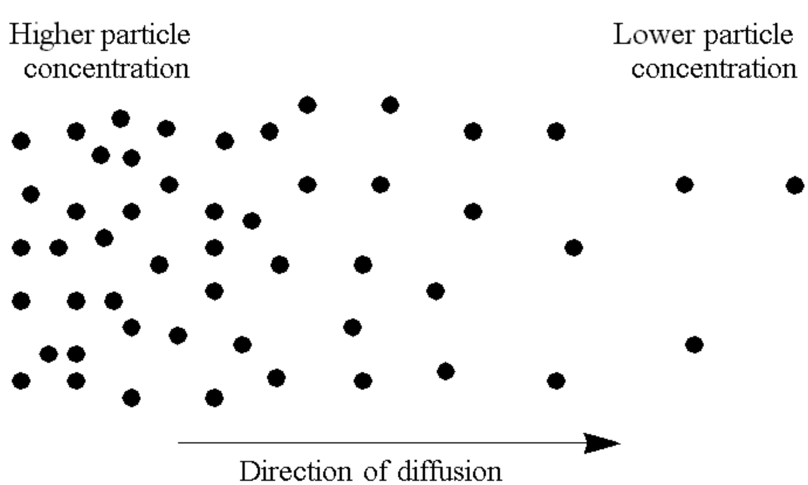
EE 116 Lectures 12-15

Diffusion of carriers

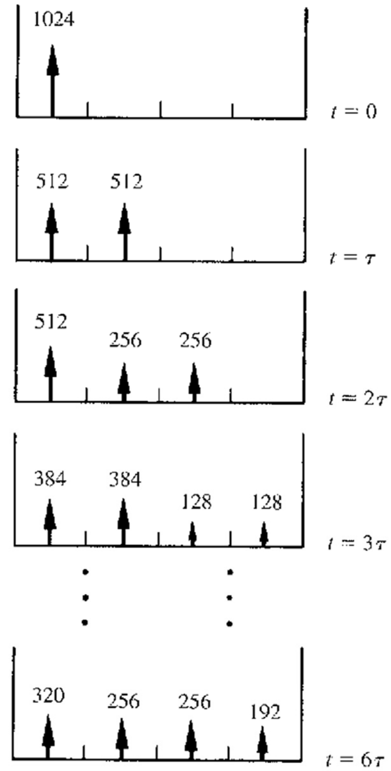
- https://truenano.com/PSD20/contents/toc2.htm
- Read section 2.7.4
- Also see CCH Ch. 2.3-2.8

- Remember Brownian motion of electrons & holes!
- When E-field = 0, but T > 0, thermal velocity v_T = ______
- But net drift velocity v_d = __________
- So net current J_d = _________

- What if there is a *concentration* or *temperature* (thermal velocity) gradient?



- Is there a net flux of particles? Is there a net current?
- Examples of diffusion:
  - ___________
  - ___________
  - ___________
- One-dimensional diffusion example:



- How would you set up diffusion in a semiconductor? You need something to drive it out of equilibrium.

- Let's look at **two types of diffusion**:

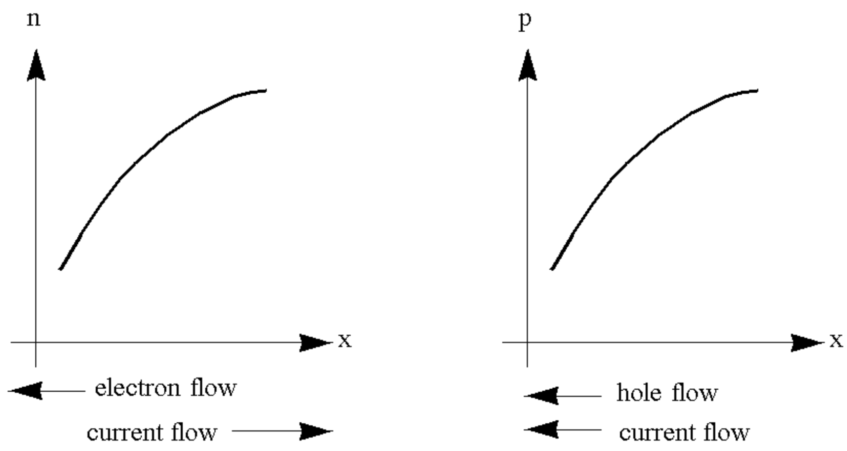
  1) Driven by carrier density gradients (∇n, ∇p)

     → Applications: ___________________________

  2) Drive by temperature gradients (∇T)

     → Applications: ___________________________

1) Diffusion driven by **gradients in carrier density** (∇n, ∇p)



Mathematically:

$$J_{\text{N,diff}} = qD_{\text{N}} \frac{dn}{dx} \qquad J_{\text{P,diff}} = -qD_{P} \frac{dp}{dx}$$

Where D_n and D_p are the *diffusion coefficients* or *diffusivity*

- Now, we can FINALLY write down the TOTAL currents…
- For electrons: $$J_{\text{N}} = J_{\text{N,drift}} + J_{\text{N,diff}} = qn\mu_n\mathcal{E} + qD_N \frac{dn}{dx}$$
- For holes: $$J_{\text{P}} = J_{\text{P,drift}} + J_{\text{P,diff}} = qp\mu_p\mathcal{E} - qD_P \frac{dp}{dx}$$
- And TOTAL current:

$$J_{\text{TOT}} = J_{\text{N}} + J_{\text{P}}$$

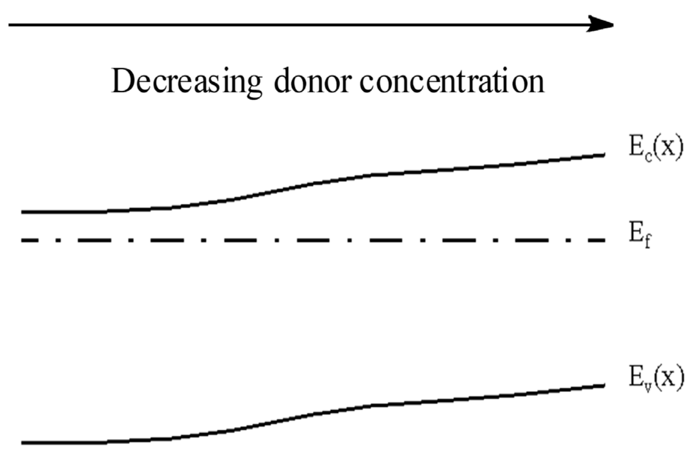
- Interesting point: minority carriers contribute little to drift current (usually, too few of them!), BUT if their gradient is high enough…

- Under <u>equilibrium</u>, open-circuit conditions, the total current must always be = <u>zero</u>
- I.e. J_{drift} = - $J_{diffusion}$
- More mathematically, for electrons:

$$J_{n,drift} + J_{n,diff} = 0 \qquad \text{in thermal equilibrium}$$

- So any disturbance (e.g. light, doping gradient, thermal gradient) which may set up a carrier concentration gradient, will also internally set up a built-in ___________________

- What is the relationship between mobility and diffusivity?
- Consider this band diagram:



- Going back to *drift* + *diffusion* = 0 in equilibrium:

$$J_N = qn\mu_n\mathcal{E} + qD_N\frac{dn}{dx} = 0$$

$$n\mu\mathcal{E} + D\frac{\partial n}{\partial x} = 0$$ (drift + diffusion current = 0 in equilibrium)

$$n \approx N_C e^{\frac{E_F - E_C}{kT}} \longrightarrow \frac{\partial n}{\partial x} \approx n\left(\frac{-1}{kT}\right)\left(\frac{\partial E_C}{dx}\right) = \frac{-n}{kT}q\mathcal{E}$$

$$n\mu\mathcal{E} - D\frac{n}{kT}q\mathcal{E} = 0$$

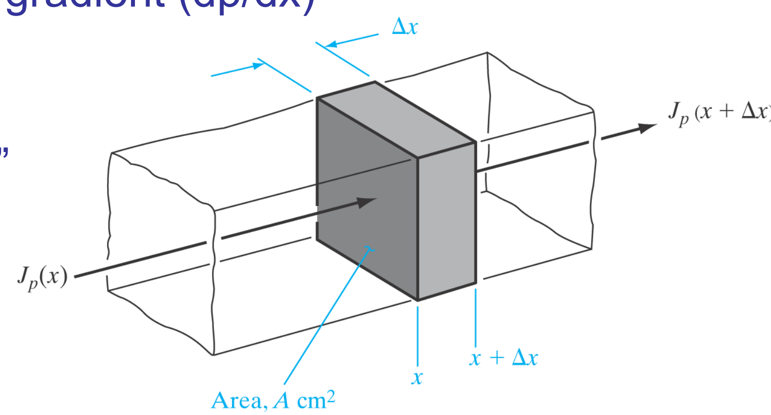
- Leads us to the Einstein Relationship: $$\frac{D}{\mu} = \frac{kT}{q}$$
  - This is very, very important because it connects diffusivity with mobility, which we already know how to look up. Plus, it rhymes in many languages so it's easy to remember.
- The Einstein Relationship (almost) always holds true.

- **Ex:** The hole density in an n-type silicon wafer ($N_D = 10^{17}$ cm^{-3}) decreases linearly from 10^{14} cm^{-3} to 10^{13} cm^{-3} between x = 0 and x = 1 µm (why?). Calculate the hole diffusion current.

- Let's recap the carrier-gradient-diffusion lessons so far:
  - Diffusion without recombination (driven by ∇n or ∇p)
  - Einstein relationship ($D/\mu = kT/q$)
  - kT/q at room temperature ~ 0.026 V (this is worth memorizing, but be careful at temperatures different from 300 K)
  - Mobility μ look up in tables, then get diffusivity (be careful with total background doping concentration, N_A+N_D)

- Next we examine:
  - Diffusion with recombination
  - The diffusion length (distance until they recombine)
  - Temperature-driven-diffusion (∇T)

- Assume holes (p) are minority carriers
- Consider simple volume element where we have both generation, recombination, and holes passing through due to a concentration gradient (dp/dx)
- Simple "bean counting" in the little volume



- Rate of "bean" or "bubble" population change = (current IN – current OUT) – bean recombination + generation

- This technique is very powerful in any Finite Element (FE) computational or mathematical model.
- So let's count "beans" ("bubbles"):
  - Recombination rate = # excess bubbles (δp) / recombination time (τ)
  - Current (#bubbles) IN – Current (#bubbles) OUT = $(J_{IN} - J_{OUT})$ / dx
  - Generation rate = # bubbles created /cm^3/s
- Note units (VERY important check)
- The continuity equation, mathematically:

$$\frac{\partial p}{\partial t} = \frac{\partial(\delta p)}{\partial t} = -\frac{1}{q}\frac{\partial J}{\partial x} - \frac{\delta p}{\tau} + G_L$$

- Notation: $p = p_0 + \delta p$

- Why is there a (diffusion) current derivative divided by q?
- Of course, e.g. for holes:

$$J_{DIFF} = -qD_p \frac{\partial p}{\partial x}$$

so,

$$-\frac{1}{q}\frac{\partial J}{\partial x} = +D_p \frac{\partial^2 p}{\partial x^2}$$

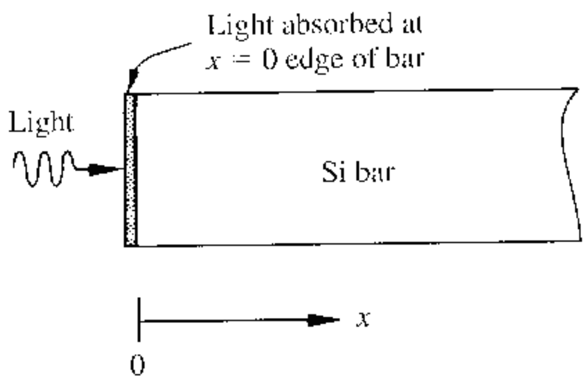
- So the diffusion equation (which is just a special case of the continuity equation above) becomes:

$$\boxed{\frac{\partial(\delta p)}{\partial t} = D_P \frac{\partial^2(\delta p)}{\partial x^2} - \frac{\delta p}{\tau} + G_L}$$

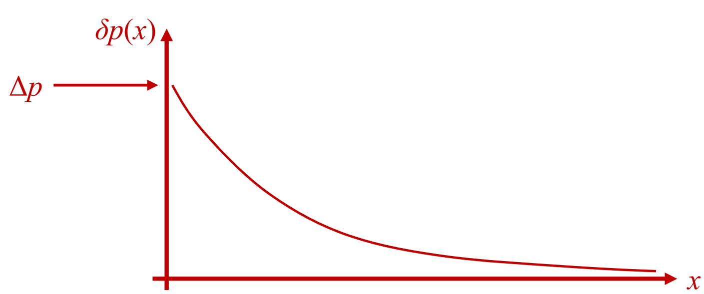
- This allows us to solve for the minority carrier concentrations *in space and time* (here, holes)

- Note, this is applicable only to minority carriers, whose net motion is entirely dominated by diffusion (gradients)
- What does this mean in *steady-state*?
- The diffusion equation in steady-state: $$\frac{\partial^2(\delta p)}{\partial x^2} = \frac{\delta p}{D_P \tau} = \frac{\delta p}{L_p^2}$$
  (with lights off, $G_L = 0$)
- Interesting: this is what a lot of other diffusion problems look like in steady-state. Other examples?
- The diffusion length $L_p = (D_p\tau)^{1/2}$ is a figure of merit.

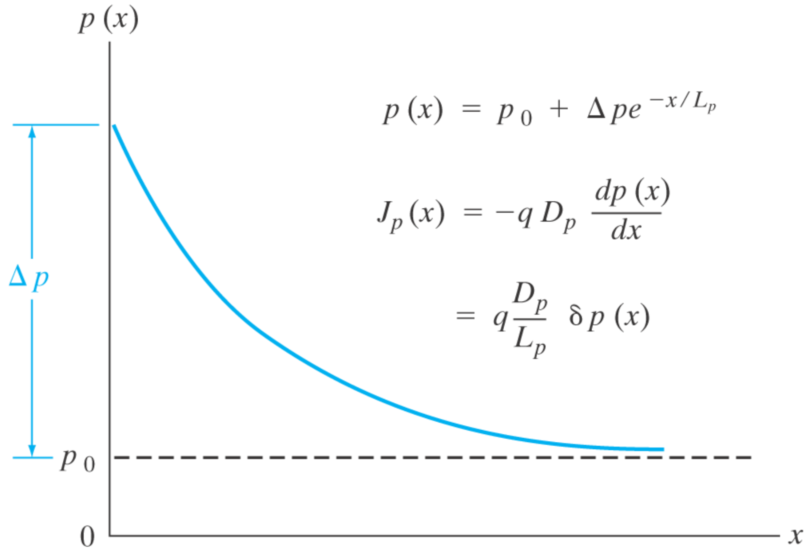
- Consider an example under steady-state illumination:



- Solve diffusion equation: excess $\delta p(x) = \Delta p \, e^{-x/L_p}$



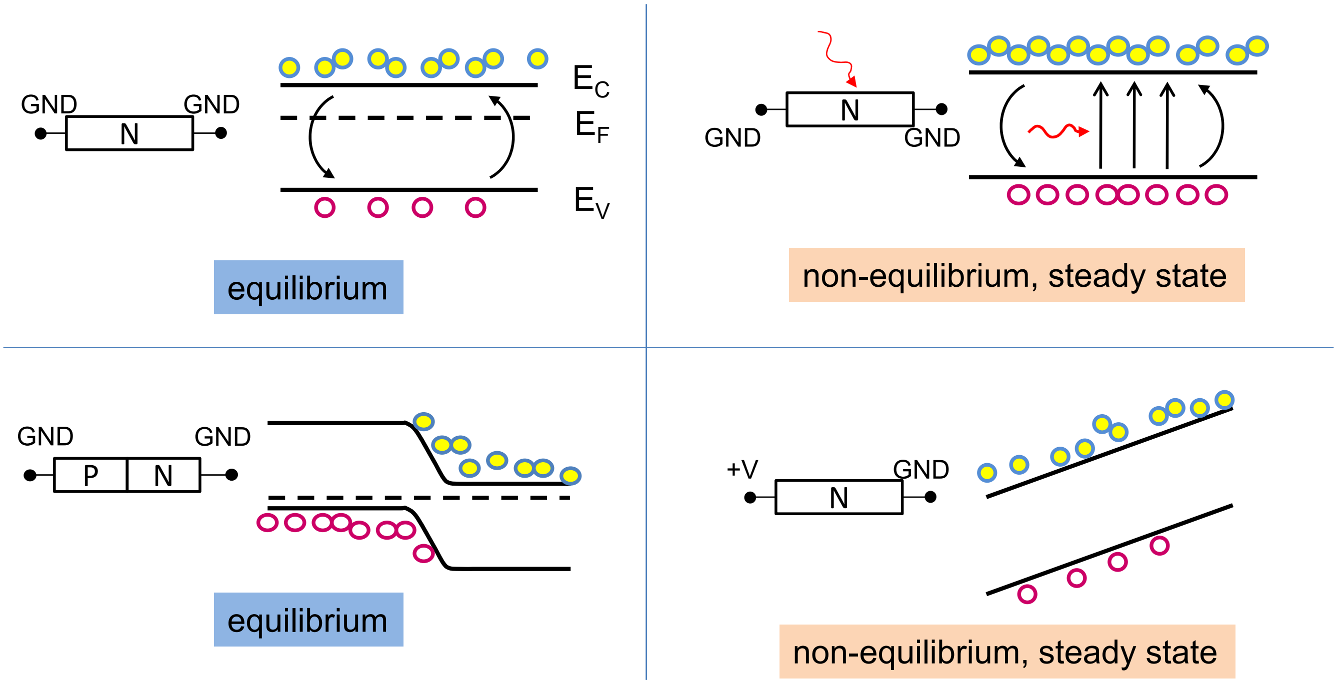
- Plot total $p(x)$:



- Physically, the diffusion lengths (L_p and L_n) are the <u>average</u> distance that minority carriers can diffuse into a sea of majority carriers before “being annihilated” (recombining).
- What devices is this useful in?! (peek ahead)

- **<u>Ex:</u>** A) Calculate minority carrier diffusion length in silicon with $N_D = 10^{16}$ cm^{-3} and τ_p = 1 μs. B) Assuming 10^{15} cm^{-3} excess holes photogenerated at the surface, what is the diffusion current at 1 μm depth?

Recap: Thermal Equilibrium vs. Steady State

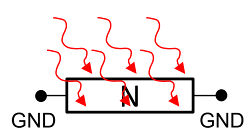


Applications of Continuity Equations to Photo-Generation

Big picture:

What kinds of problems do we want to solve?

What are the appropriate models and how to apply?



Uniform generation:

no spatial dependence and we study its temporal dependence

Usually looks like an R-C transient problem in 101B

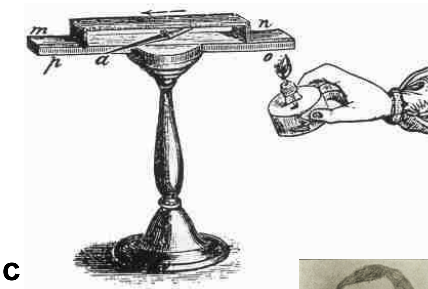
Localized generation:

We usually only consider steady-state (d/dt = 0), spatial dependence

Localized generation sets a boundary condition for the problem

2) Diffusion driven by **gradients in temperature** (∇T)

Seebeck effect (1821):

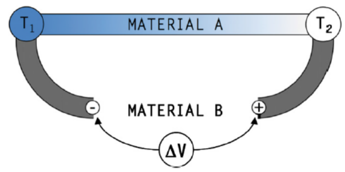


- Loop of Cu and Bi wires (thermocouple)
- Heating one end deflected magnetic needle, initial confused with thermomagnetism
- Ørsted (1823) correctly explained that **electric flow occurred due to temperature gradient**

Thomas Seebeck

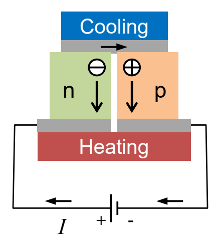
$$\Delta V \equiv (S_B - S_A)\Delta T$$

- $S_{A,B}$ = Seebeck coefficient = thermopower specific to material A or B (units of μV/K)
- Ex: ΔS ~ 300 μV/K and ΔT = 100 K, we generate 30 mV
- *Q: how do we generate 1.5 V like AA battery?*



Peltier effect (1834):

- Opposite of Seebeck effect
- **Electric current flow through a junction of materials A and B can be used to heat or cool!**



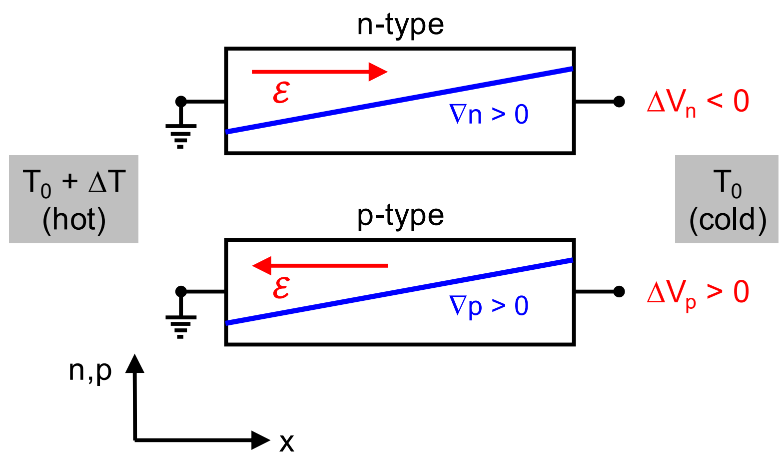
$$Q \equiv \Pi_{AB} I = (S_B - S_A)TI$$

- Π_{AB} = $S_{AB}T$ = Peltier coefficient of junction
- Heating and cooling are reversible, depending on the direction (± sign) of the current *I*
- Ex: I = 1 mA, ΔS ~ 300 μV/K and T = 300 K gives us cooling power of 90 μW
- *Q: how do we generate greater cooling (or heating) power?*

Jean Peltier

Seebeck in a semiconductor:

- Hot end will have thermal velocity v_{th} (hot) > v_{th} (cold)
- This will set up a gradient of electron or hole density
- …which will set up an internal electric field (at open circuit)

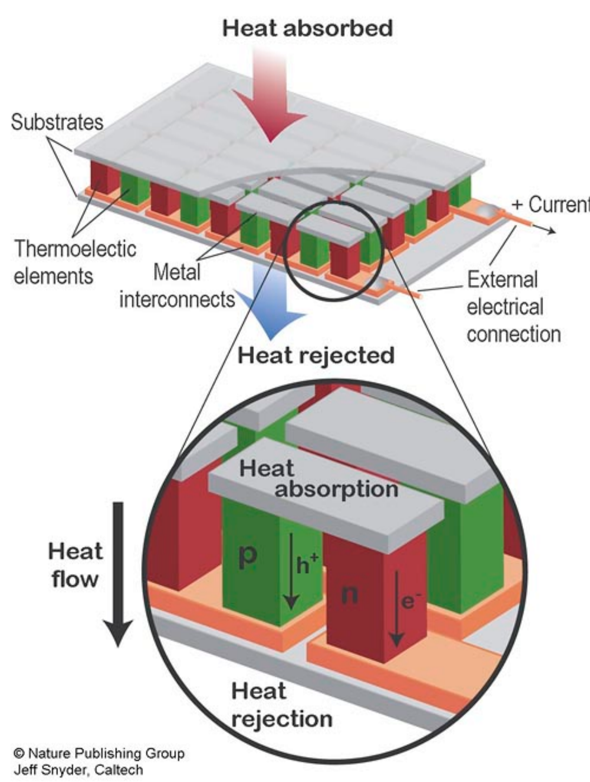


Peltier → electrons & holes carry kinetic energy (in addition to charge) as they move with current flow

- Explains why we prefer higher σ, i.e. highly doped semiconductors

- Thermoelectric (TE) modules are typically arranged in a series of alternating "n" and "p"-doped semiconductor legs

- TE legs are "electrically in series" and "thermally in parallel"



Combining TE, Joule and Heat Flow Effects

- Electric field:

$$\mathbf{E} = -\nabla V = \frac{\mathbf{J}}{\sigma} + S\nabla T$$

Ohm Seebeck

- Heat flux:

$$Q'' = -k\nabla T + STJ$$

- Local current density:

$$\mathbf{J} = \sigma\left(-\nabla V - S\nabla T\right)$$

- Heat diffusion with Seebeck effects and Joule heating

$$-Q''' = \nabla \cdot \left(k\nabla T\right) + \mathbf{J}\cdot\mathbf{E} - T\mathbf{J}\cdot\nabla S$$

So What is the Seebeck Coefficient?

- Seebeck coefficient can be thought of as the heat per carrier per degree K (specific heat per carrier), S ≈ C/q
- In classical electron gas (recall k_B/q = 86 μV/K):

$$S_{classic} \approx \frac{3}{2}\frac{k_B}{q} \approx 130\ \mu\text{V/K}$$

- In normal metals only small fraction around E_F contribute, so the thermopower is very small:

$$S_{metal} \approx \left(\frac{k_B T}{E_F}\right)\frac{k_B}{q} \approx 1\ \mu\text{V/K}$$

- In semiconductors, energy carriers can be “far” from E_F, so the thermopower can be large:

$$S_{semi} \approx \left|\frac{E - E_F}{qT}\right| \approx 1\ \text{mV/K}$$

Common Seebeck Coefficients

Material	Seebeck coefficient S *relative to platinum* (μV/K)
Selenium	900
Tellurium	500
Silicon	440
Germanium	330
Antimony	47
Nichrome	25
Molybdenum	10
Cadmium, tungsten	7.5
Gold, silver, copper	6.5
Rhodium	6.0
Tantalum	4.5
Lead	4.0
Aluminium	3.5
Carbon	3.0
Mercury	0.6
Platinum	0 (definition)
Sodium	-2.0
Potassium	-9.0
Nickel	-15
Constantan	-35
Bismuth	-72

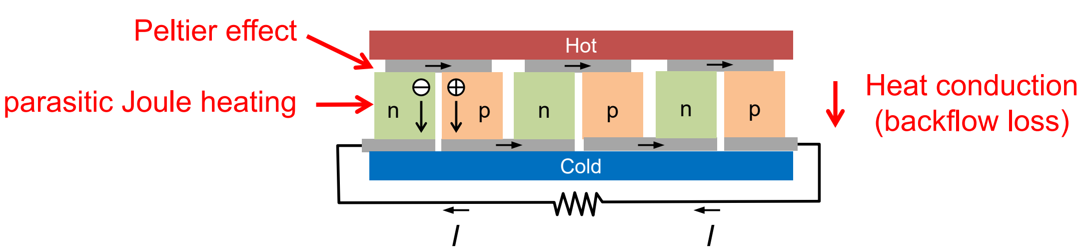
semiconductors tend to have high |S|, but magnitude and sign depend on doping ($S_p > 0$ and $S_n < 0$)

metals tend to have low S

Thomas Seebeck's original junction

Thermoelectric Figure of Merit (ZT)

How efficient are TEs?



Obtain highest

$$Q = STI - I^2\left(\frac{L}{\sigma A}\right) - \frac{kA\Delta T}{L}$$

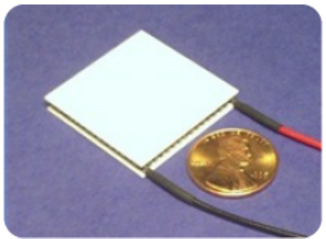
Peltier Joule loss Heat backflow

When maximizing

$$ZT = \frac{S^2 \sigma T}{k}$$

$k_e + k_L$

Thermoelectric Applications



Electric Cooling

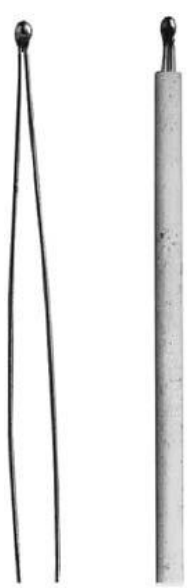




Power Generation

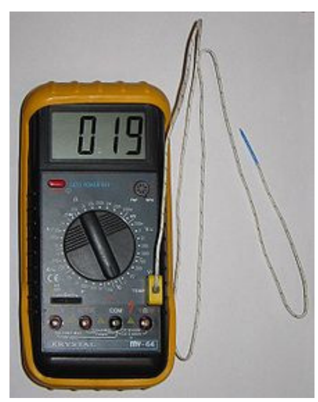



Thermocouples



inside water heater

inside meat thermometer



connected to multimeter

- Junction of two dissimilar materials, used to measure temperature (based on Seebeck's original experiment)

Recap: Thermoelectric Modules

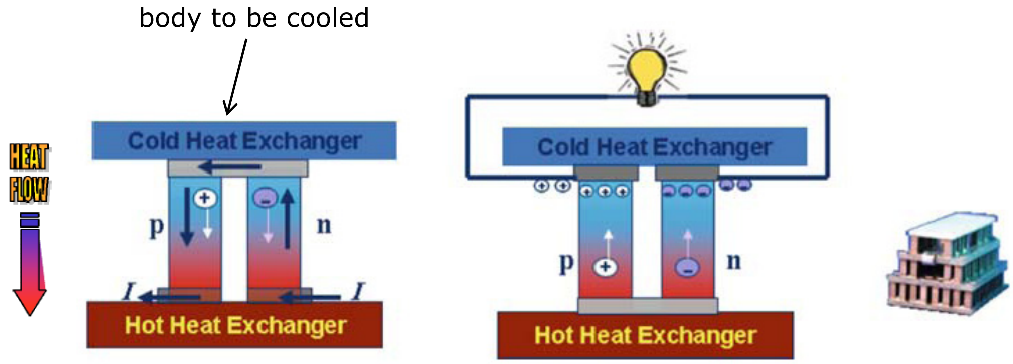


Fig. 9.1 Thermoelectric devices. *Left*: Cooler based on Peltier effect. *Center*: Power generator based on Seebeck effect. *Right*: An actual module

- Use electrons and holes to carry heat and cool a body (e.g. cup holder)
  - Must have good electron and hole conductivity (high σ, S)
  - Must block heat "backflow" through p and n legs (low k)
- Use temperature gradient (e.g. hot engine to ambient) to generate power
- No moving parts (=quiet and reliable), no freon (=clean)

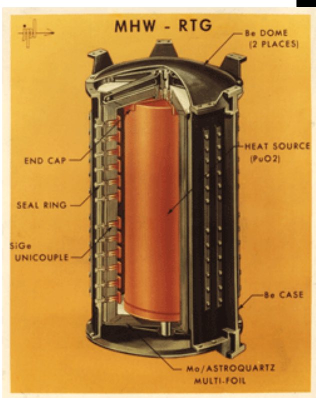
- During and after world wars TE research grew
- Some advances could not be shared or were slow (US vs. USSR)
- 1950s: cooling from ambient to 0°C demonstrated (with Bi_2Te_3)
- Energy harvesting from oil lamp or camp fire to power radios

Kerosene Radio Made in Moscow for use in rural areas, this all-wave radio is reportedly powered by the kerosene lamp hanging above it. A group of thermocouples is heated internally to 570 degrees by the flame. Fins cool the outside to about 90 degrees. The temperature differential generates enough current to operate the low-drain receiver. Regular listeners may want fur-lined union suits, though: It works best in a room with open windows.

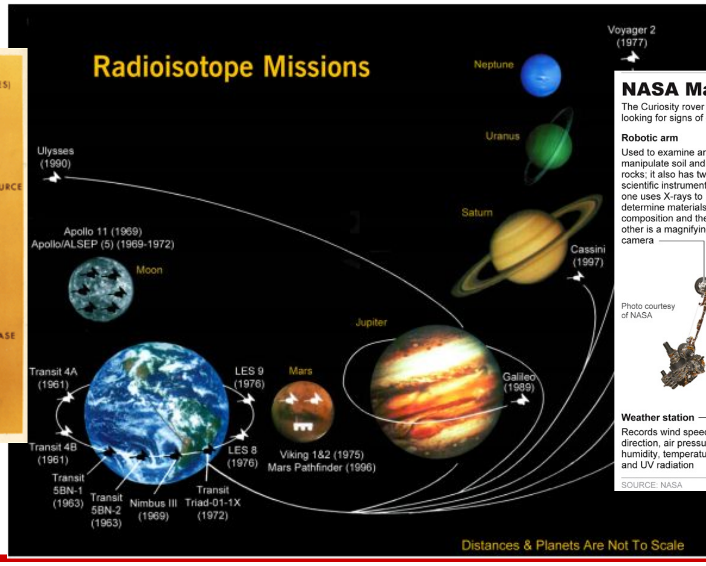
Today: the BioLite camp stove phone charger ($130 at REI.com)

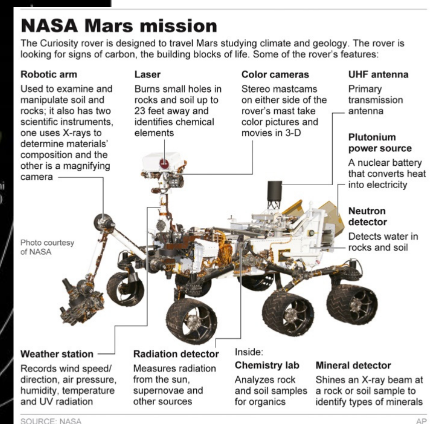
Radioisotope Thermoelectric Generators (RTGs)

- For remote applications (e.g. lighthouses) and space exploration, electrical power provided by RTG
- RTG converts heat from decaying Pu-238 into electricity
  - Half-life of 90 years and 1 g sufficient for ~0.5 W power
- NASA used RTGs to power Apollo, Voyager, Viking, Curiosity…

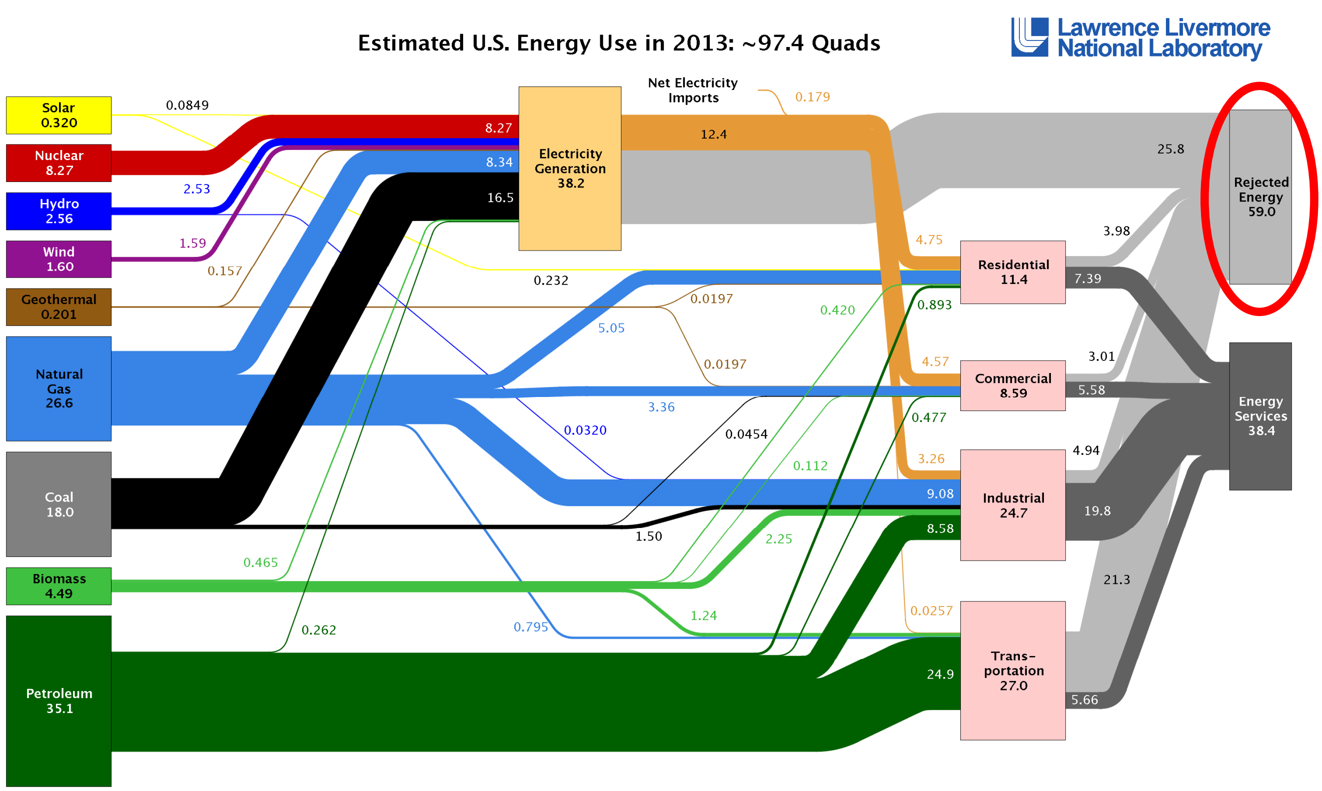


RTG for Voyager 1, 2





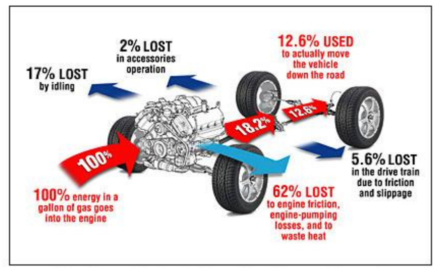
Back on Earth…



Energy Harvesting from Waste Heat

- Almost everything we do wastes heat
  - Power generation
  - Transportation (engine + friction)
  - Computing

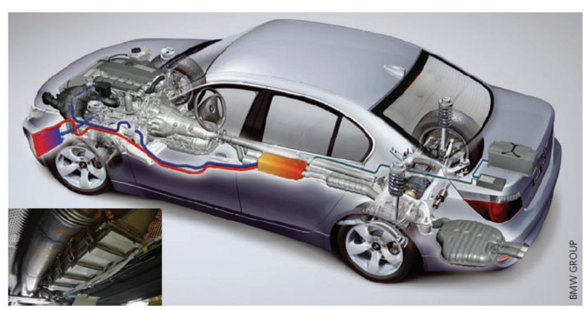
- 15 TW (60%) wasted as heat in the world*
- Most is "low-grade" $T \leq 200\ ^{o}C$
- Recovering even a few percent would be HUGE, equivalent of several power plants (GW)

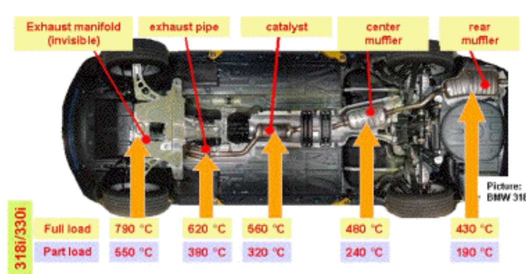


thermoelectrics could be a solution

*Dept. of Energy (2012). **By comparison, ALL data center power consumption world-wide is ~30 GW!**

- About 75% of energy from combustion lost as heat in exhaust or coolant
- Catalytic converters reach 300-500 C and TEGs can be used to harvest 100s of W
- Small fraction power recovery (consider 1 HP ≈ 750 W) but sufficient to power radio or AC and lessen alternator load





Power Consumption

desktop PC ~ 100 W
notebook PC ~ 10 W
low-power sensor, μchip ~ μW – mW
human body output at rest ~ 100 W

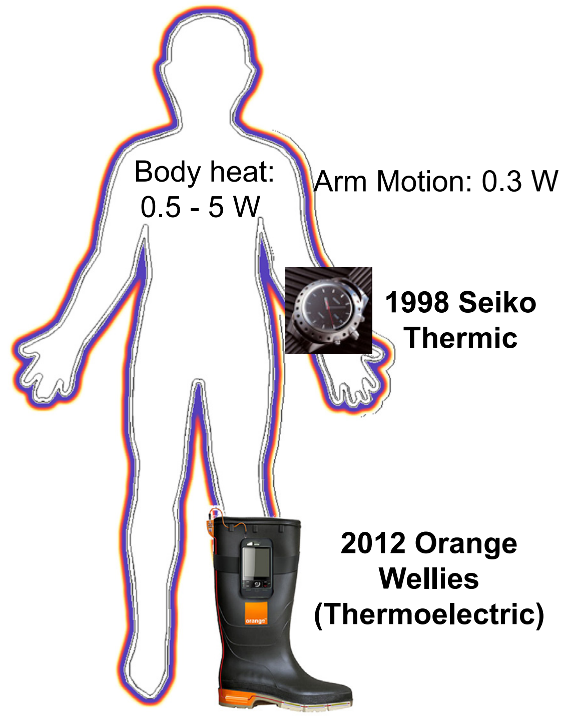
What's The Upper Limit (Carnot)?

$$\eta_{carnot} = \frac{T_{body} - T_{ambient}}{T_{body}} = \frac{310 - 293\ K}{310\ K} \approx 5\%$$

$$\boxed{\eta_{carnot} \times \eta_{TE} \approx 0.5\%}$$

must maximize $ZT = \frac{S^2 \sigma T}{k_{th}}$

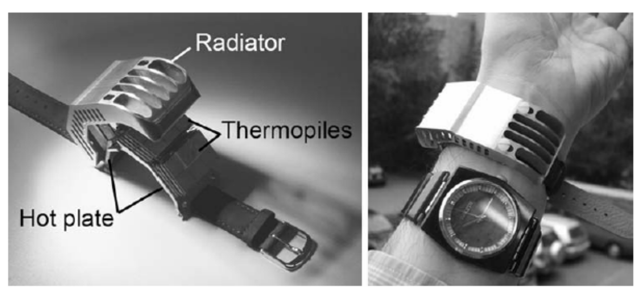
Usable Power From The Body:

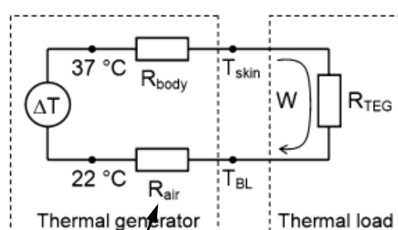


T. Starner, *IBM Systems Journal*, **35** (1996)

Optimizing Human Energy Harvesting

- Body heat powered watches, boots already demonstrated
- Maximum power harvested is ~180 μW/cm[2] between skin (34 °C) and air (22 °C)
- However, full ΔT = 12 °C is not dropped across TEG
- Key is maximizing internal TEG thermal resistance (R_{TEG}) and minimizing TEG-air thermal resistance (R_{air})
- Most also minimize TEG contact resistance (flex-TEG)





parasitics!

source: V. Leonov (2009)