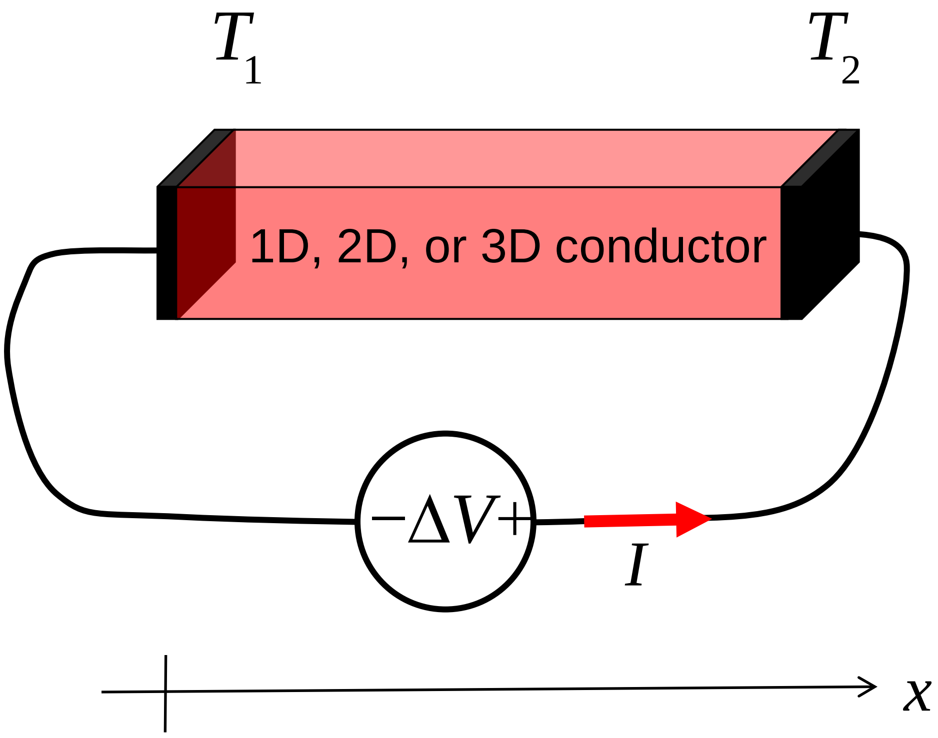
ECE-656: Fall 2009

Lecture 9: Coupled Current Equations

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

charge and heat currents



$$I = G\Delta V - [SG]\Delta T$$

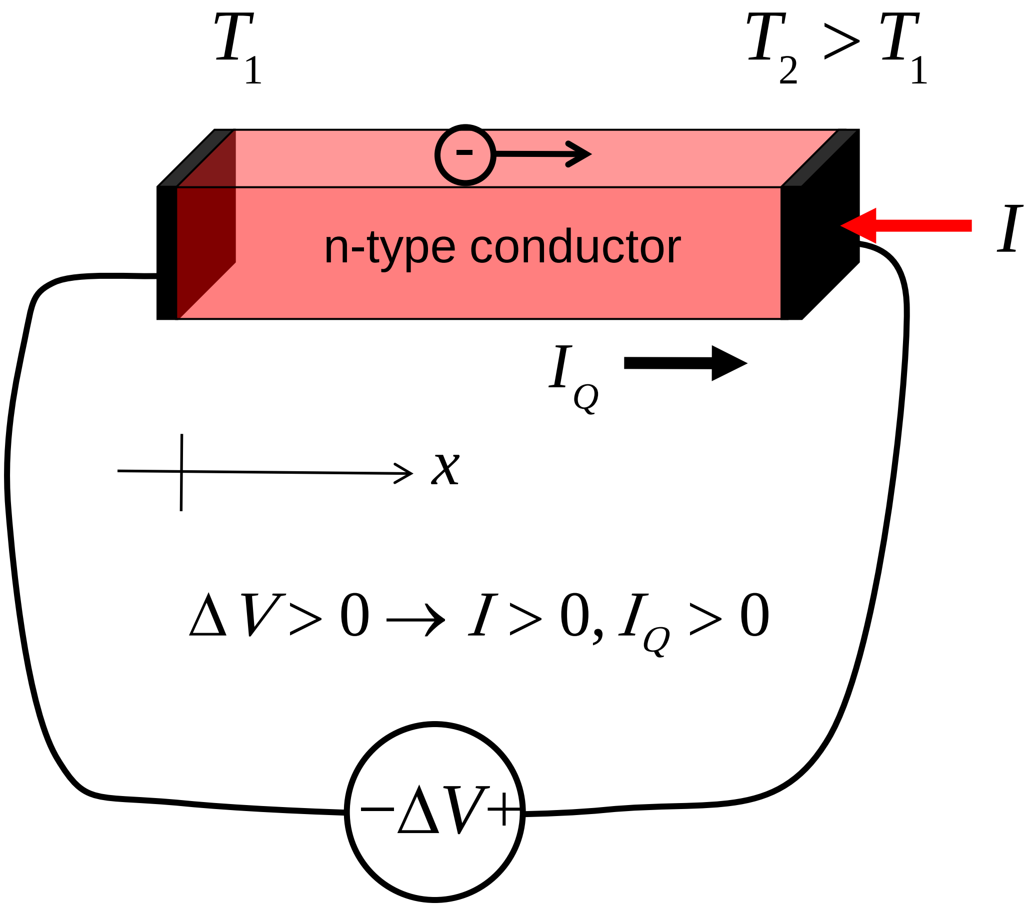
$$I_Q = T[SG]\Delta V - K_0\Delta T$$

driving "forces:"

1) differences in voltage
(electrochemical potential)

2) differences in <u>temperature</u>

signs of the coefficient



$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0 \Delta T$$

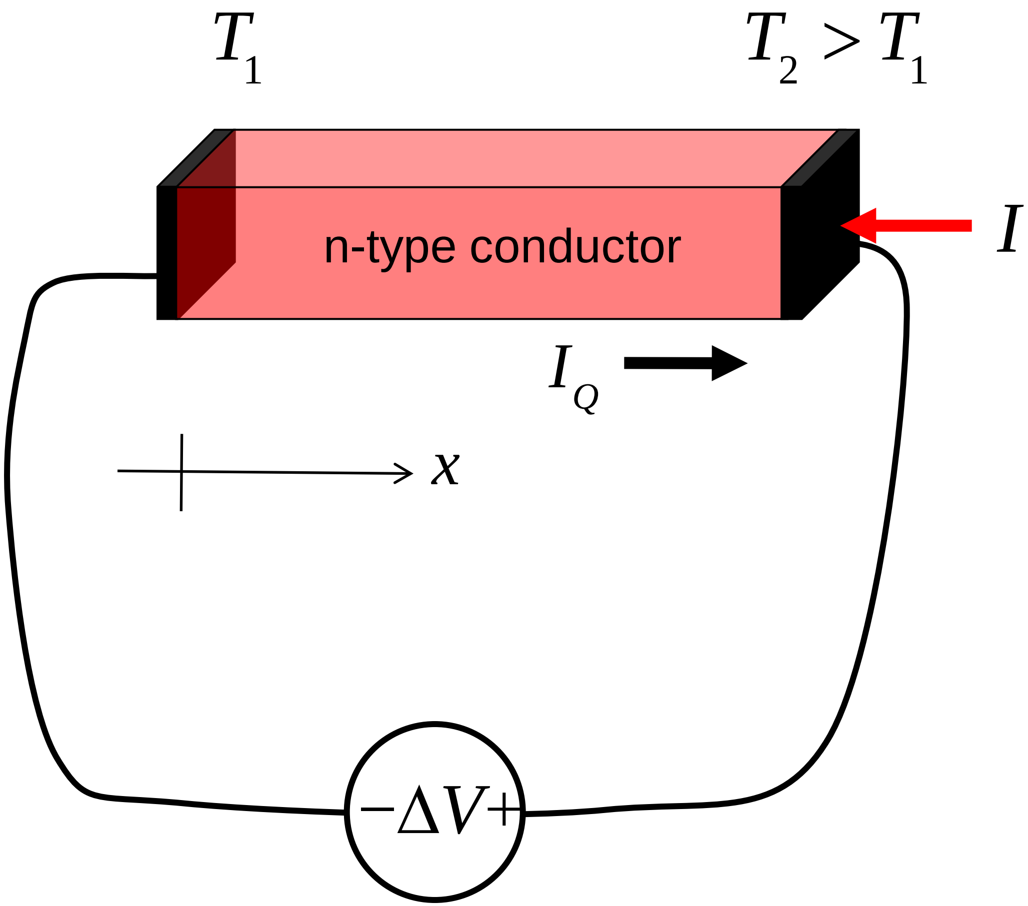
$G > 0$

$[SG] > 0$

$K_0 > 0$

(electronic) thermal conductance for $\Delta V = 0$

conductance vs. conductivity



$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0 \Delta T$$

3D conductors

$$G = \sigma \frac{A}{L}$$

$$K_0 = \kappa_0 \frac{A}{L}$$

etc.

temperature gradients

$$I \propto \left(f_1 - f_2\right) = \left(f_1 - f_2\right)_T + \left(f_1 - f_2\right)_{E_F}$$

$$\left.\left(f_1 - f_2\right)\right|_T = -\left(\frac{\partial f_0}{\partial E_F}\right)\Delta E_F = \left(-\frac{\partial f_0}{\partial E}\right)\left(q\Delta V\right)$$

$$\left.\left(f_1 - f_2\right)\right|_{E_F} = \left(-\frac{\partial f_0}{\partial \Theta}\right)\Delta\Theta$$

$$= k_B T\left(-\frac{\partial f_0}{\partial E}\right) \times \frac{\left(E - E_F\right)}{k_B}\Delta\left(\frac{1}{T}\right)$$

$$f_0 = \frac{1}{1 + e^{\left(E - E_F\right)/k_B T}}$$

$$f_0 = \frac{1}{1 + e^{\Theta}}$$

$$\Theta = \left(E - E_F\right)/k_B T$$

The proper driving forces are changes in the electrochemical potential and in the inverse temperature.

coupled flows

$$I = L_{11}\Delta\left(E_F\right) + L_{12}\Delta\left(\frac{1}{T}\right)$$

$$I_Q = L_{21}\Delta E_F + L_{22}\Delta\left(\frac{1}{T}\right)$$

$$I_1 = L_{11}\left(\vec{B}\right)F_1 + L_{12}\left(\vec{B}\right)F_2$$

$$I_2 = L_{21}\left(\vec{B}\right)F_1 + L_{22}\left(\vec{B}\right)F_2$$

I_1, I_2 “generalized fluxes”

F_1, F_2 “generalized forces”

$L_{12} = L_{21}$ Onsager relation

example

temperature differences produce heat currents

pressure differences produce matter currents

heat flow per pressure difference = matter flow per temperature difference

Lars Onsaeger, Nobel Prize in Chemistry, 1968.

http.en.wikipedia.org/wiki/Onsaeger_reciprocal_relations

for more about this topic

A.C. Smith, J.F. Janak, and R.B. Adler, *Electronic Conduction in Solids*, McGraw-Hill, New York, 1967.

Irreversible thermodynamics: Chapter 2

Onsager relations: Chapter 3

outline

1) Onsager relations

2) **Measurement considerations**

3) Thermoelectric devices

measurements

$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0\Delta T$$

$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e\Delta T$$

two forms of the equations

$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0\Delta T$$

$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e\Delta T$$

$$\pi = TS < 0$$

$$K_e = K_0 - T\frac{[SG]^2}{G} > 0$$

electronic thermal conductance for *I* = 0

$$\Delta V = \frac{1}{G} I + \frac{[SG]}{G}\Delta T$$

$$R = 1/G \qquad S = -[SG]/G$$

$$\Delta V = RI - S\Delta T$$

$$I_Q = T[SG](RI - S\Delta T) - K_0\Delta T$$

$$I_Q = T\frac{[SG]}{G} I - (K_0 + T[SG]S)\Delta T$$

$$I_Q = -TSI - \left(K_0 - T\frac{[SG]^2}{G}\right)\Delta T$$

resistivity / conductivity measurements

$$I = G\Delta V - [SG]\Delta T$$

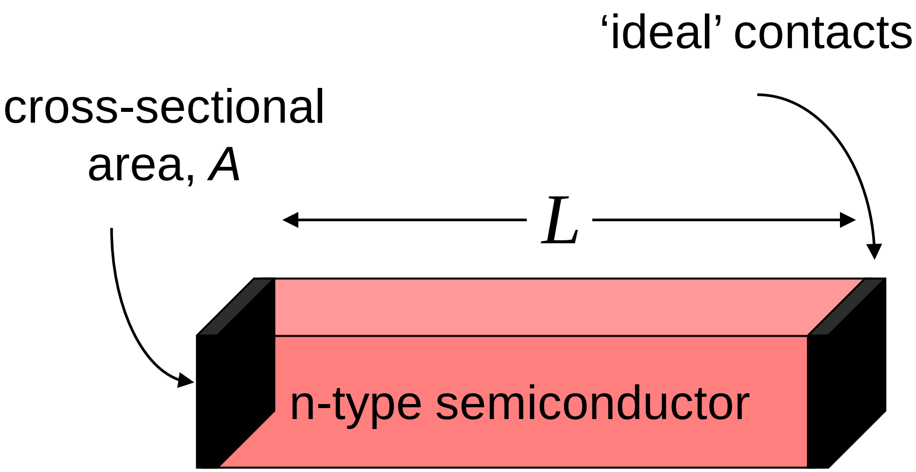
$$I_Q = T[SG]\Delta V - K_0 \Delta T$$

$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e \Delta T$$

People generally measure **resisitivity** (or **conductivity**) because for bulk materials, these parameters depend on material properties and not on the length of the resistor or its width or cross-sectional area.

resistance and resistivity



How does the resistivity depend on the parameters of the semiconductor?

$$I = V/R$$

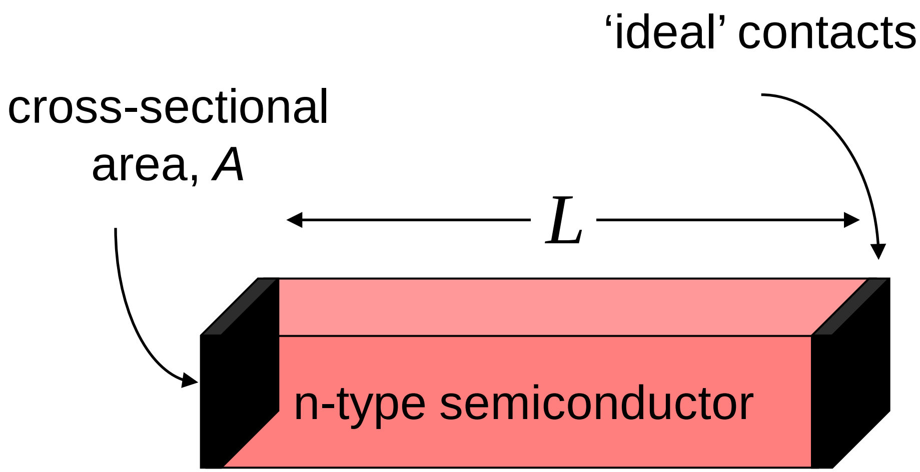
$$R \propto \frac{L}{A}\ \Omega$$

$$R = \rho \frac{L}{A}\ \Omega$$

resistivity:

ρ ½-m

conductance and conductivity



$$I = GV = V/R$$

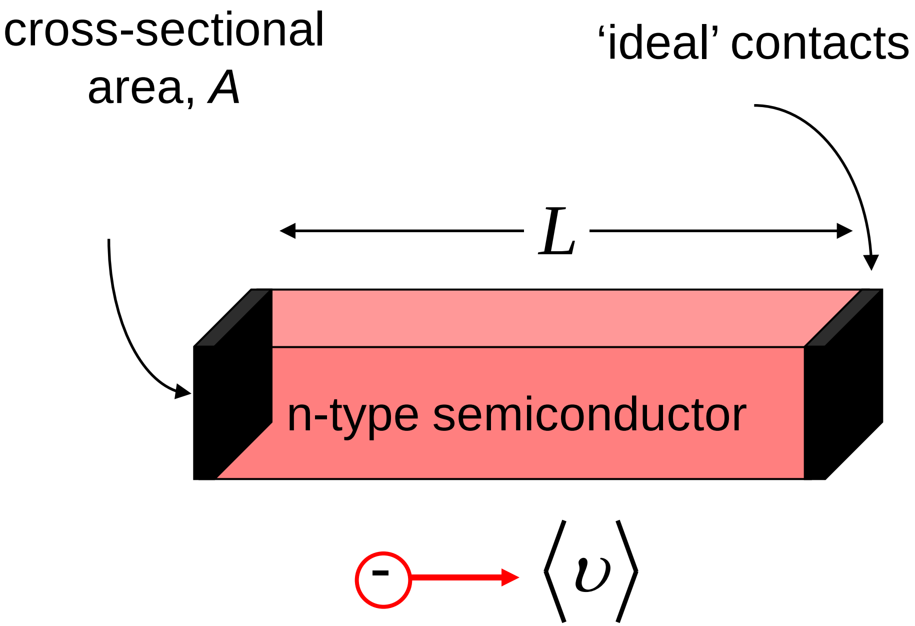
$$G = \frac{1}{R} \propto \frac{A}{L}\ \mathrm{S}\ (\Omega)^{-1}$$

$$G = \sigma \frac{A}{L}$$

conductivity:

$$\sigma = \frac{1}{\rho}\ \ \mathrm{S/m}$$

traditional conductance and conductivity



$$\langle \upsilon \rangle$$

$$Q = (qn)AL$$

$$I = GV \equiv \frac{Q}{\tau} \text{ Amperes}$$

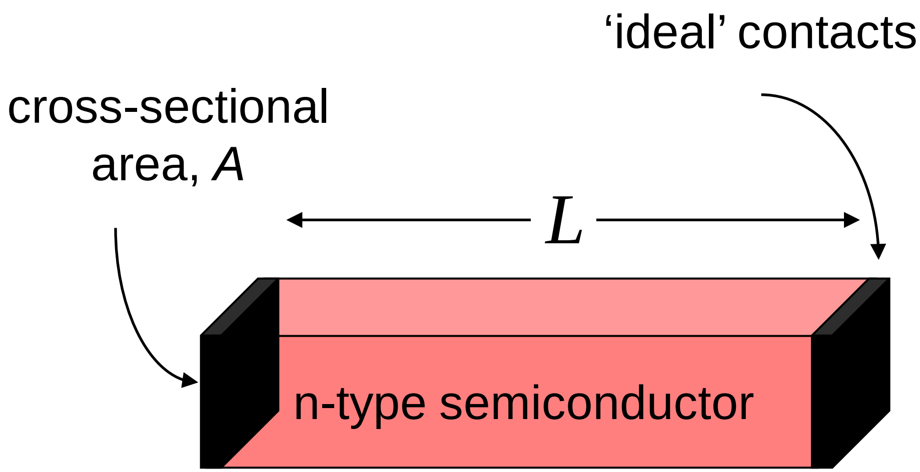
$$\langle \upsilon \rangle = \mu_n E = \mu_n \frac{V}{L} \text{ cm/sec}$$

$$\tau = \frac{L}{\langle \upsilon \rangle} = \frac{L^2}{\mu_n V}$$

$$I = \left\{ (nq\mu_n)\frac{A}{L} \right\} V = GV$$

$$G = \sigma \frac{A}{L} \qquad \sigma = nq\mu_n$$

Landauer conductance and conductivity



$$G = \frac{2q^2}{h}\left(\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right)$$

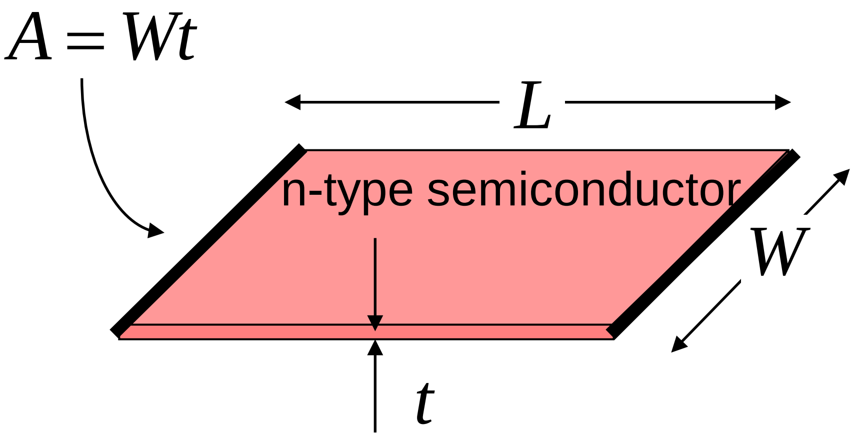
$$I = GV$$

$$G \propto \frac{A}{L}\, \mathrm{S}\,(\Omega)^{-1}$$

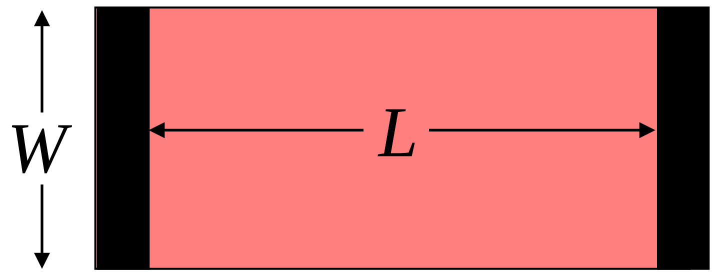
$$G = \sigma\frac{A}{L} \qquad \sigma = \frac{1}{\rho}\ \mathrm{S/m}$$

$$\sigma = \frac{G}{A/L} = \frac{2q^2}{h}\left(\int \lambda(E)\frac{M(E)}{A}\left(-\frac{\partial f_0}{\partial E}\right)dE\right) \qquad \left(T(E) \approx \lambda(E)/L\right)$$

sheet conductance



Top view



$$I = GV$$

$$G = \sigma \frac{A}{L} \qquad \sigma = nq\mu_n$$

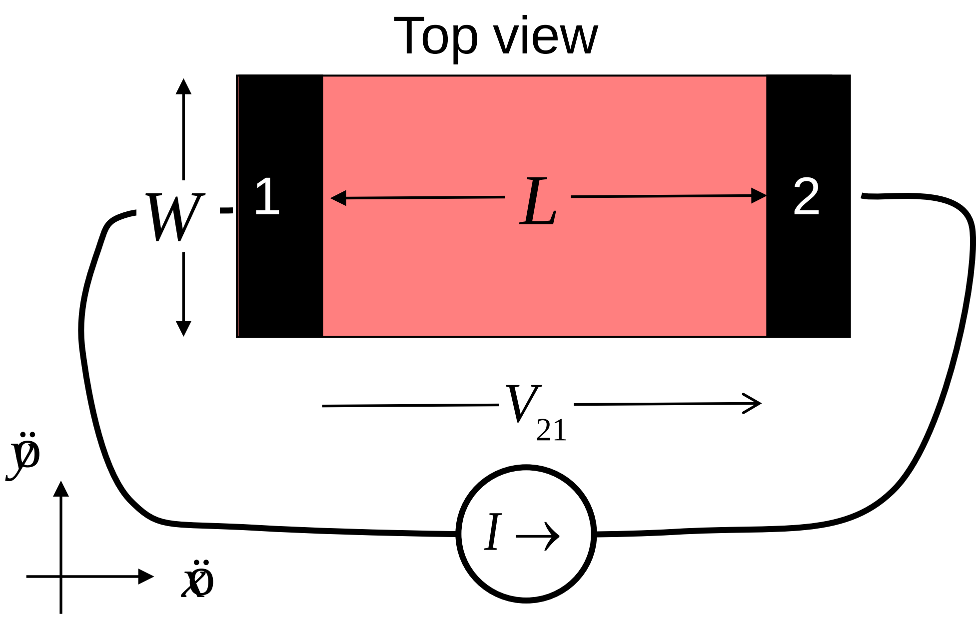
$$G = \sigma \left(\frac{Wt}{L} \right) = nq\mu_n t \left(\frac{W}{L} \right)$$

$$G = \sigma_S \left(\frac{W}{L} \right)$$

$$\sigma_S = n_S \, q \, \mu_n$$

'sheet conductance'

2-probe measurements



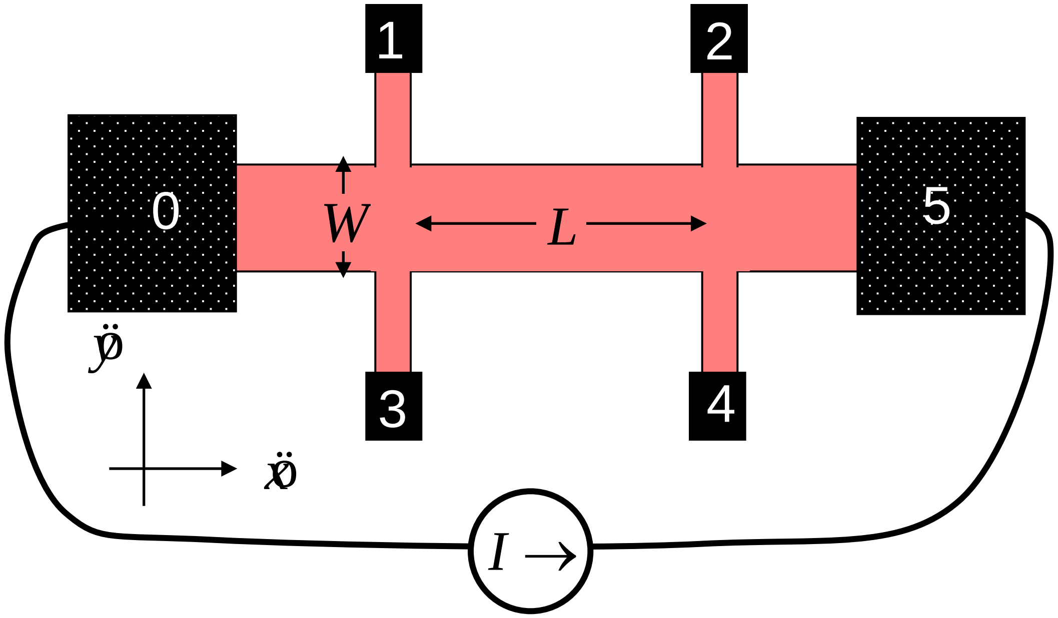
$$R_{DEV} = \rho_S \frac{L}{W}$$

$$V_{21} = I\left(2R_C + R_{DEV}\right)$$

$$R_{DEV} \neq \frac{V_{21}}{I}$$

4-probe measurements

Top view



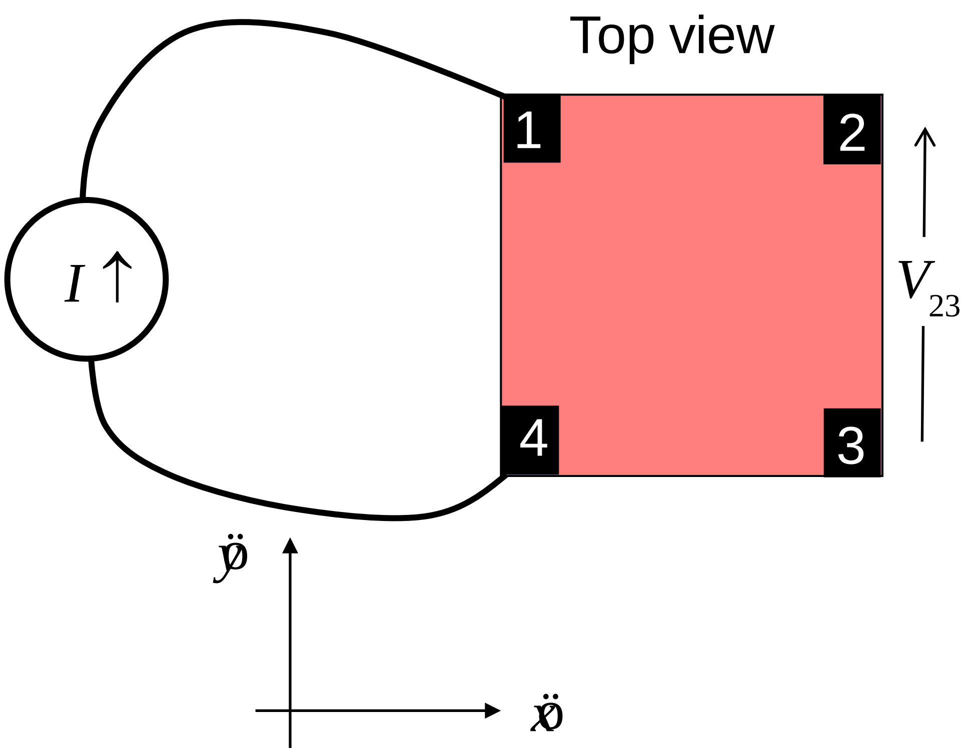
$$R_{DEV} = \rho_S \frac{L}{W}$$

$$V_{21} = I\left(R_{DEV}\right)$$

(high impedance voltmeter)

"Hall bar geometry"

van der Pauw technique



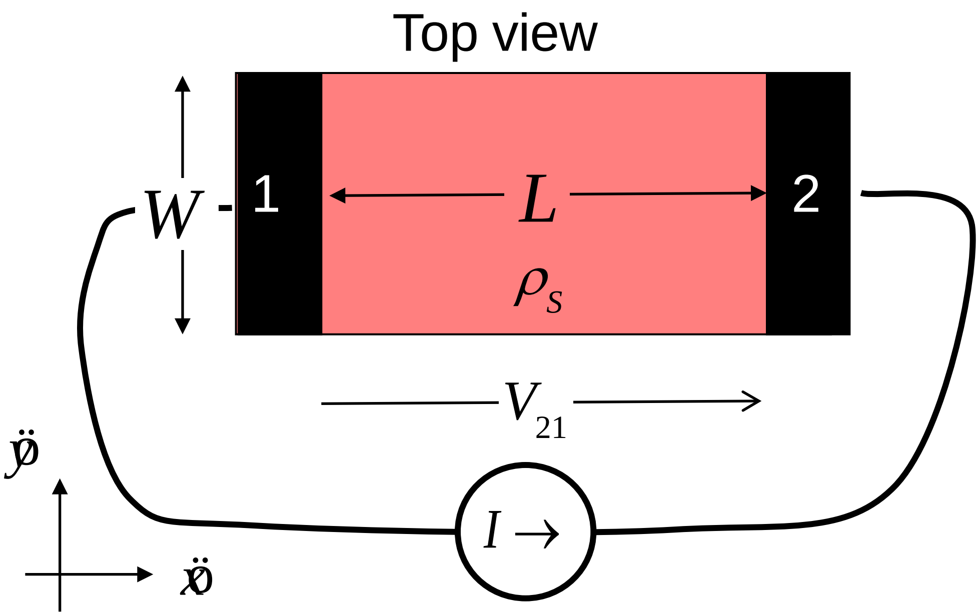
$$R_{1,4/2,3} \equiv \frac{V_{23}}{I_{14}} \qquad R_{2,1/3,4} \equiv \frac{V_{34}}{I_{21}}$$

$$e^{-\frac{\pi}{\rho_S} R_{1,4/2,3}} + e^{-\frac{\pi}{\rho_S} R_{2,1/3,4}} = 1$$

$$\Rightarrow \rho_S$$

Force *I* through two contacts, measure *V* between the other two contacts.

isothermal vs. adiabatic



$$R_{DEV} = \rho_S \frac{L}{W}$$

$$V_{21} = R_{DEV} I - S \Delta T$$

$$I_Q = -\pi I - K_e \Delta T$$

i) $\Delta T = 0$

$$V_{21} = R_{DEV} I \rightarrow R_{DEV} = V_{21}/I$$

ii) $I_Q = 0$

$$\Delta T = \left(-\pi / K_e\right) I$$

$$V_{21} = R_{DEV} I + \left(S^2 T / K_e\right) I$$

$$V_{21}/I = R_{DEV} + \left(S^2 T / K_e\right)$$

for more about low-field measurments

D.C. Look, *Electrical Characterization of GaAs Materials and Devices*, John Wiley and Sons, New York, 1989.

L.J. van der Pauw, “A method of measuring specific resistivity and Hall effect of discs of arbitrary shape,” *Phillips Research Reports*, vol. 13, pp. 1-9, 1958.

Lundstrom, Chapter 4, Sec. 7

outline

1) Onsager relations

2) Measurement considerations

3) Thermoelectric devices

thermoelectric devices: cooling

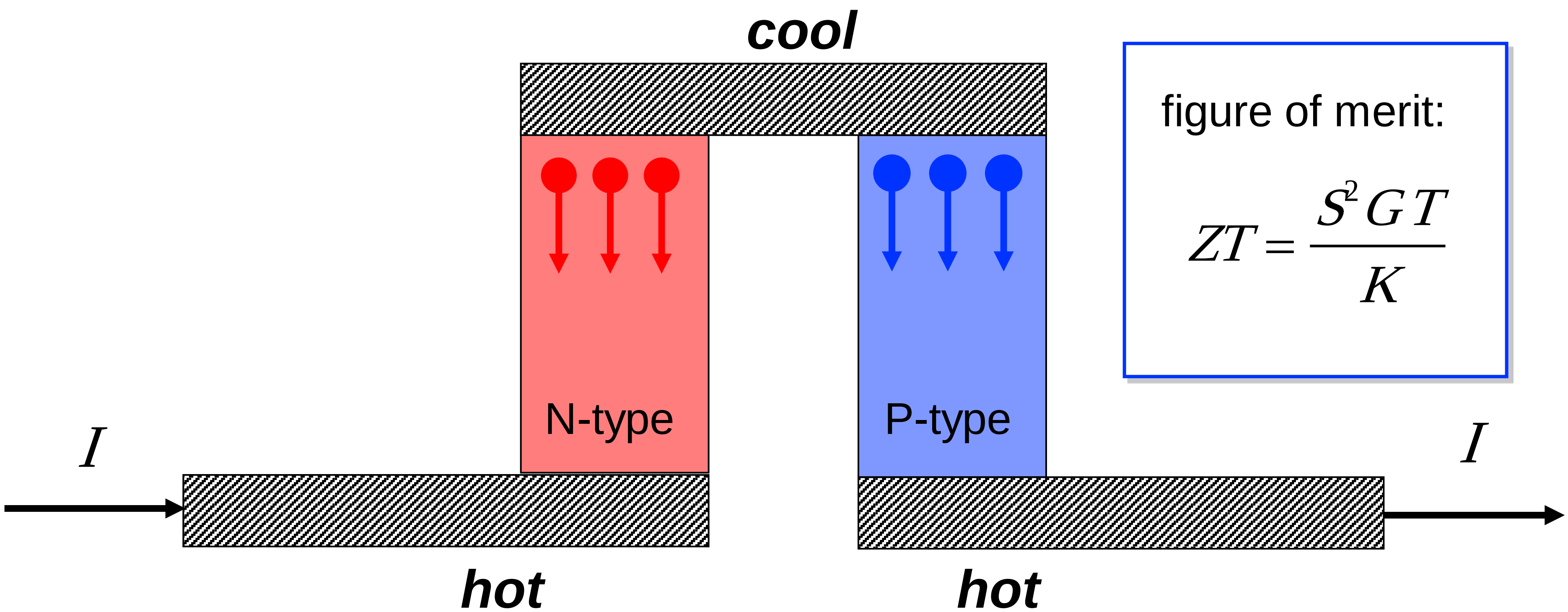


figure of merit:

$$ZT = \frac{S^2 G T}{K}$$

thermoelectric devices: power generation

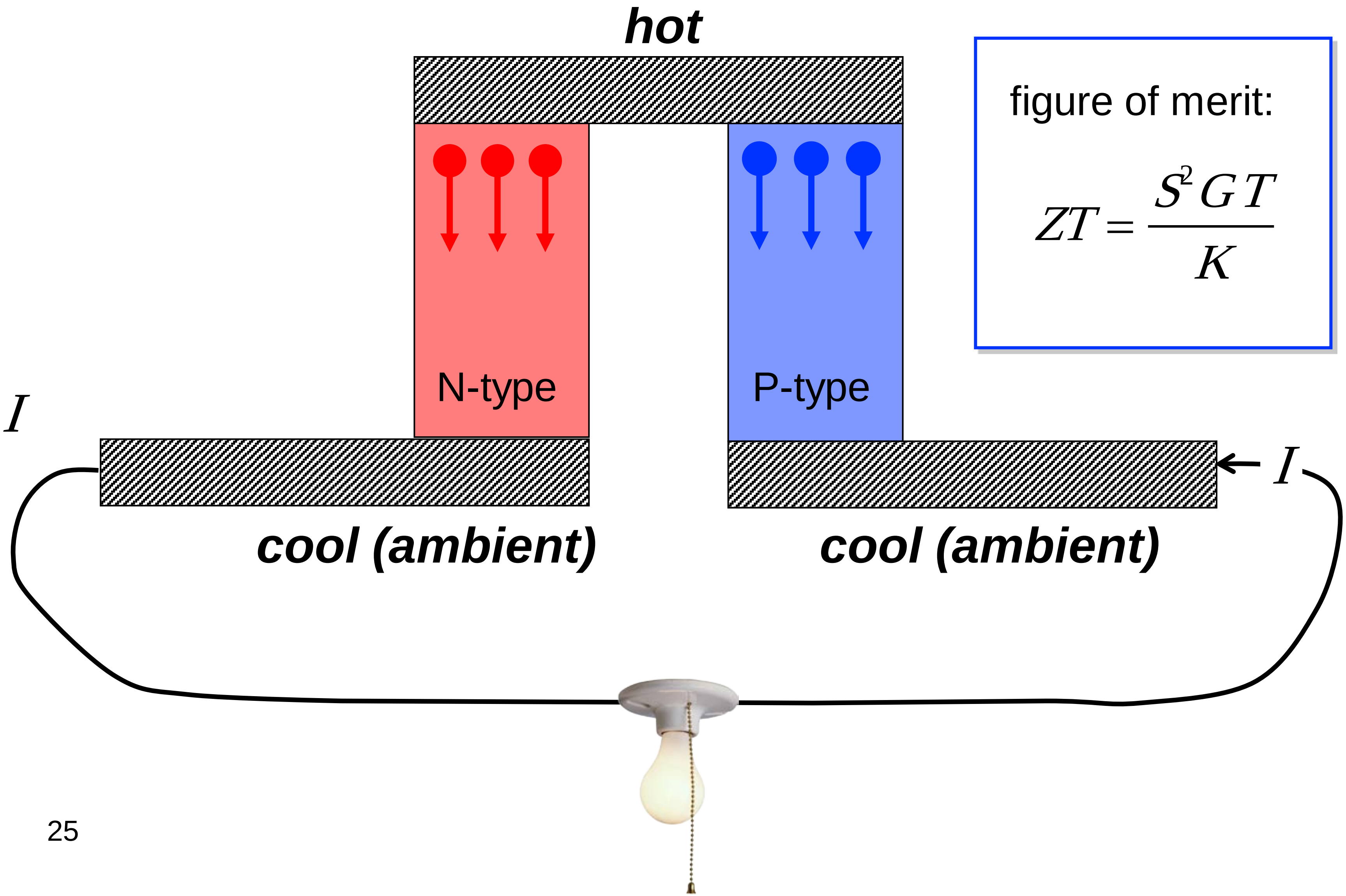


figure of merit:

$$ZT = \frac{S^2 G T}{K}$$

the TE industry: 2009

1) NASA: Radioisotope Thermoelectric Generators for deep-space missions.

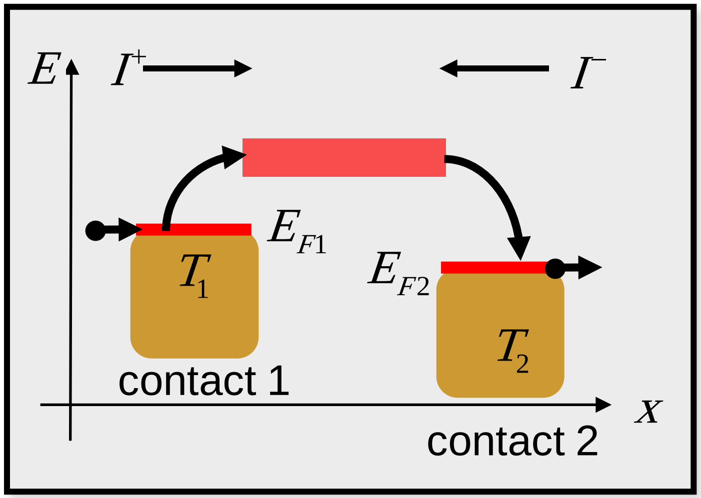
2) DOD: cooling for lasers, night vision, sensors, guidance systems, etc.

1) World market for commercial TE power generation: $30-50M/yr

2) World market for commercial TE cooling: $200-250M/yr

Automobile market (seat cooler/heater) is growing. Vehicle waste heat recovery to improve fuel efficiency is a potential ‘killer-app.’

TE heat engine



If we heat contact 1, and keep contact 2 cool, what is the maximum efficiency with which we can heat into useful work?

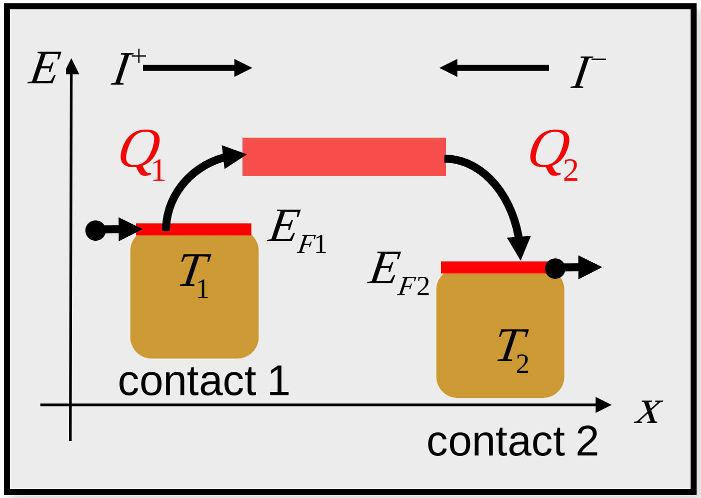
Answer:

Maximum efficiency:

$$\eta_{\max} = 1 - \frac{T_2}{T_1} = 1 - \frac{T_{COLD}}{T_{HOT}}$$

Carnot's theorem

what's necessary for current to flow?



$$I(E) = \frac{2q}{h} T(E) M(E) (f_1 - f_2)$$

Current flows when there is a difference in Fermi levels.

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

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

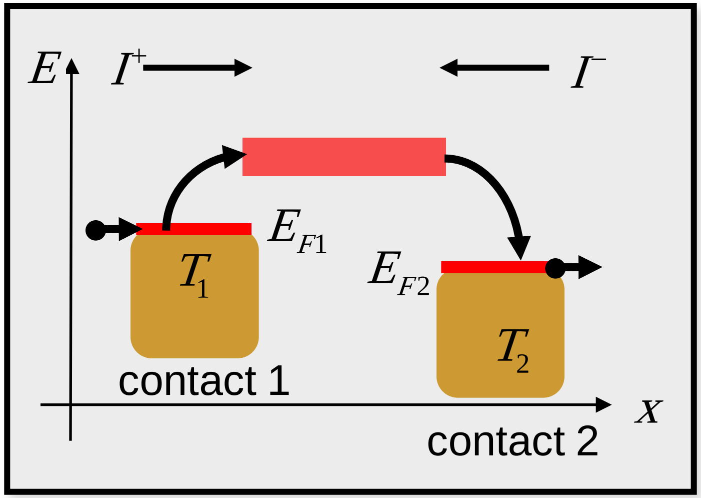
$$\boxed{\frac{Q_1}{T_1} < \frac{Q_2}{T_2}}$$

for current to flow

$$I(E) > 0 \Rightarrow f_1 > f_2$$

$$\Rightarrow \frac{(E - E_{F1})}{k_B T_1} < \frac{(E - E_{F2})}{k_B T_2}$$

maximum efficiency of a TE heat engine



$$Q_1/T_1 < Q_2/T_2$$

Maximum efficiency:

$$\boxed{\eta_{\max} = 1 - \frac{T_2}{T_1} = 1 - \frac{T_{COLD}}{T_{HOT}}}$$

Carnot's theorem

Thermal energy absorbed from contact 1:

$$Q_1 = (E - E_{F1})$$

Thermal energy dissipated into contact 2:

$$Q_2 = (E - E_{F2})$$

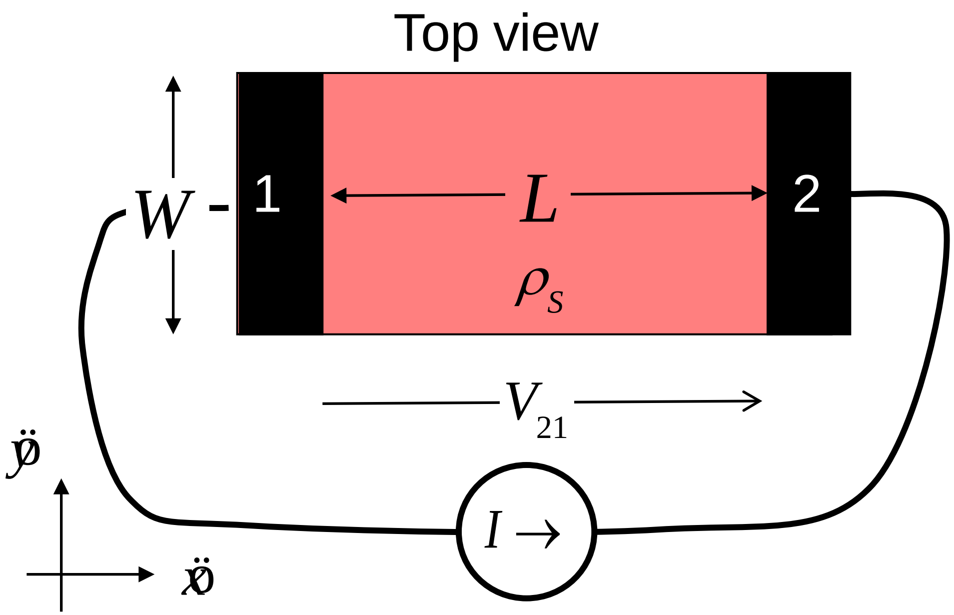
Net thermal energy absorbed from contact 1 that can be converted into useful work:

$$Q_1 - Q_2$$

Efficiency:

$$\eta = \frac{Q_1 - Q_2}{Q_1} = 1 - \frac{Q_2}{Q_1} = 1 - \frac{Q_2/T_2}{Q_1/T_1}\left(\frac{T_2}{T_1}\right)$$

maximum temperature difference

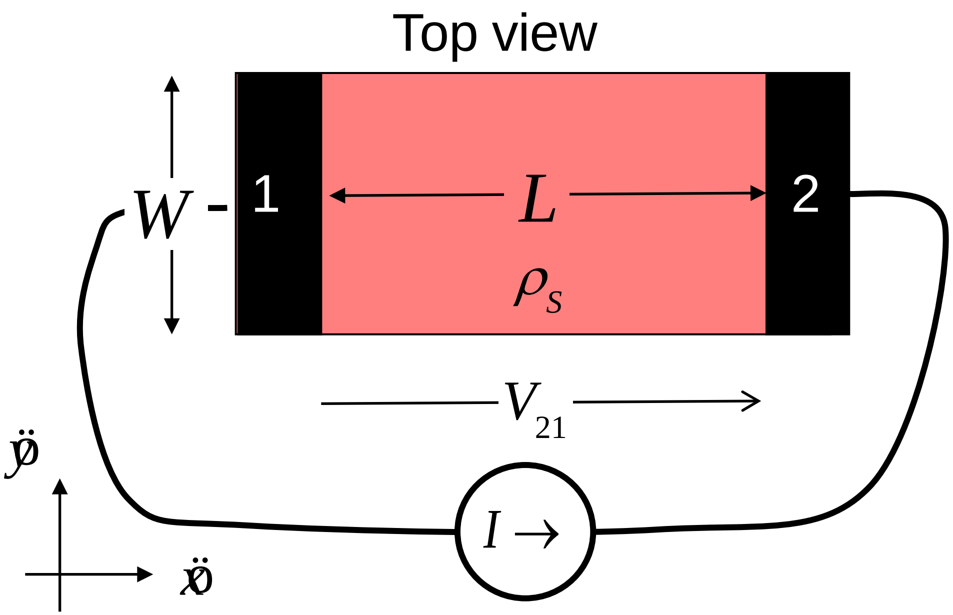


$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e \Delta T$$

If we force a current through this thermoelectric device, what is the maximum temperature difference, $\Delta T = T_2 - T_1$, that we can produce?

maximum temperature difference



$$\Delta V = RI - S\Delta T$$

$$I_Q = -\pi I - K_e \Delta T$$

$$I_{Q1} = -TSI - K_e \Delta T - \frac{1}{2} I^2 R$$

For a fixed current, the temperature will rise until $I_Q = 0$

$$\Delta T = -\frac{\left(TSI + I^2 R/2\right)}{K_e}$$

$$\frac{\partial \Delta T}{\partial I} = -\frac{\left(TS + IR\right)}{K_e} = 0$$

$$I_{opt} = -TS/R$$

$$\Delta T\big|_{\max} = \frac{1}{2}\frac{T^2 S^2 G}{K}$$

maximum temperature difference

$$\Delta T\Big|_{\max} = \frac{1}{2}\frac{T^2 S^2 G}{K}$$

$$\left.\frac{\Delta T}{T}\right|_{\max} = \frac{1}{2}\frac{S^2 GT}{K} = \frac{1}{2} ZT$$

$$ZT = \frac{S^2 GT}{K_e + K_L}$$

dimensionless figure of merit

K_e: electronic heat conductance

K_L: lattice heat conductance

figure of merit

Power factor:

-large Seebeck coefficient

-high conductance

-depends on material parameters

$$ZT = \frac{S^2 GT}{K_e + K_L}$$

thermal conductance:

-$K_L > K_e$

-need short mfp for phonons

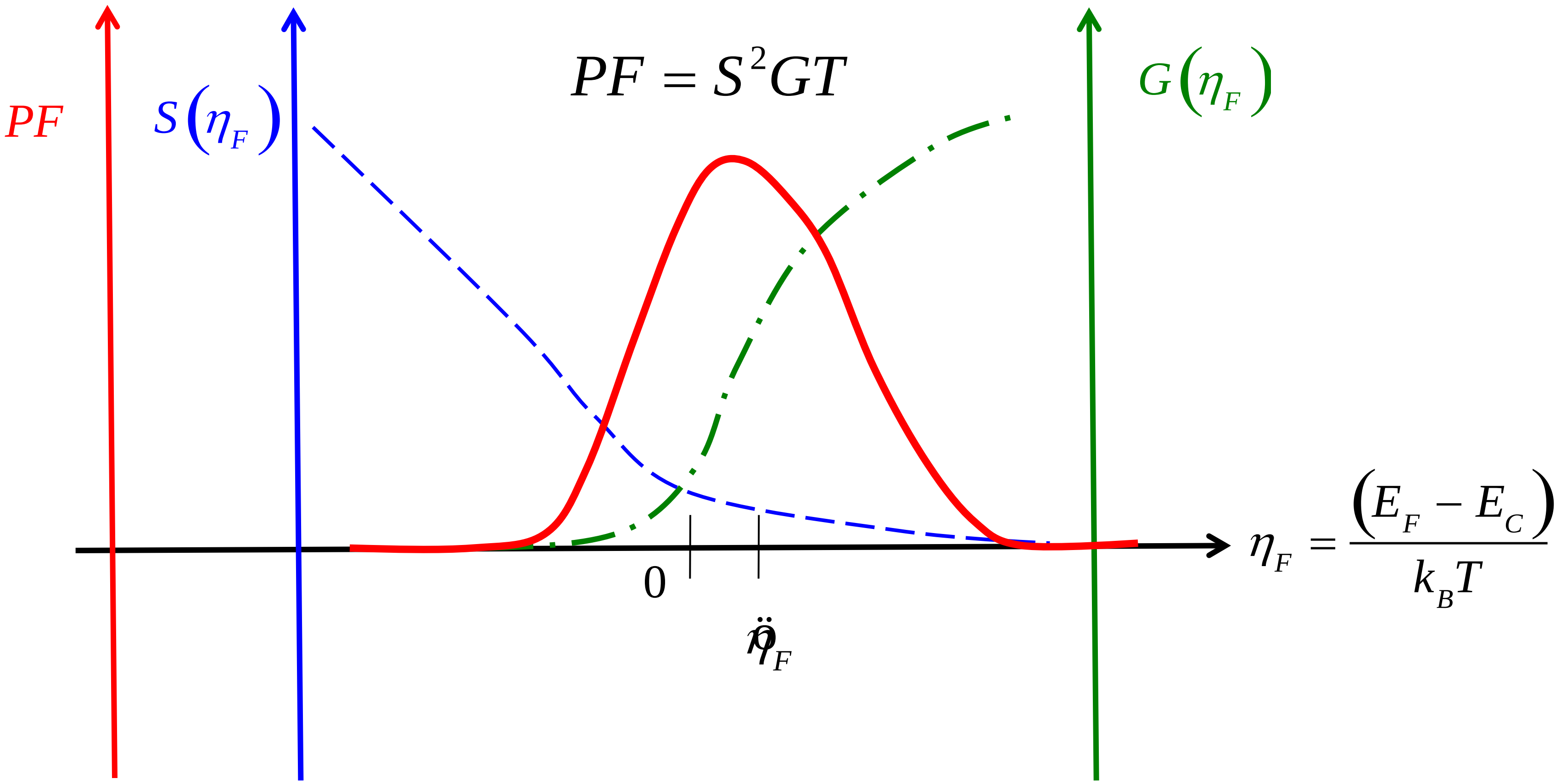
(alloys with large mass difference – e.g. Bi_2Te_3, SiGe)

-nanostructuring for reducing mfp

-"phonon glass electron crystal"

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

optimal power factor

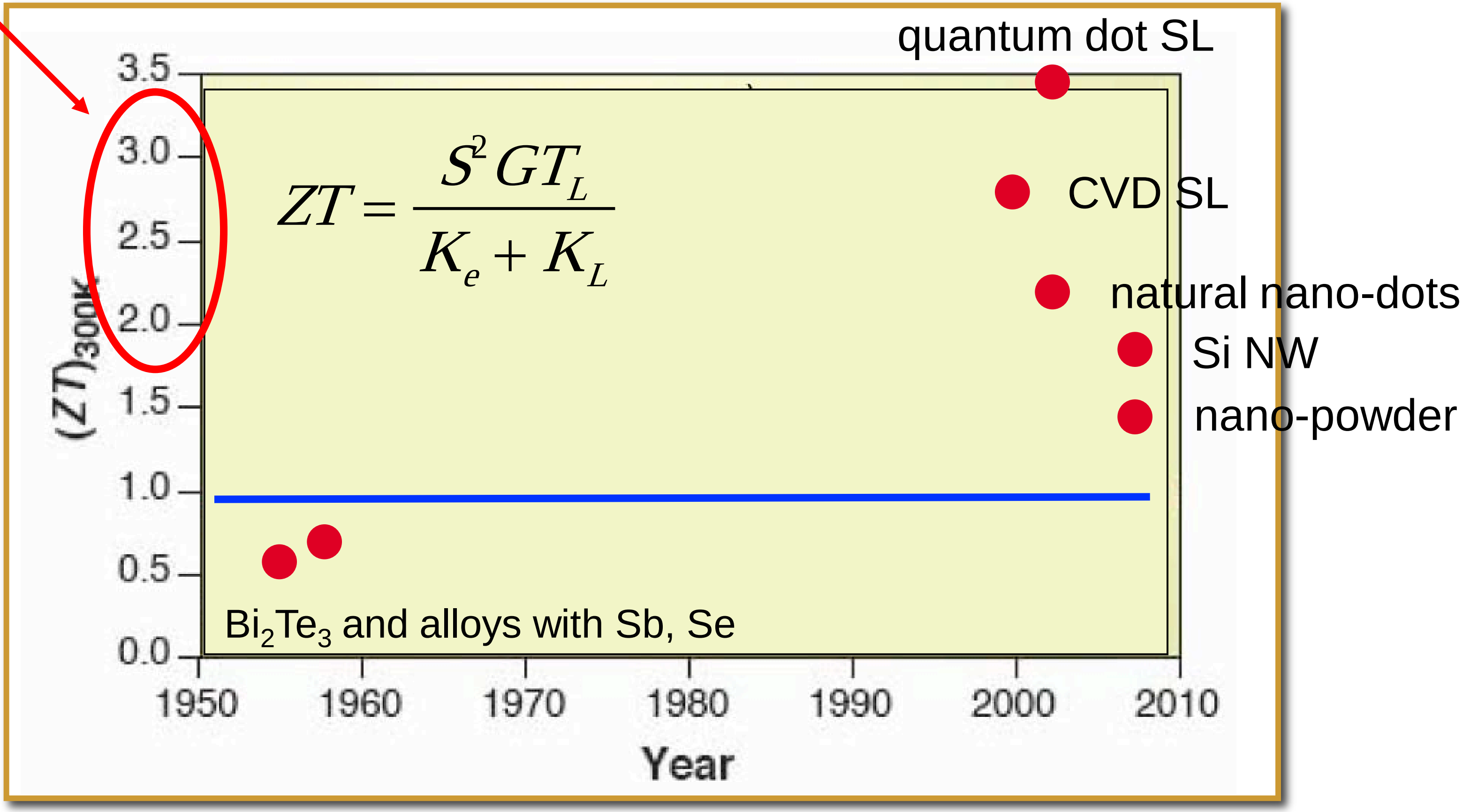


The optimum power factor occurs when E_F is near E_C.

history and prospects

holy grail

nanostructured thermoelectrics



Majumdar, *Science*, **303**, 777 (2004)

questions

1) Onsager relations

2) Measurement considerations

3) Thermoelectric devices