Thermoelectricity: From Atoms to Systems

Week 2: Thermoelectric Transport Parameters

Lecture 2.0: **Short Introduction**

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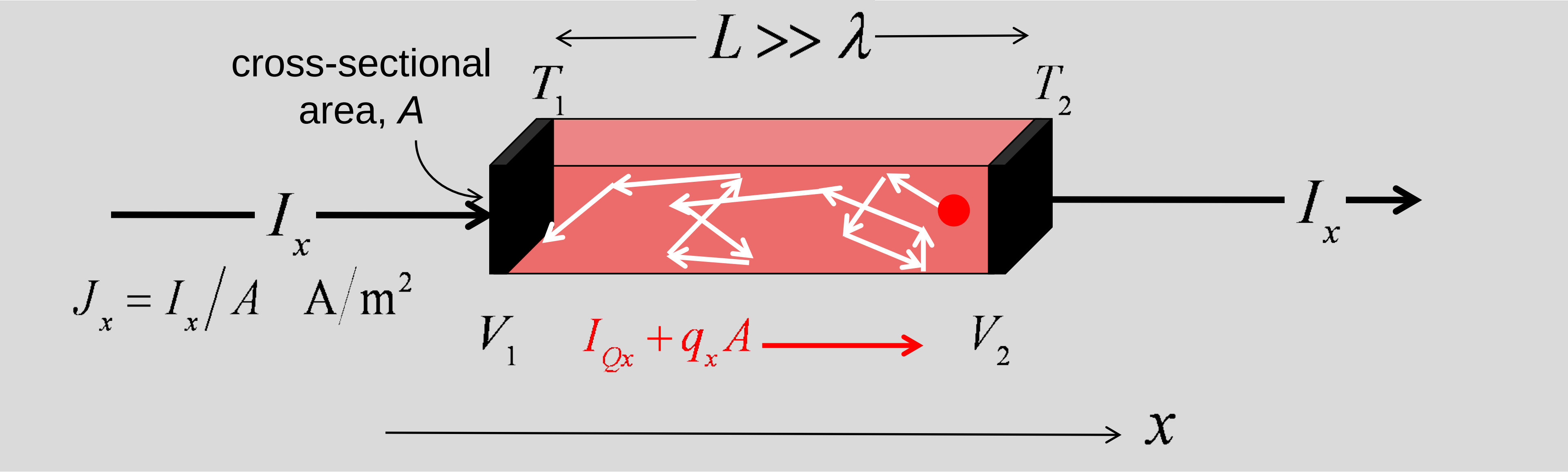
the experiment:

1) Force a current: I_x

2) Impose a temperature gradient:

$$dT/dx = (T_2 - T_1)/L$$



3) Measure the voltage, $V_2 - V_1$ or electric field: $\mathcal{E}_x = (V_2 - V_1)/L$

4) Measure the heat current (electronic plus lattice): $I_{Qx} + q_x A$

coupled charge and heat currents

electrical current:

$$\mathcal{E}_x = \rho J_x + S\frac{dT}{dx}$$

heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

heat current (lattice):

$$q_x = -\kappa_L \left(\frac{dT}{dx}\right)$$

transport coefficients (3D)

ρ resistivity Ω-m

S Seebeck coefficient V/K

π Peltier coefficient V

κ_e electronic thermal conductivity W/m-K

κ_L lattice thermal conductivity W/m-K

coupled charge and heat currents

electrical current:

$$\mathcal{E}_x = (1/\sigma) J_x + S \frac{dT}{dx}$$

heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

heat current (lattice):

$$q_x = -\kappa_L \left(\frac{dT}{dx} \right)$$

Temperature differences produce voltage differences.

Current flow produces temperature differences.

coupled charge and heat currents

electrical current:

$$\mathcal{E}_x = (1/\sigma) J_x + S \frac{dT}{dx}$$

heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

heat current (lattice):

$$q_x = -\kappa_L \left(\frac{dT}{dx} \right)$$

More generally: $\mathcal{E}_x \rightarrow \frac{1}{q} \frac{dF_n}{dx}$

F_n: quasi-Fermi level (electrochemical potential)

expressions for the TE transport coefficients

$$\sigma = q^2 \int \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\Sigma(E) = \frac{1}{\Omega} \sum_{\vec{k}} \upsilon_x(\vec{k})^2 \, \tau(\vec{k}) \, \delta\left(E - E(\vec{k})\right)$$

"transport distribution function"

$$S = -\frac{q}{T\sigma} \int (E - E_F) \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\pi = TS$$

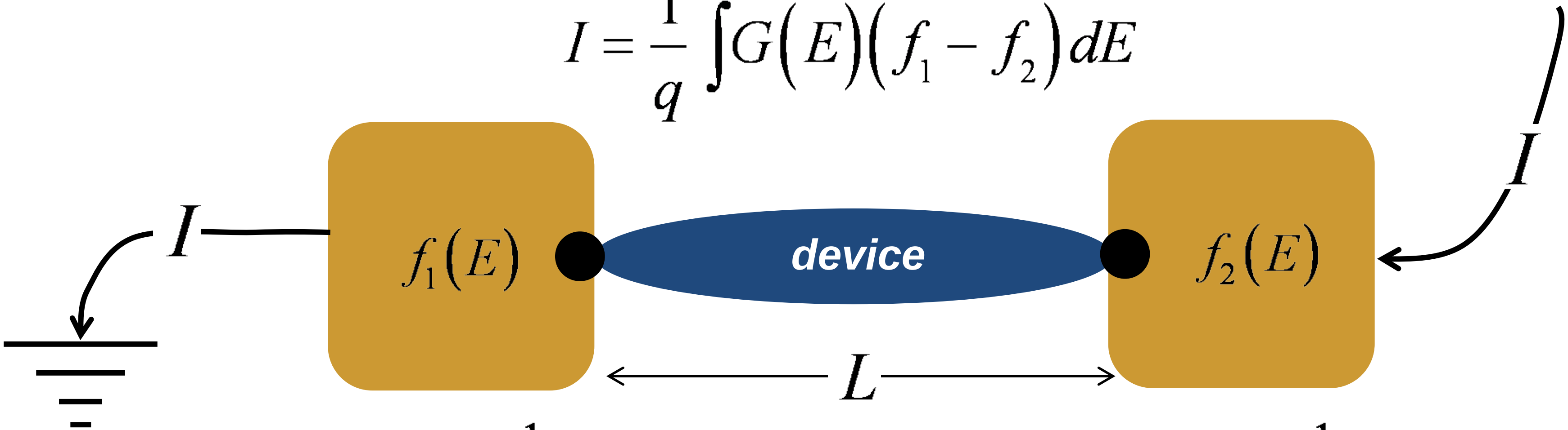
$$\kappa_0 = \frac{1}{T} \int (E - E_F)^2 \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\kappa_e = \kappa_0 - T\sigma S^2$$

G.D. Mahan and J.O. Sofo, "The Best Thermoelectric," *Proc. Nat. Acad. Sci.*, **93**, pp. 7436-7439, 1996.

Landauer-Boltzmann expression for current

$$I = \frac{1}{q}\int G(E)\left(f_1 - f_2\right) dE$$



$$f_1(E) = \frac{1}{1 + e^{(E - E_{F1})/k_B T_1}}$$

$$f_2(E) = \frac{1}{1 + e^{(E - E_{F2})/k_B T_2}}$$

$$I = \frac{2q}{h}\int \mathcal{T}(E) M(E)\left(f_1 - f_2\right) dE$$

transmission, modes (channels), differences in Fermi-levels

expressions for the TE transport coefficients

$$\sigma = q^2 \int \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E) dE$$

$$\Sigma(E) = \frac{1}{\Omega} \sum_{\vec{k}} \upsilon_x(\vec{k})^2 \tau(\vec{k}) \delta\left(E - E(\vec{k})\right)$$

"transport distribution function"

$$S = \frac{q}{T\sigma} \int (E - E_F) \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E) dE$$

$$\Sigma(E) = \frac{2}{h} \left(M(E)/A \right) \lambda(E)$$

$$\pi = TS$$

$$\kappa_0 = \frac{1}{T} \int (E - E_F)^2 \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E) dE$$

G.D. Mahan and J.O. Sofo, "The Best Thermoelectric," *Proc. Nat. Acad. Sci.*, **93**, pp. 7436-7439, 1996.

$$\kappa_e = \kappa_0 - T\sigma S^2$$

coupled charge and heat currents

electrical current:

$$\mathcal{E}_x = (1/\sigma) J_x + S \frac{dT}{dx}$$

heat current (electronic):

$$J_{Qx} = \pi J_x - \kappa_e \frac{dT}{dx}$$

heat current (lattice):

$$q_x = -\kappa_L \left(\frac{dT}{dx} \right)$$

$$\sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle$$

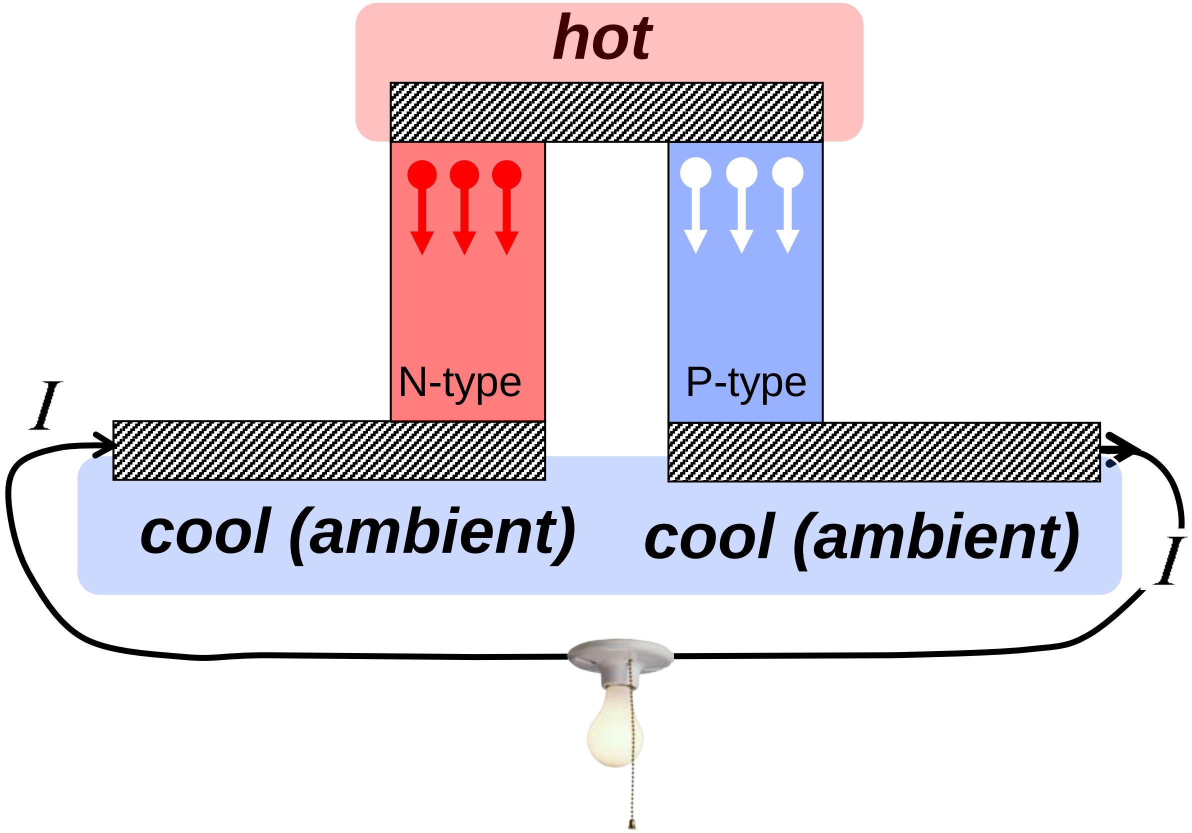
$$S = \pi / T$$ Kelvin relation

$$\pi = -\frac{1}{q}\left(E_J - E_F \right)$$

$$\kappa_e = T \left(\frac{k_B}{q} \right)^2 \mathcal{L} \sigma$$

$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \langle M_{ph}/A \rangle \langle \langle \lambda_{ph} \rangle \rangle$$

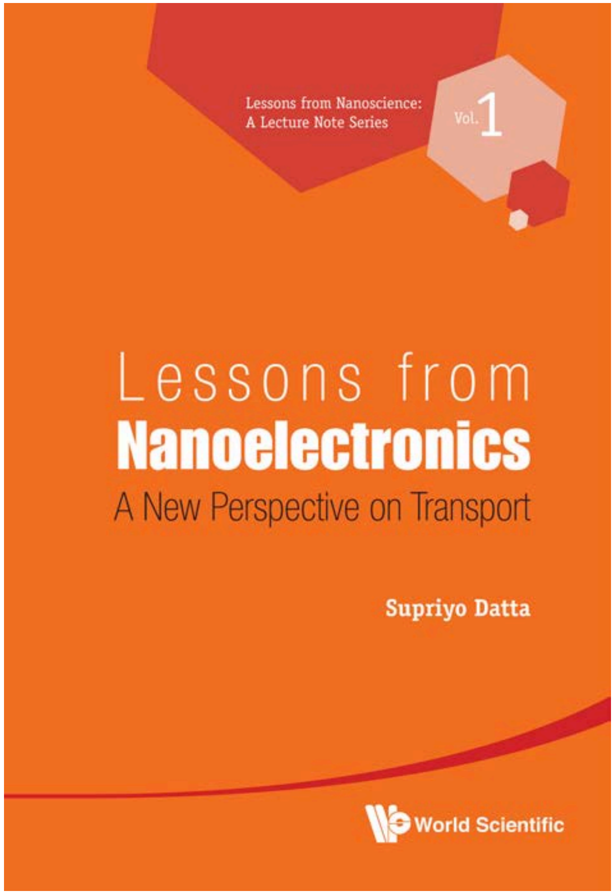
devices and the thermoelectric figure of merit



$$ZT = \frac{S^2 \sigma T}{\kappa_L + \kappa_e}$$

references

Chapters 4, 5, and 9



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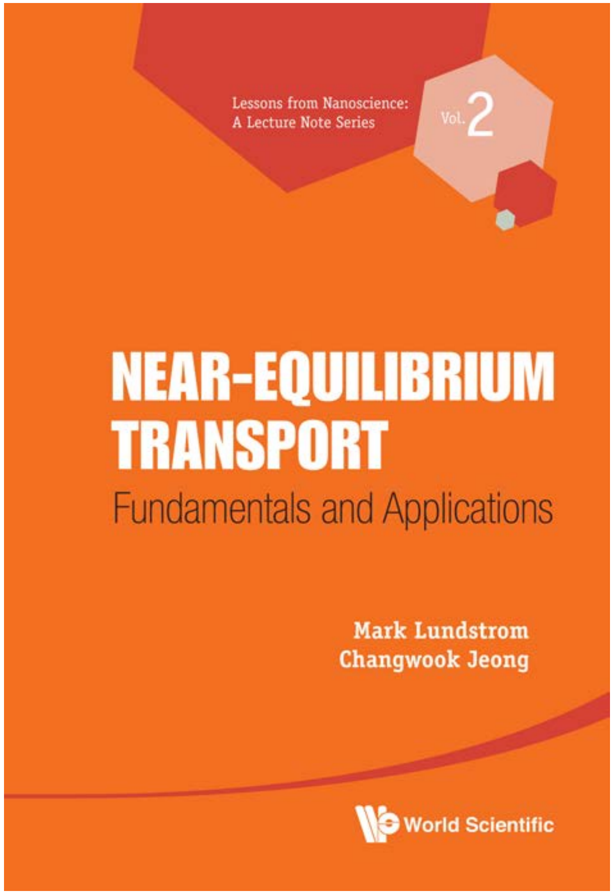

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week 2 lectures

1) The Landauer-Boltzmann Approach
2) The Thermoelectric Transport Coefficients
3) Devices, FOM, and Material Trade-offs
4) Novel Materials and Structures
5) Lattice Thermal Conductivity
6) The Boltzmann Transport Equation
7) First-principles thermoelectrics (Dr. Jesse Maassen)