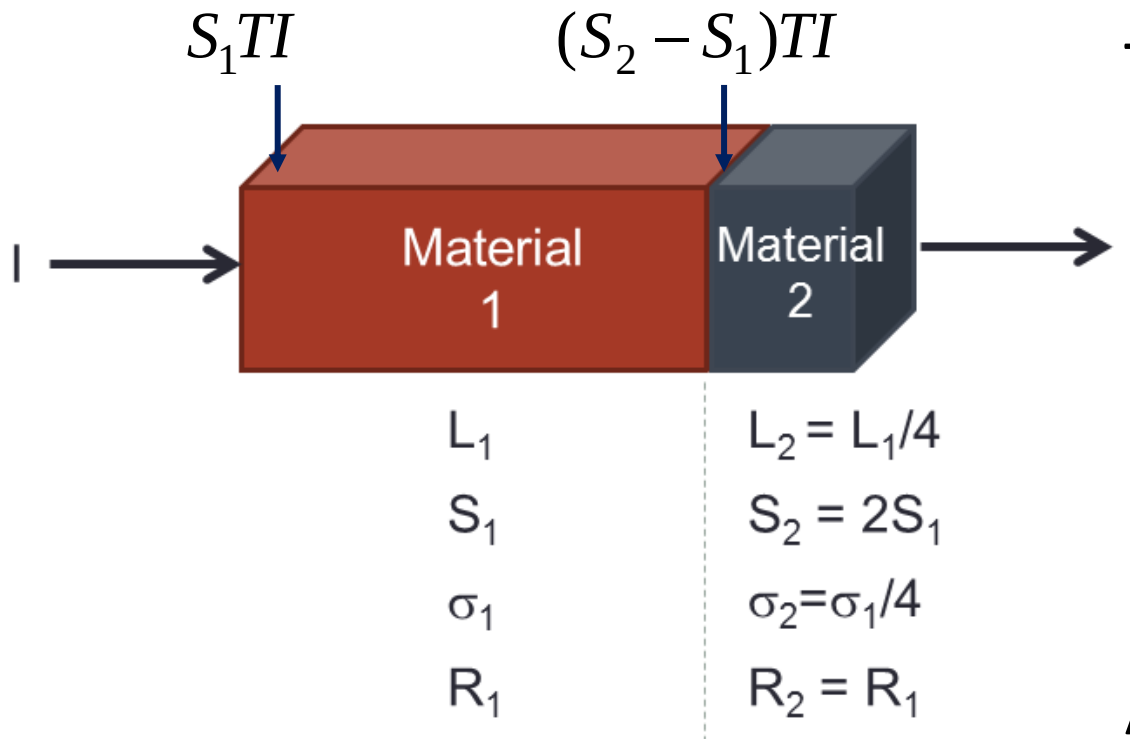
Prob. 3. Thermoelectric cooler

3-5. With substrate with spreading effect on T_2



Prob. 4. Segmented TE element

In a single material: $\Delta T_{\max} = \frac{1}{2} Z T_C^2$ when $I = \frac{S T_C}{R}$ or $I^2 R = S T_C I$
 (Joule)=(Peltier)



To keep this condition

$$S_1 T I = (S_2 - S_1) T I$$

$$\therefore S_2 = 2S_1$$

$$R_1 = R_2$$

$$\text{Also, } S_1^2 \sigma_1 = S_2^2 \sigma_2$$

Prob. 4. Segmented TE element

Material 1

Property	Value
Seebeck Coefficient, TF [microV/K]	200
Thermal Conductivity, TF [W/(m*K)]	2
Electrical Conductivity, TF [1/(ohm*cm)]	1000
Thickness, TF [micrometers]	50
Area, TF [micrometers^2]	10000

Material 2

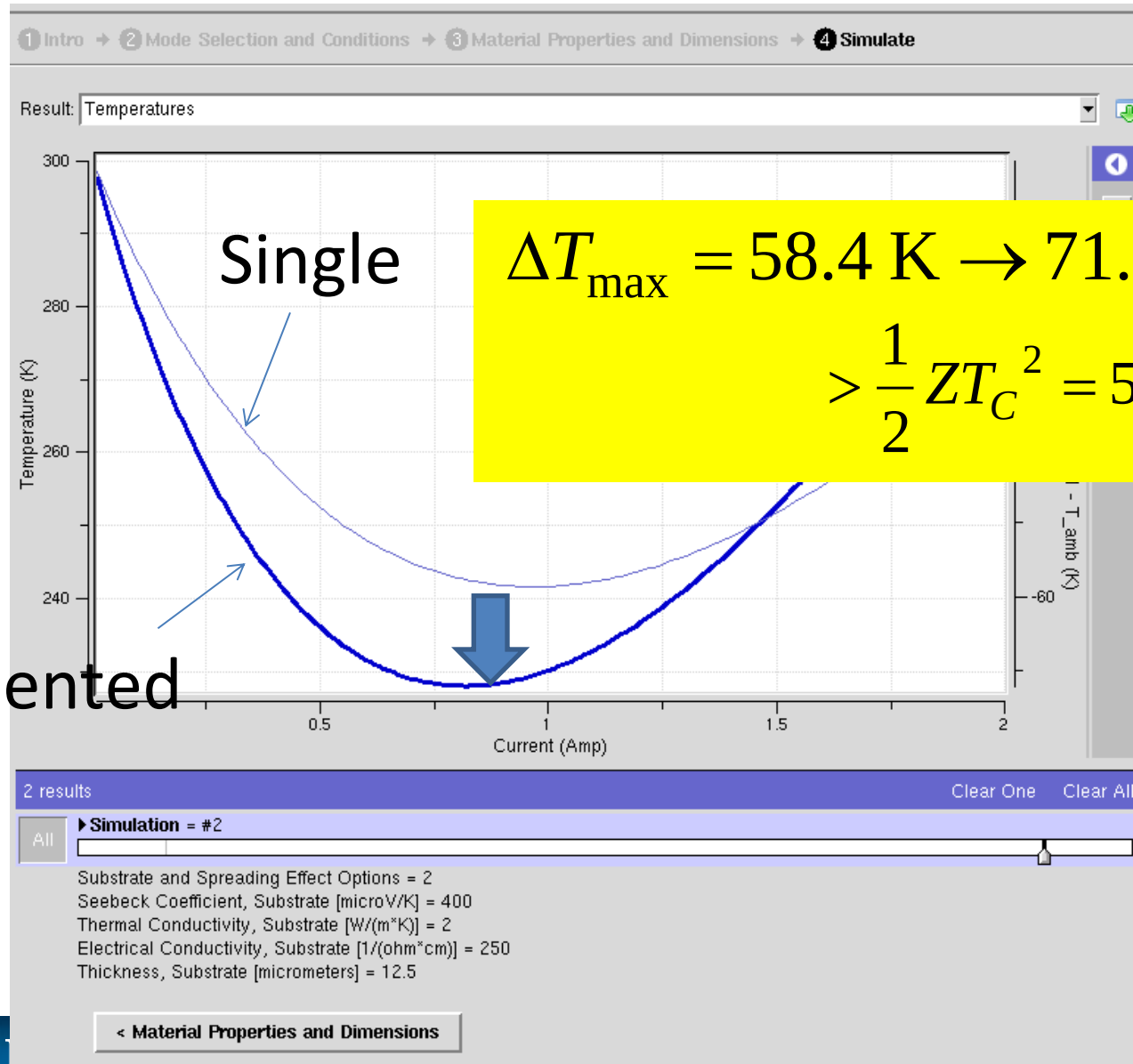
Property	Value
Seebeck Coefficient, Substrate [microV/K]	400
Thermal Conductivity, Substrate [W/(m*K)]	2
Electrical Conductivity, Substrate [1/(ohm*cm)]	250
Thickness, Substrate [micrometers]	12.5

< Mode Selection and Conditions

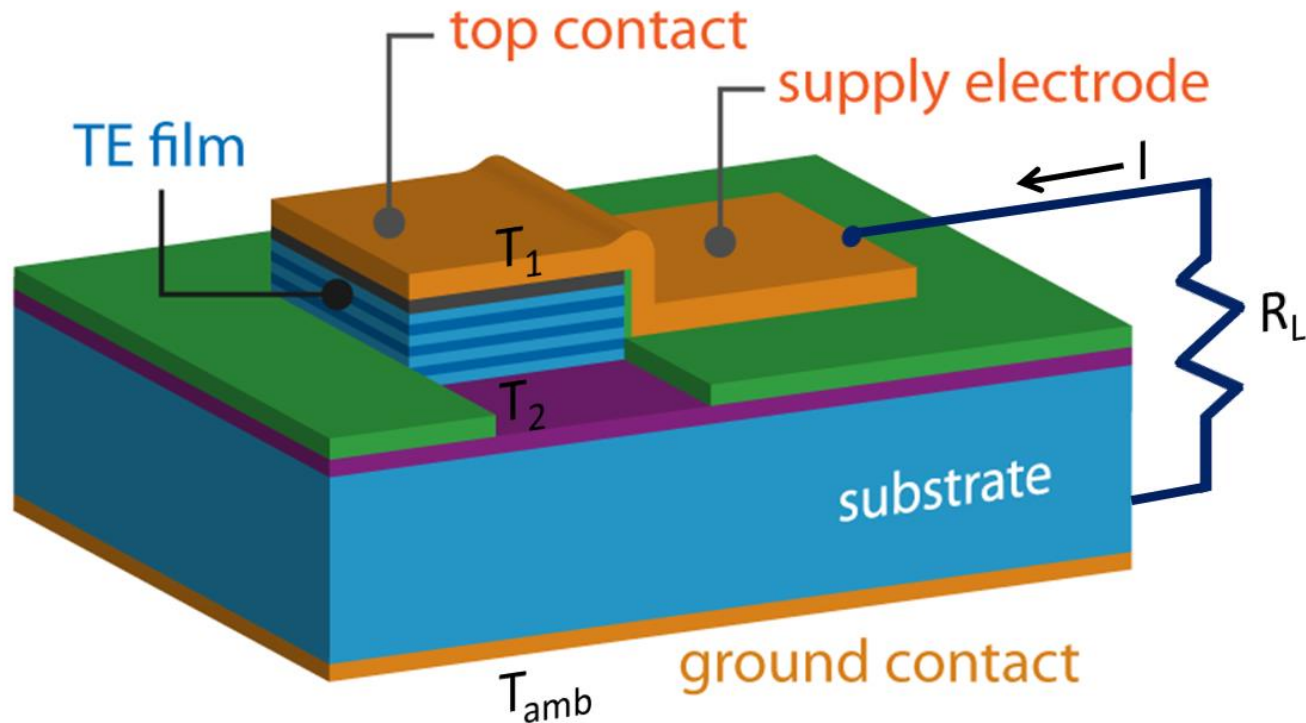
Simulate >

Prob. 4. Segmented TE element

Segmented

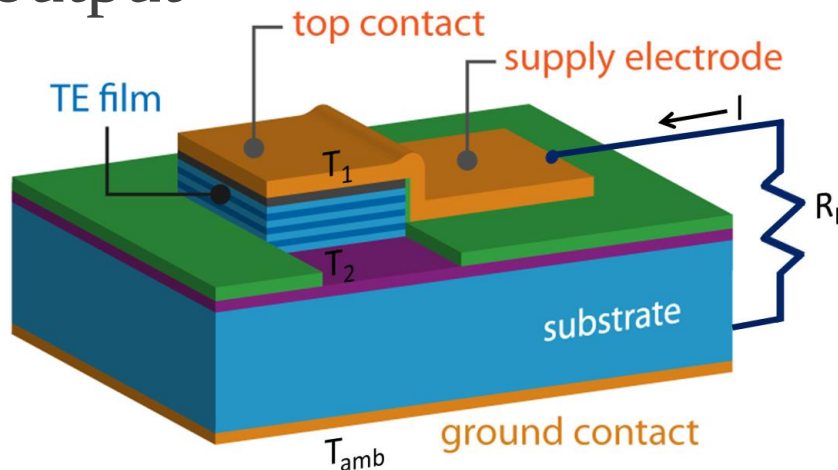


Prob. 5. TE power generator

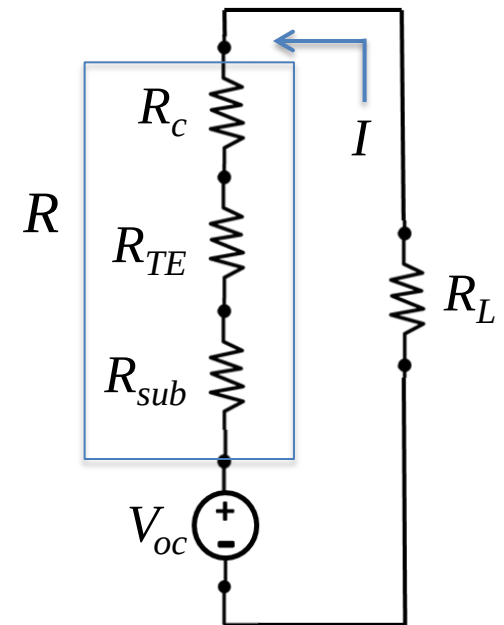


Prob. 5. TE power generator

5-1. Power output



< Electrical resistance network for power generation >



Seebeck effect: $V_{oc} = S_{TE}(T_1 - T_2) + S_{sub}(T_2 - T_{amb})$

$V_{oc} = S_{TE}\Delta T$ (without substrate)

Ohmic law: $V_{oc} = I(R + R_L) = S_{TE}\Delta T$

$$\therefore I = \frac{S(T_H - T_C)}{R + R_L}, P_{out} = \frac{S^2(\Delta T)^2 R_L}{(R + R_L)^2}$$

Prob. 5. TE power generator

5-2. Maximum power output

$$P_{\text{out}} = \frac{S^2 (\Delta T)^2 R_L}{(R + R_L)^2}$$

Differentiate P_{out} with respect to R_L

$$\frac{dP_{\text{out}}}{dR_L} = \frac{S^2 (\Delta T)^2 \left[(R + R_L)^2 - 2R_L (R + R_L) \right]}{(R + R_L)^4} = 0$$

$$\therefore R_L = R$$

$$P_{\text{out,max}} = \frac{S^2 (\Delta T)^2}{4R}$$

Prob. 5. TE power generator

5-3. Maximum efficiency

$$\eta = \frac{I(S\Delta T - IR)}{ST_H I - \frac{1}{2}RI^2 + K\Delta T} \quad (a)$$

Differentiate η with respect to I , and $\frac{d\eta}{dI} = 0$

$$(S\Delta T - 2RI)(K\Delta T + SIT_H - 1/2I^2R) - I(S\Delta T - RI)(ST_H - RI) = 0$$



$$\begin{aligned} I &= \frac{K\Delta T}{ST_M}(\gamma - 1) = \frac{S\Delta T}{ZT_M R}(\gamma - 1) \quad \text{where} \quad \gamma = \sqrt{1 + ZT_M} \\ &= \frac{S\Delta T}{R} \frac{(\gamma - 1)}{(\gamma^2 - 1)} = \boxed{\frac{S\Delta T}{R(\gamma + 1)}} \quad (b) \end{aligned}$$
$$ZT_M = \gamma^2 - 1$$

Prob. 5. TE power generator

5-3. Maximum efficiency (cont'd)

Plug (b) into (a) to get

$$\therefore \eta_{\max} = \frac{(\gamma - 1)}{\left[(\gamma + 1) - \frac{\Delta T}{T_H} \right]} \frac{\Delta T}{T_H}$$

From $I = \frac{S\Delta T}{R(\gamma + 1)} = \frac{S\Delta T}{R + R_L}$

$$\therefore R_L = \gamma R$$

5-4. (Carnot limit)

$$\eta_{\max} = \frac{(\gamma - 1)}{\left[(\gamma + 1) - \frac{\Delta T}{T_H} \right]} \frac{\Delta T}{T_H} = \frac{\Delta T}{T_H}$$

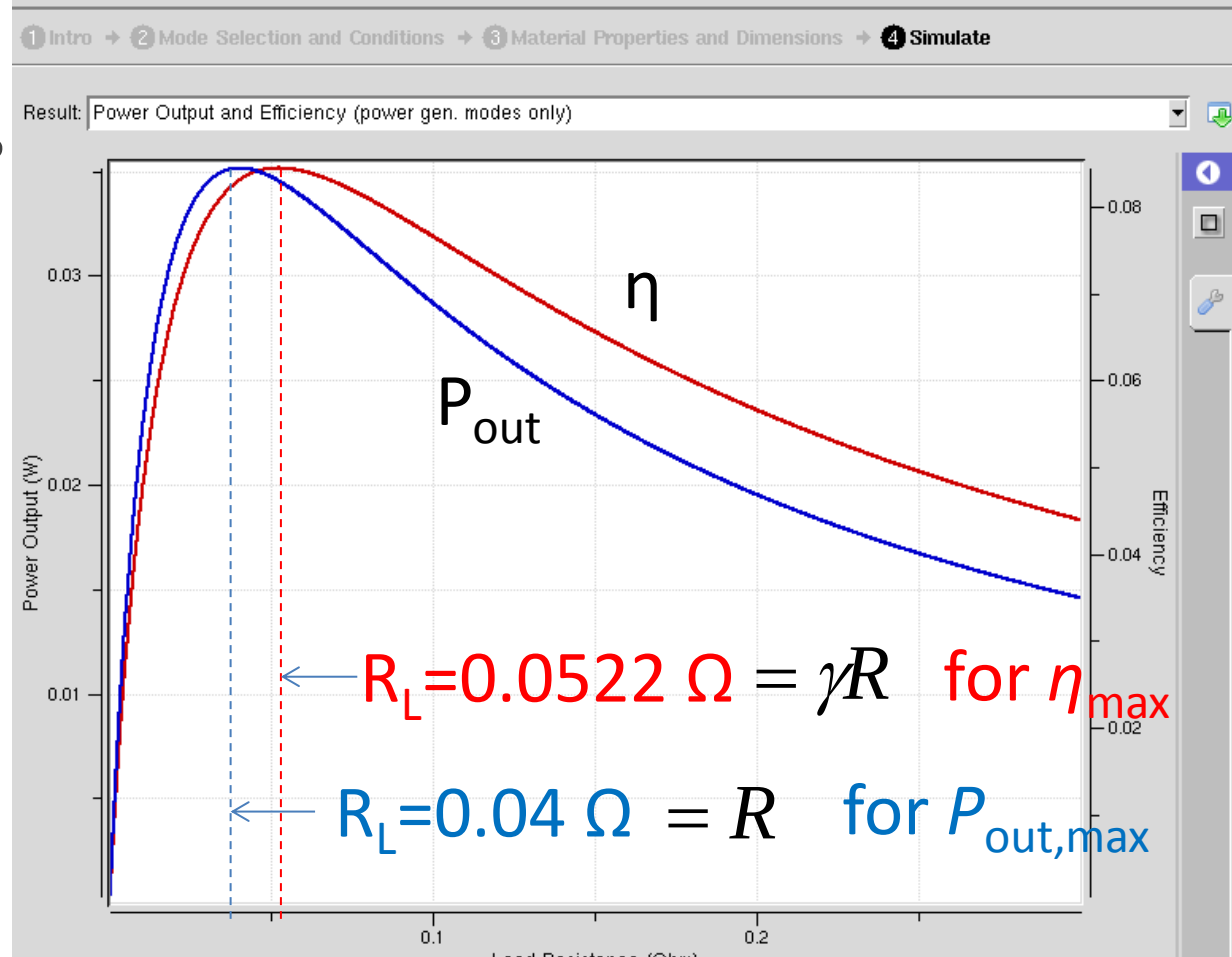

$$(\gamma - 1) = (\gamma + 1) - \frac{\Delta T}{T_H}$$

True only if $\gamma = \infty$

or $ZT_M = \infty$

Prob. 5. TE power generator

5-5 & 5-6 Simulations



$$Z = \frac{(250 \times 10^{-6} \text{ V/K})^2 (50000 \Omega^{-1} \text{ m}^{-1})}{(2 \text{ W/mK})} = .001563$$

$$T_M = 450 \text{ K}$$

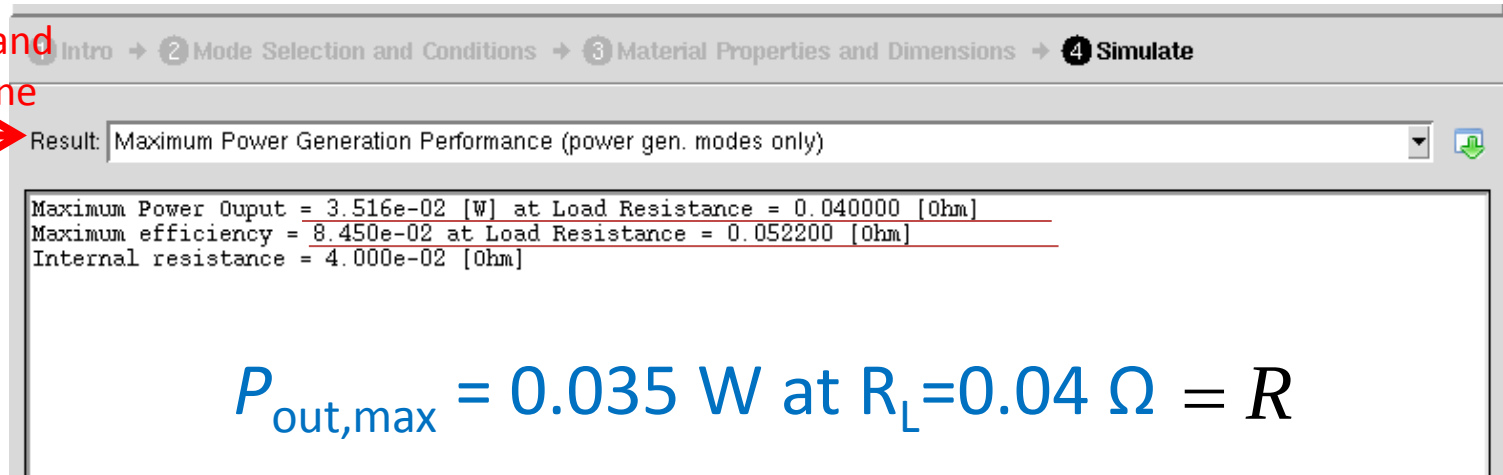
$$\therefore ZT_M = 0.70$$

$$\gamma = \sqrt{1 + 0.70} = 1.305$$

Prob. 5. TE power generator

5-5 & 5-6 (cont'd)

Click the menu and
select the last one



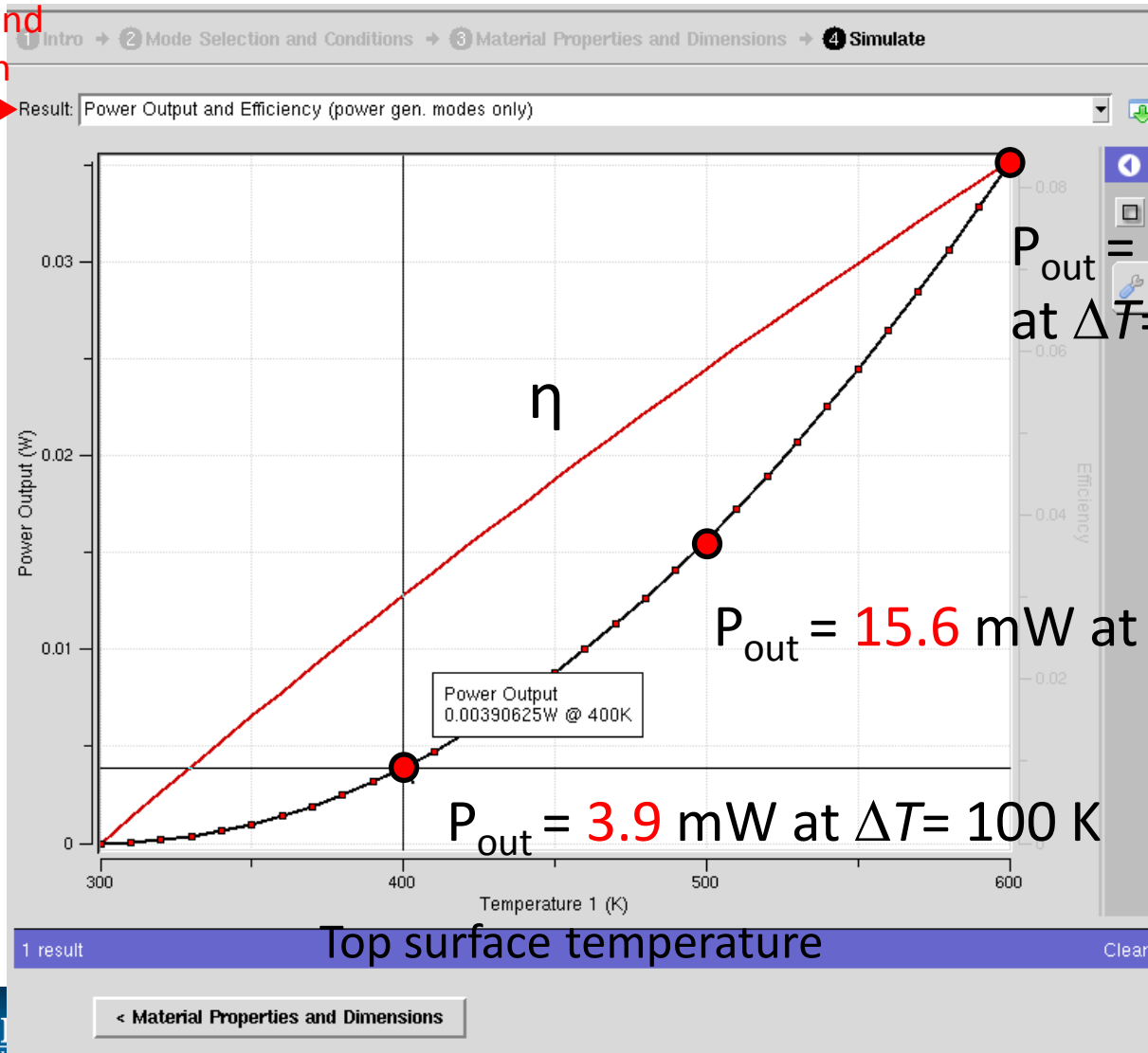
$$P_{\text{out,max}} = 0.035 \text{ W at } R_L = 0.04 \, \Omega = R$$

$$\eta_{\text{max}} = 0.085 \text{ at } R_L = 0.0522 \, \Omega = \gamma R$$

Prob. 5. TE power generator

5-7. Power output as a function of ΔT

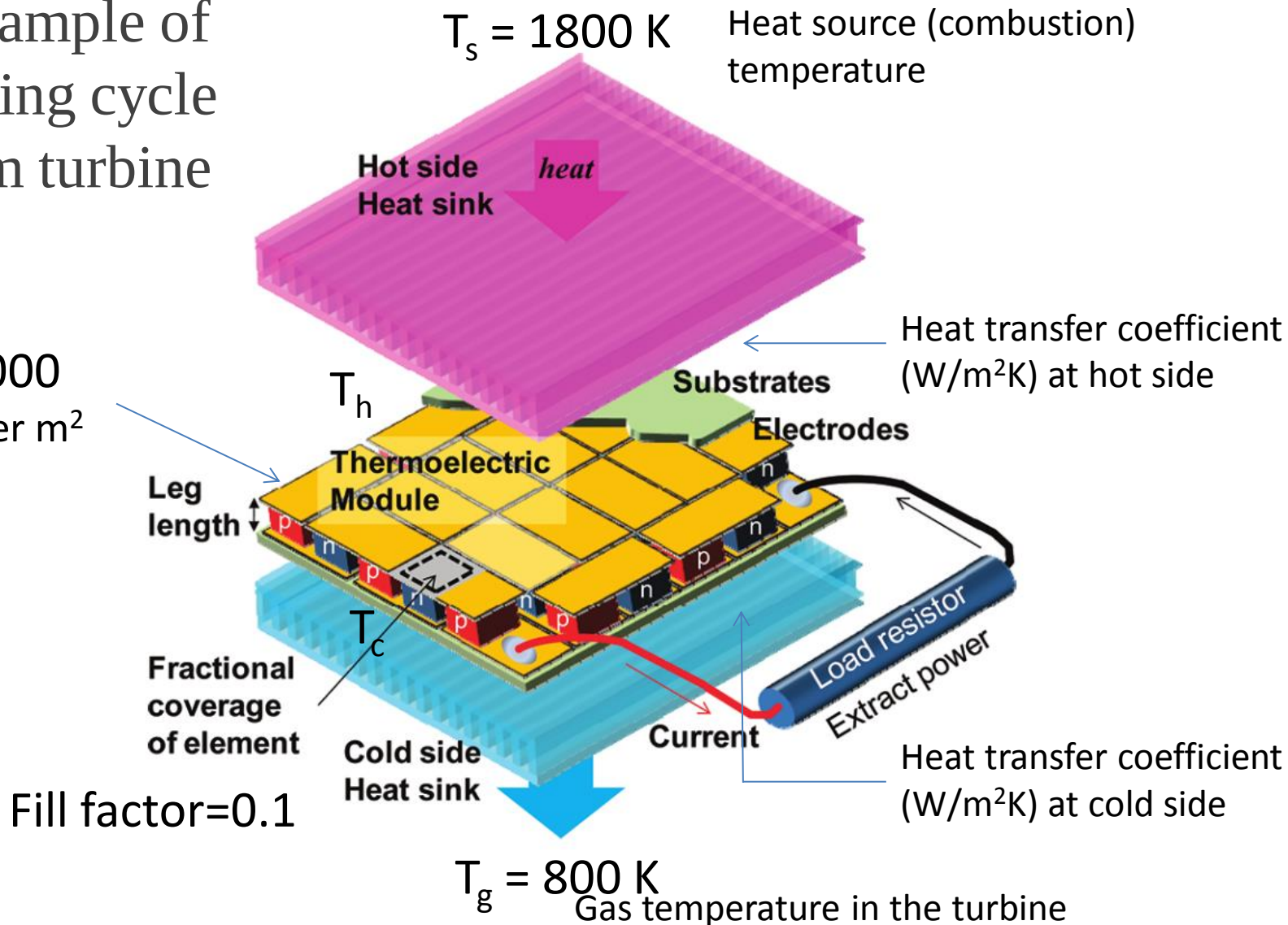
Click the menu and select this option



Prob. 6. Thermoelectric system

* An example of TE topping cycle on steam turbine

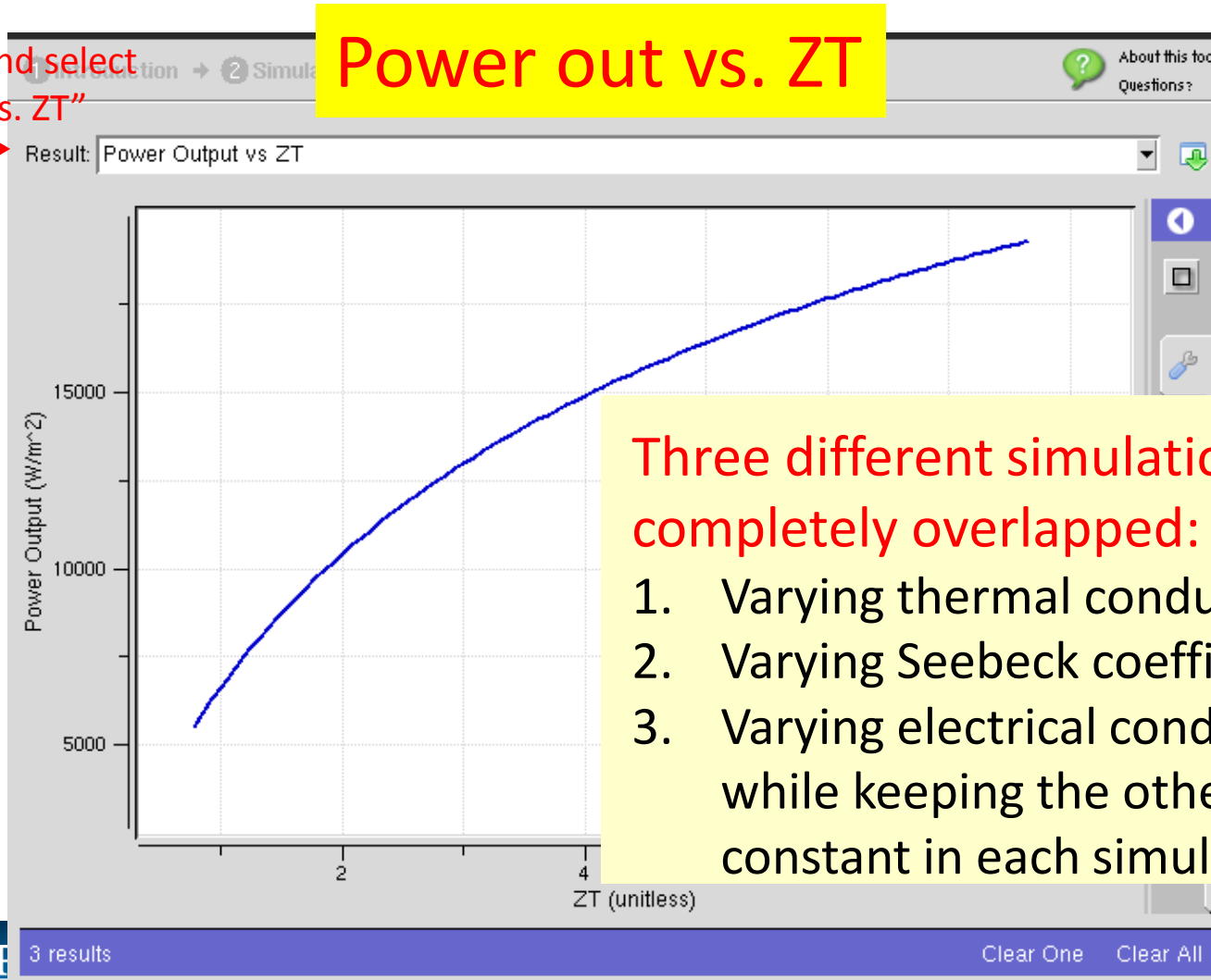
1000 x 1000
elements per m²



Prob. 6. Thermoelectric system

6-1. Power output as a function of material properties and heat transfer coefficients

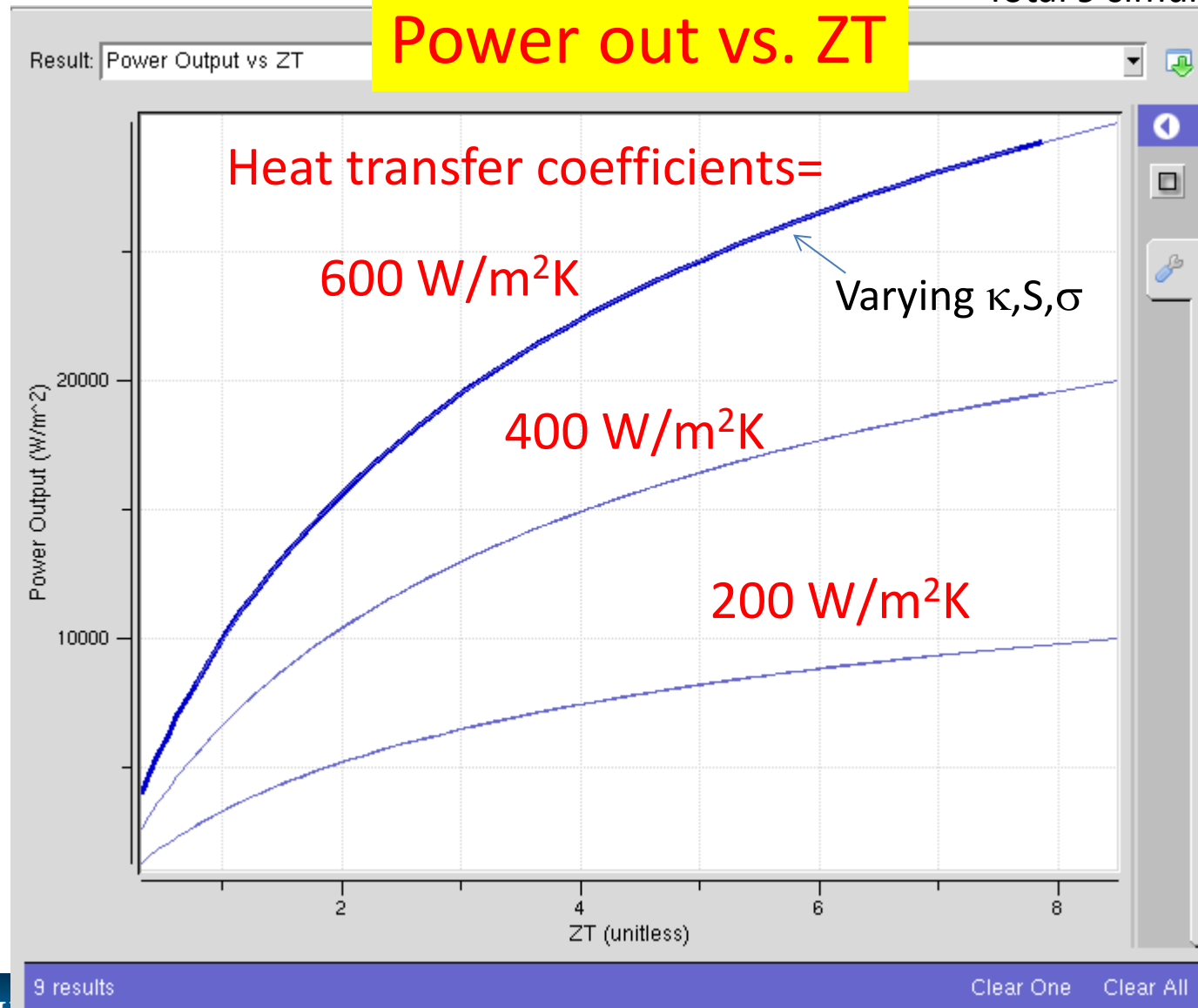
Click the menu and select
"Power Output vs. ZT"



Prob. 6. Thermoelectric system

6-1.
(cont'd)

Total 9 simulations



Prob. 6. Thermoelectric system

6-1. (cont'd) which statement is correct?

- a. The higher the heat transfer coefficient is, the lower the power output is generated.
- b. Optimal power output is only a function of the heat transfer coefficients, and not of the material properties.
- c. Optimal power output does not change with varying any of the three individual material properties and the heat transfer coefficients as long as the ZT value remains the same.
- d. Optimal power output does not change with varying any of the three individual material properties as long as the ZT value and the heat transfer coefficients remain the same.
- e. None of the above.

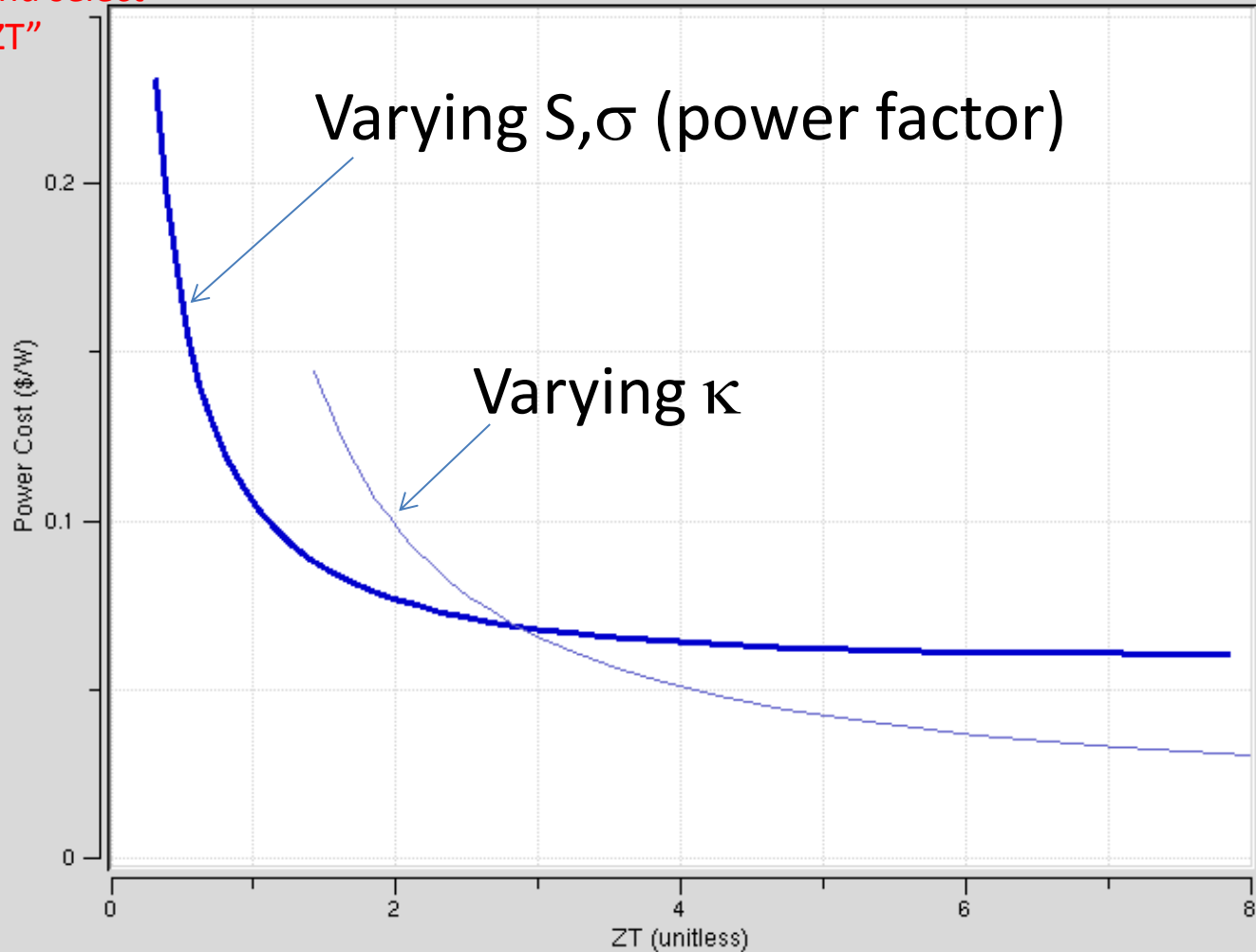
Prob. 6. Thermoelectric system

6-2. Cost analysis

Power cost (\$/W) vs. ZT

Result: Power Cost vs ZT

Click the menu and select
"Power cost vs. ZT"



Prob. 6. Thermoelectric system

6-2. (Cost analysis, cont'd) which statement is correct?

- a. Materials produce the same power cost if their ZT values are the same.
- b. In the high ZT regime (e.g. ZT higher than ~ 3.0), lowering the thermal conductivity is more desired than enhancing the power factor in terms of power cost if ZT remains the same.
- c. In the high ZT regime (e.g. ZT higher than ~ 3.0), enhancing the power factor is more desired than lowering the thermal conductivity in terms of power cost if ZT remains the same.
- d. Power cost increases with increasing ZT.
- e. Power cost decreases with decreasing efficiency.