Thermoelectricity: From Atoms to Systems

Week 2: Thermoelectric Transport Parameters

Lecture 2.3: **Devices and Materials**

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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):

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

$$\sigma'(E) = \frac{2q^2}{h}\lambda(E)\left(M(E)/A\right)\left(-\frac{\partial f_0}{\partial E}\right)$$

$$\sigma = \int_{-\infty}^{+\infty}\sigma'(E)dE \qquad \rho = 1/\sigma$$

$$S = -\frac{1}{q}\frac{\int_{-\infty}^{+\infty}(E-E_F)\sigma'(E)dE}{\int \sigma'(E)dE} = -\frac{E_J - E_F}{qT}$$

$$\pi = TS$$

$$\kappa_e = \kappa_0 - T\sigma S^2 \quad \kappa_0 = \frac{1}{q^2T}\int_{-\infty}^{+\infty}(E-E_F)^2\sigma'(E)dE$$

review: 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):

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

$$\sigma = \frac{2q^2}{h}\langle M_{el}/A\rangle\langle\langle\lambda_{el}\rangle\rangle = n_0 q\mu_n$$

$$S = -\left(\frac{k_B}{q}\right)\left(\frac{E_J - E_F}{k_B T}\right)$$

$$\pi = TS$$

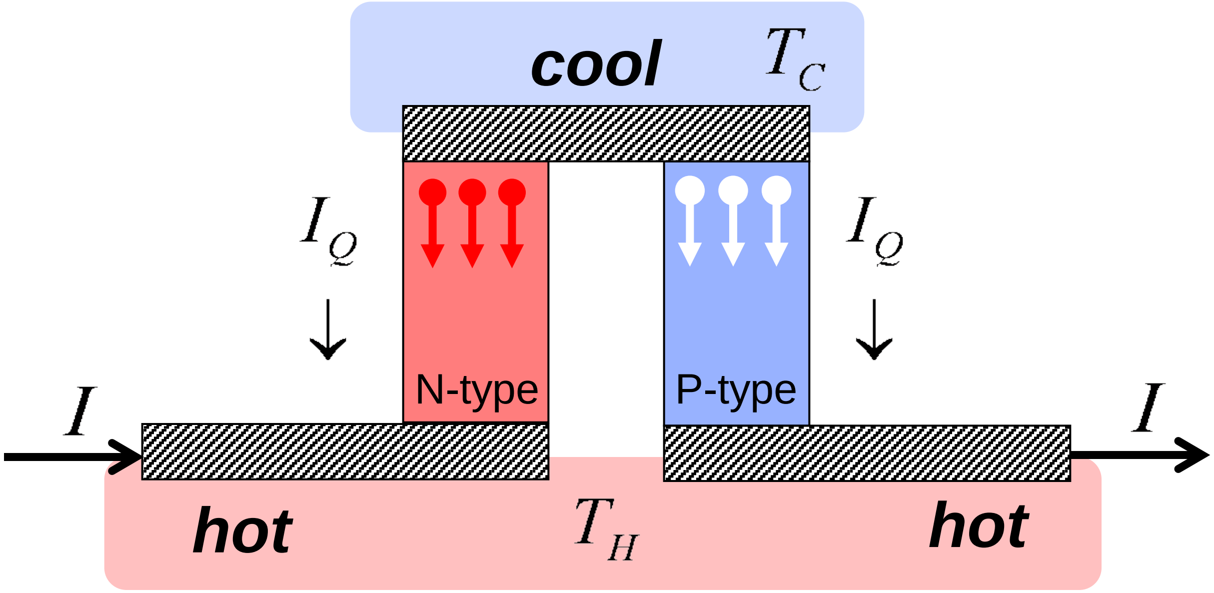
$$\kappa_e = T\sigma\mathcal{L}$$

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

lecture 3 topics

1) Thermoelectric devices
2) TE figure of merit, *ZT*
3) Material trade-offs

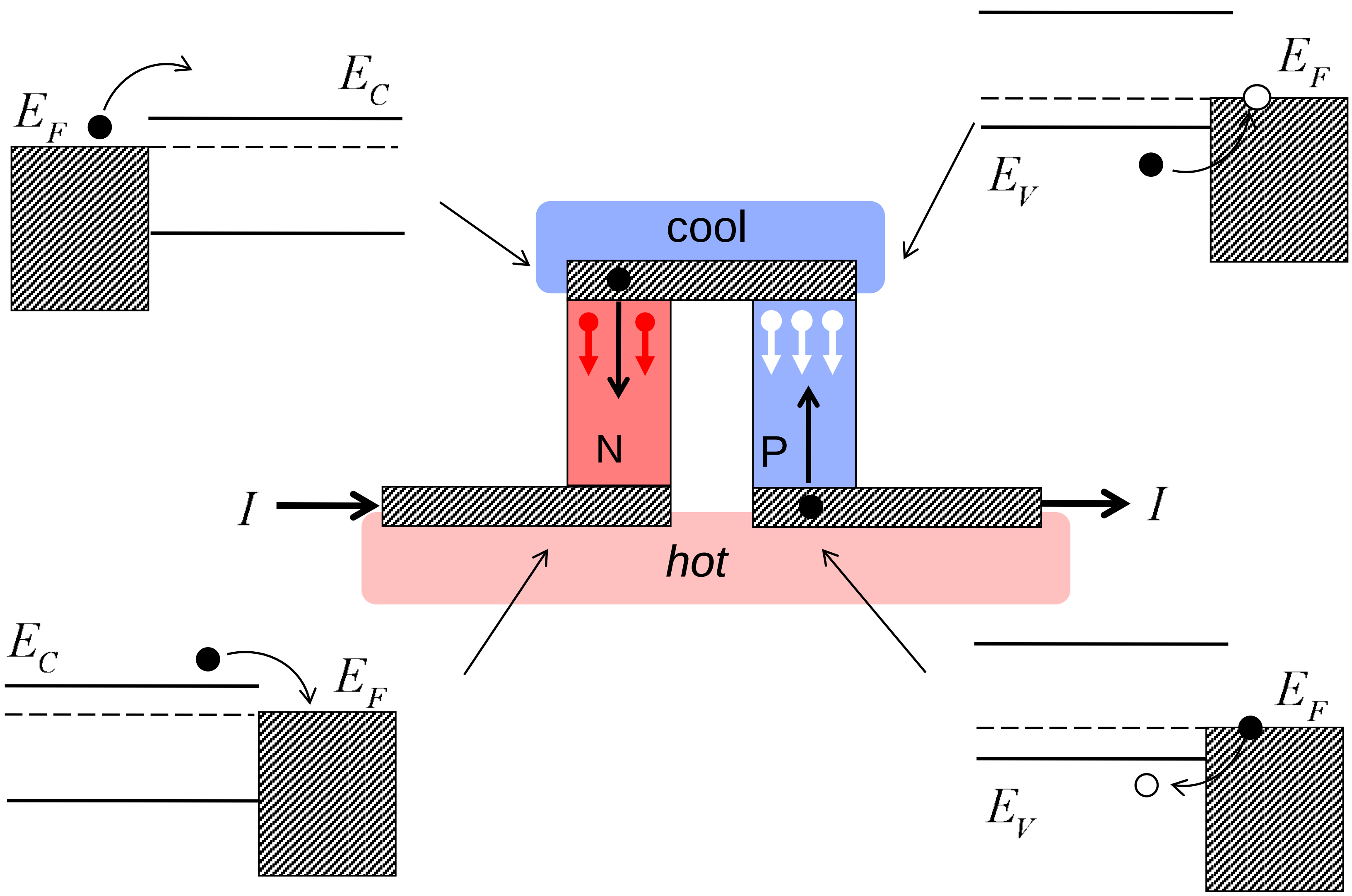
thermoelectric cooling



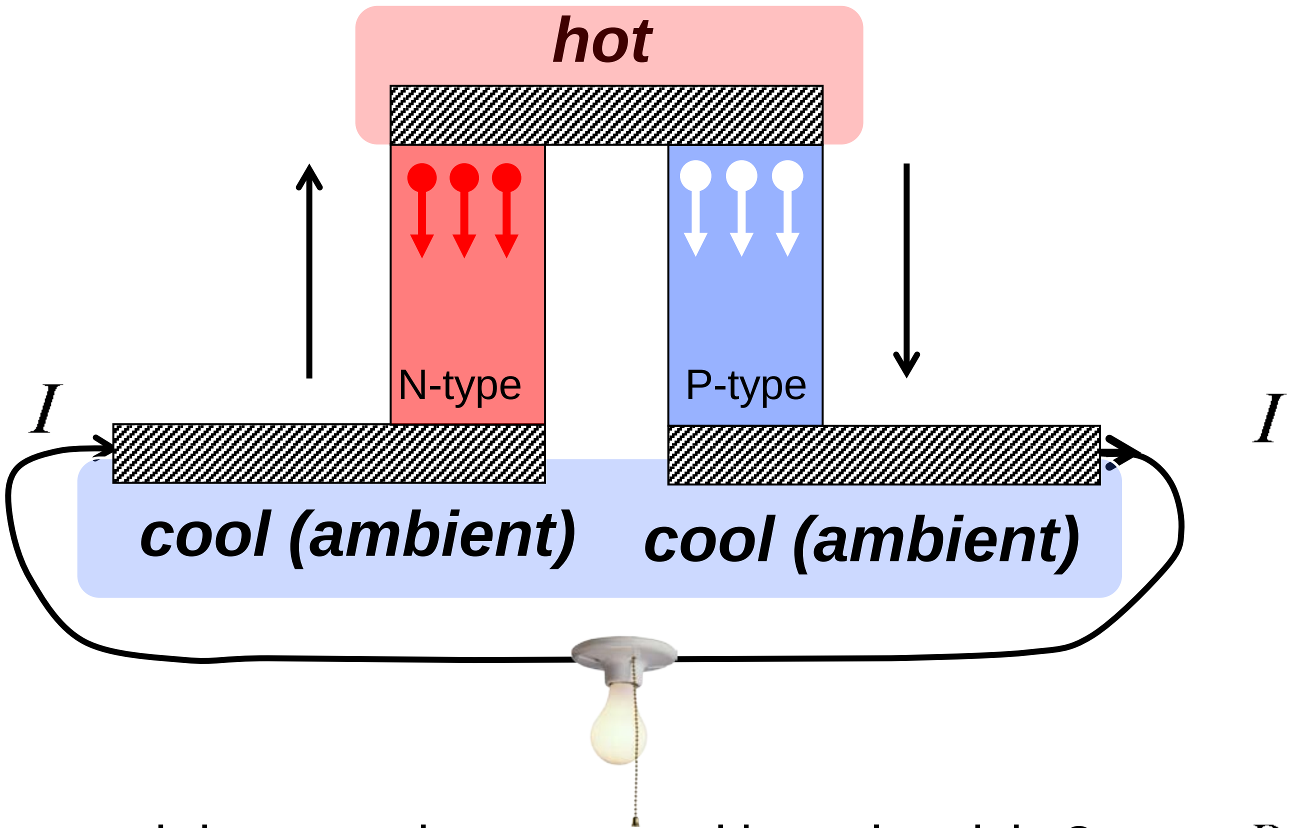
1) What determines the maximum temperature difference?
2) How much heat can be pumped?
3) What is the coefficient of performance (COP)?

COP at maximum cooling power: $\eta = q_C^{\max} / P_{in}$

inside view (electrons)



thermoelectric power generation



1) How much heat can be converted into electricity?
(what determines the efficiency?)

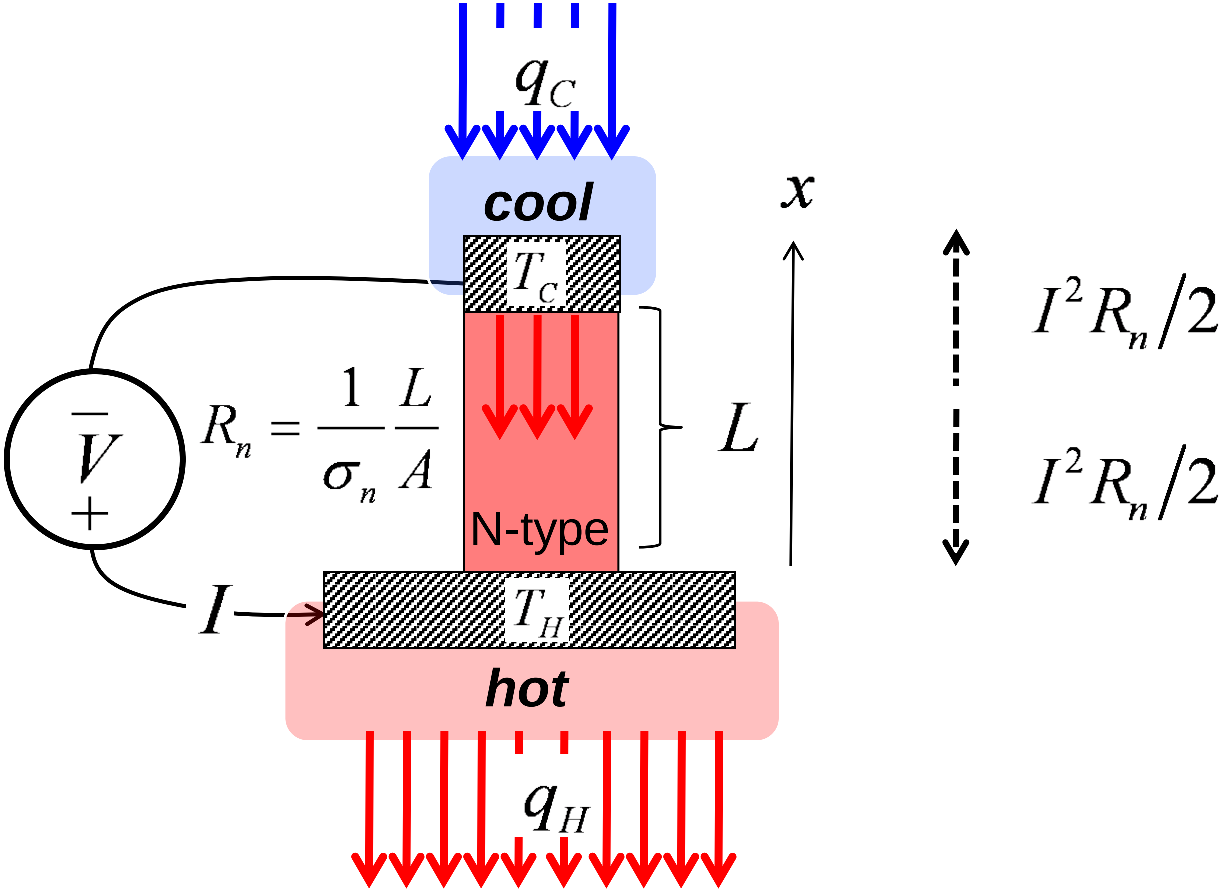
$$\eta = \frac{P_{out}}{P_{in}} = \frac{I^2 R_L}{A q_{in}}$$

FOM

Analysis of thermoelectric coolers and power generators shows that their efficiencies are related to a dimensionless, materials figure of merit (FOM), ZT

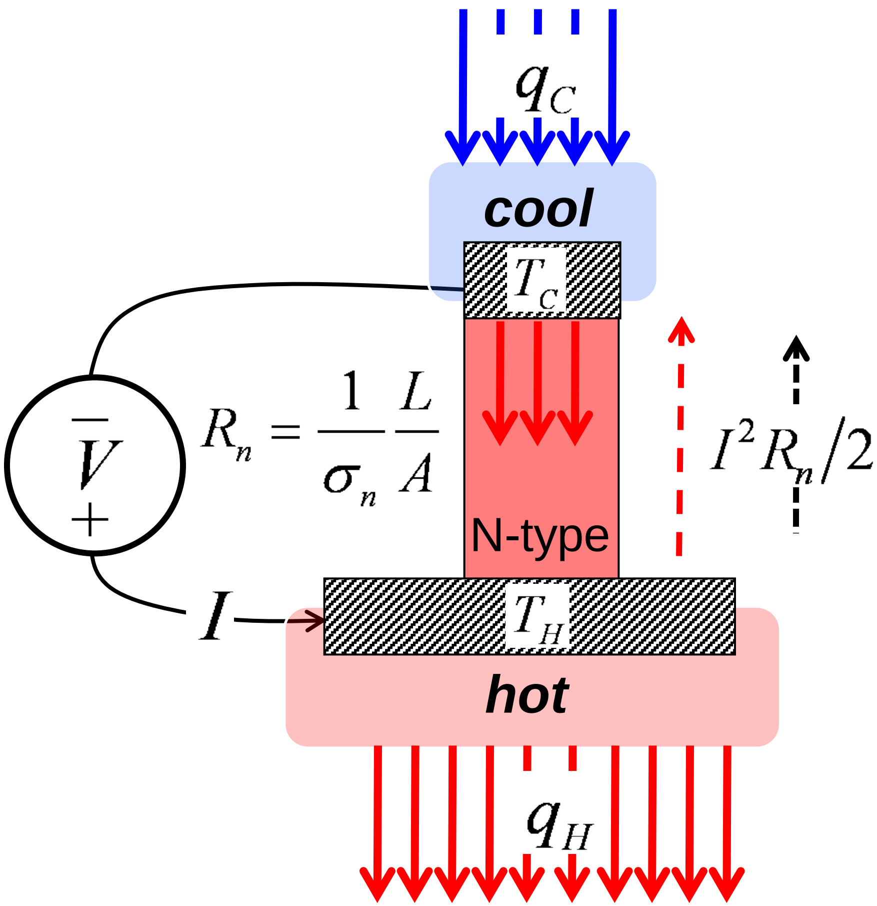
Next, we will do a simple analysis to derive ZT.

simplified TE device (one leg)



What is the maximum ΔT that can be achieved?

simplified TE cooling device (one leg)



1) heat extracted from the cold side

=

2) heat pumped by Peltier effect

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3) heat diffusing down the thermal gradient

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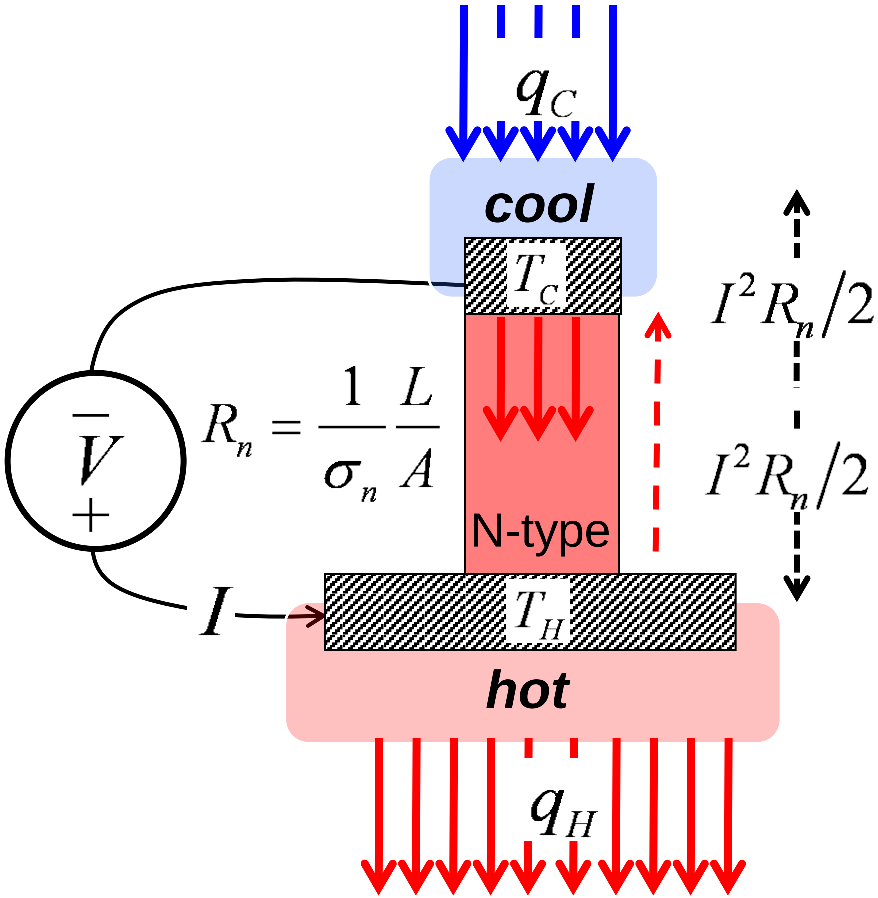
4) heat generated by Joule heating

simplified TE cooling device (one leg)



$$q_C = \pi_n \frac{I}{A} - \kappa \frac{dT}{dx} - \frac{I^2 R_n}{2A} \quad \left(\frac{\mathrm{W}}{\mathrm{m}^2}\right)$$

$$\frac{dq_C}{dI} = 0 \rightarrow I_{\max},\ q_{C\max}$$

$$q_{C\max} = 0 \rightarrow \Delta T_{\max}$$

$$\Delta T_{\max} = \frac{1}{2} Z \left(T_C\right)^2 \quad Z = \frac{S_n^2 \sigma_n}{\kappa}$$

TE figure of merit (FOM)

FOM

The performance of a TE device is related to a dimensionless figure of merit, *ZT*

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

Denominator mostly determined by lattice thermal conductivity. (Lecture 5) $\kappa_L >> \kappa_e$

dimensionless figure of merit

1) What material properties are needed for a high *ZT*?
2) Given a material, how can we optimize *ZT*?

power factor

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

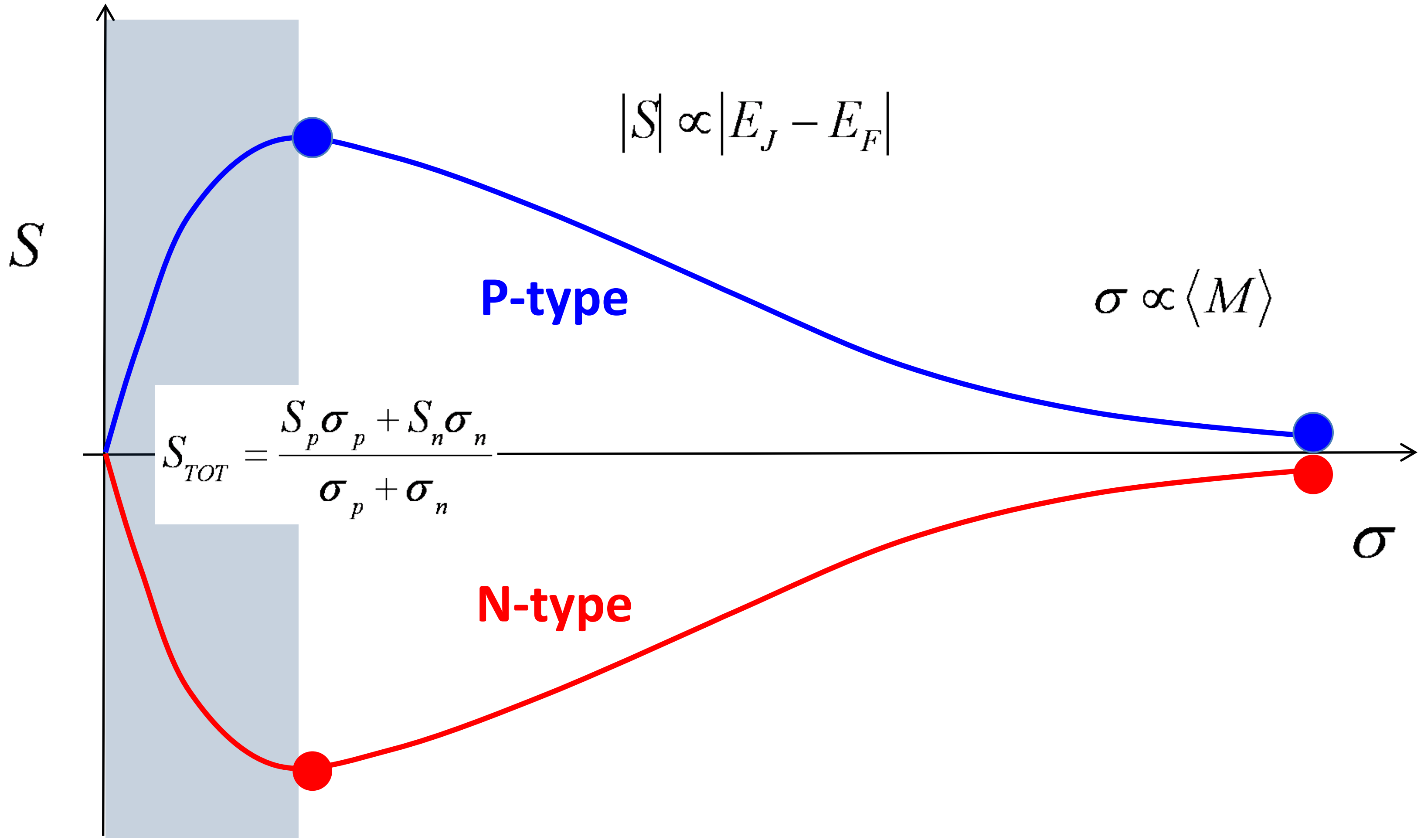
The quantity: $S^2\sigma$ is known as the "power factor."

Need a large *S* and a large σ.

$$S_n(T) = -\left(\frac{k_B}{q}\right)\frac{\left(E_J - E_F\right)}{k_B T}$$ need $E_F \ll E_C$

$$\sigma_n = \left(\frac{2q^2}{h}\right)\langle M \rangle \langle\langle \lambda \rangle\rangle = n_0 q \mu_n$$ need $E_F \gg E_C$ and large m.f.p.

Seebeck vs. conductivity trade-off

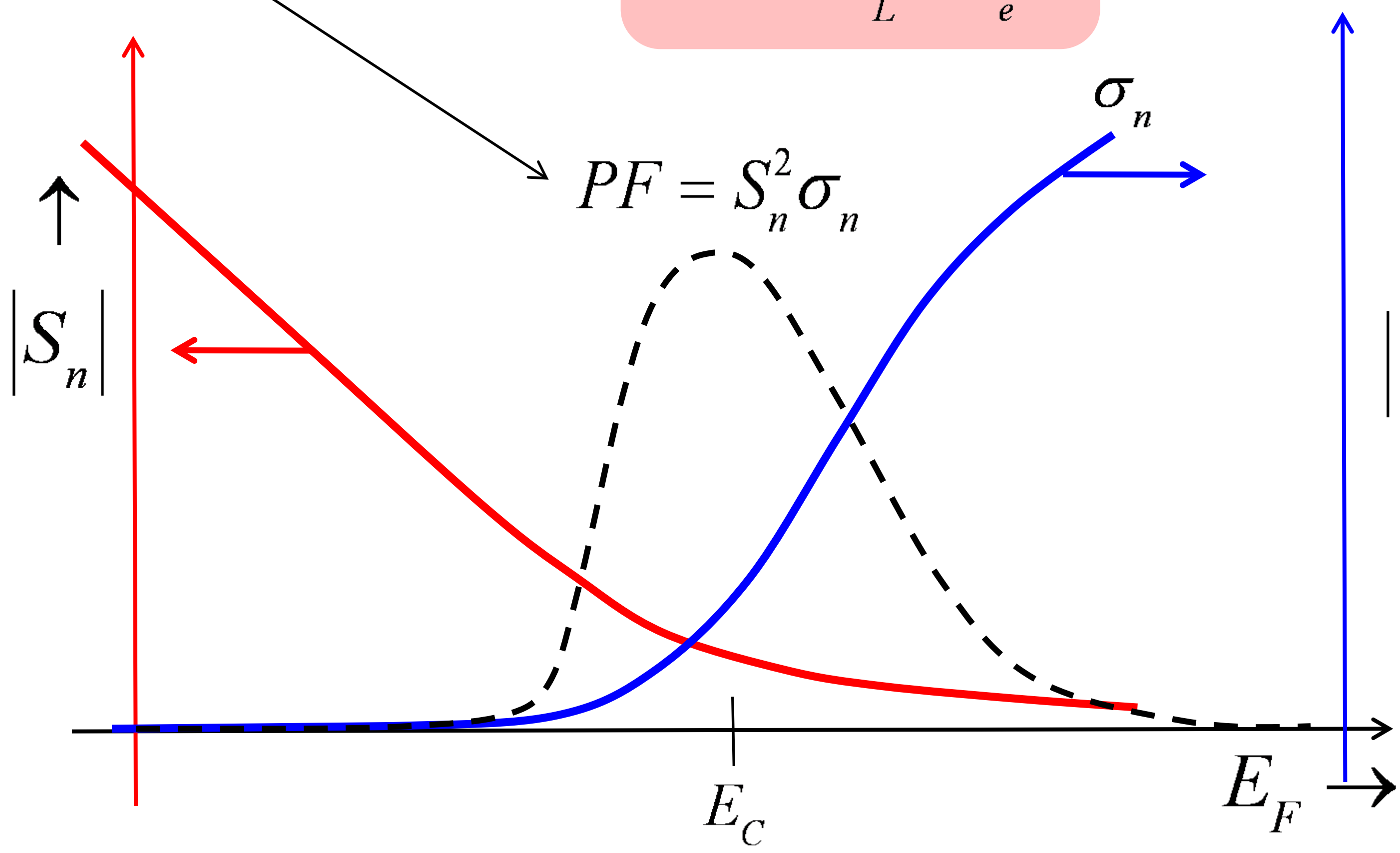


bipolar conduction

FOM: PF vs. Fermi level

The peak PF occurs when E_F is near the band edge.

$$ZT = \frac{S_n^2 \sigma_n T}{\kappa_L + \kappa_e}$$



PF in different materials

For a given material, we aim to optimize the PF with doping that positions the Fermi level near the band edge, but how does the optimum power factor vary between materials?

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

$$\frac{\text{increase the mean-free-path} \quad \text{improve the } S \text{ vs. } \sigma \text{ trade-off}}{\textbf{decrease the lattice thermal conductivity}}$$

ZT of Bi_2Te_3 vs. Si

Why is Bi_2Te_3 a good thermoelectric with ZT ~ 1?

Why is Si a poor thermoelectric with ZT ~ 0.01?

Answer: Mostly because of the difference in lattice thermal conductivities.

$$\kappa_L(\mathrm{Si}) \approx 150 \text{ W/m-K}$$

$$\kappa_L(\mathrm{Bi_2Te_3}) \approx 1.5 \text{ W/m-K}$$

We will explain why in Lecture 5

thermoelectric FOM

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

Good thermoelectrics have very low lattice thermal conductivities.

Recent progress in thermoelectric performance has largely been due to engineering materials to lower the lattice thermal conductivity.

Many ideas for PF engineering have been proposed and explored, but so far, success has been limited.

lecture 3 topics

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