3.225 Electrical,Optical, and Magnetic Properties of Materials

- Professor Eugene Fitzgerald
- Purpose: connect atoms and structure to properties
- Semi-historical context
  - What was understood first from the micro to the macro?
  - What was missing to explain other materials?

Origin of Conduction

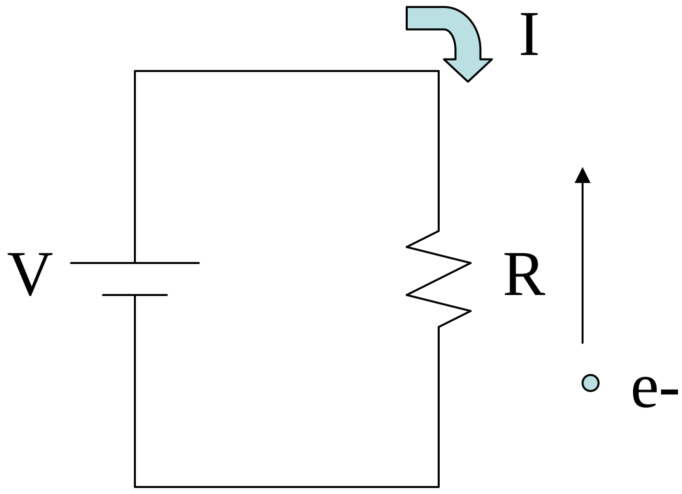
Range of Resistivity

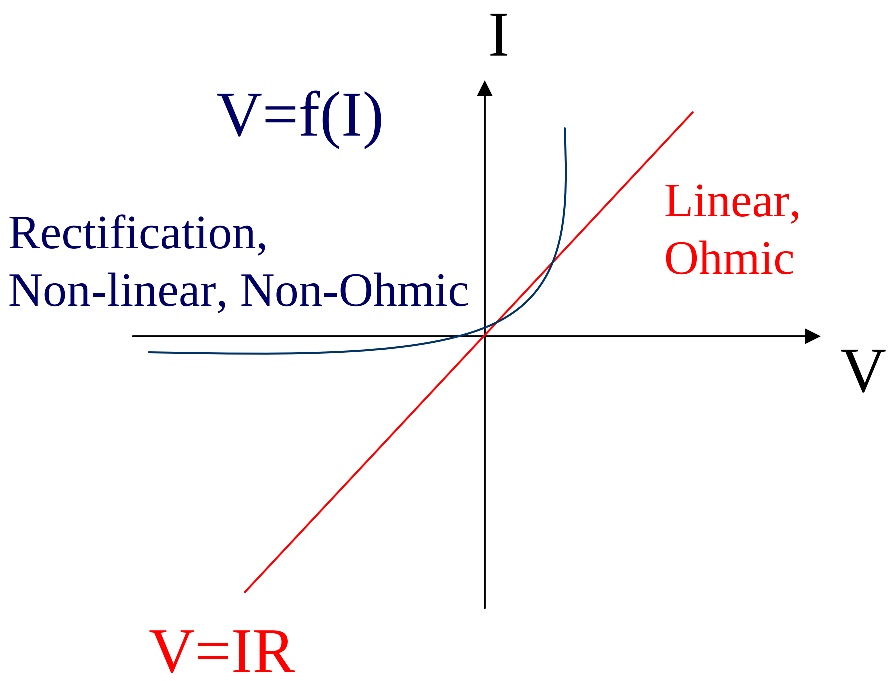
Why?

Electrical Resistivity (ohm-m)	Log		Electrical Conductivity (S/m)
	-8	8	
intercalated graphite	-7	7	copper, silver iron
	-6	6	stainless steel, metallic glass
graphite (in-plane) graphite (out of plane)	-5	5	$YBa_2Cu_3O_7$ (ab plane)
polyacetylene (doped)	-4	4	$YBa_2Cu_3O_7$ (c-axis)
	-3	3	silicon (doped)
TTF-TCNQ	-2	2	ZnO (doped) seawater
	-1	1	Fe_3O_4
	0	0	germanium
	1	-1	
	2	-2	
	3	-3	silicon
	4	-4	lnSb
	5	-5	water AgCl
polyacetylene (undoped)	6	-6	
	7	-7	
	8	-8	ZnO (undoped)
	9	-9	
	10	10	
Bakelite	11	-11	NaCl
polypyrrole	12	-12	
	13	-13	
Lucite (PMMA)	14	-14	Al_2O_3
polyvinyl chloride	15	-15	mica silica
polyethylene, teflon	16	-16	diamond

Figure by MIT OpenCourseWare.

Response of material to applied potential

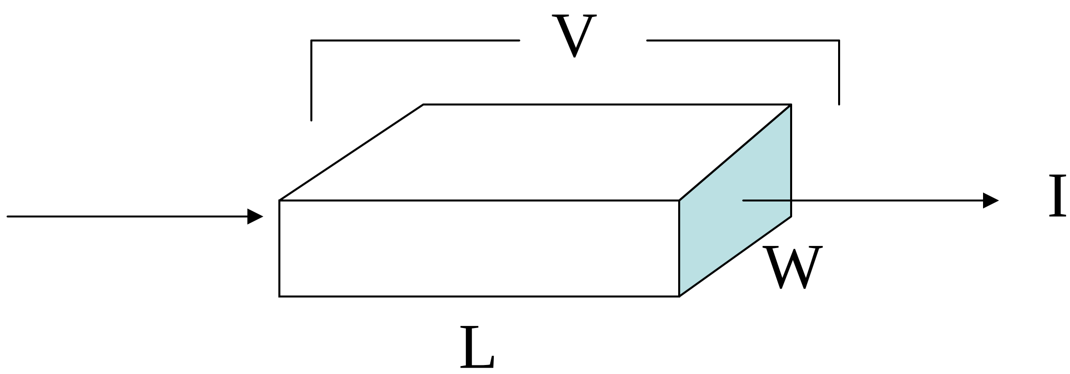




Metals show Ohmic behavior

Microscopic origin?

Remove geometry of material



V=IR=IR/L R=L/(σA)

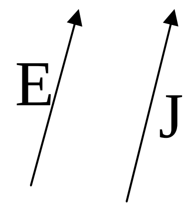
$J=\sigma E$

In general,

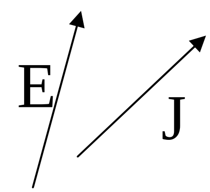
$$\vec{J} = \tilde{\sigma}\vec{E}$$

All material info

Isotropic material



Anisotropic material



In cubic material,

$$\begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

Microscopic Origin: Can we predict Conductivity of Metals?

- Drude model: Sea of electrons
  - all electrons are bound to ion atom cores except *valence* electrons
  - ignore cores
  - electron *gas*

$J=\sigma E=-nev$, by definition of flux through a cross-section

n=number of electrons per volume

v=velocity of the carriers *due to electric field*--> *drift velocity*

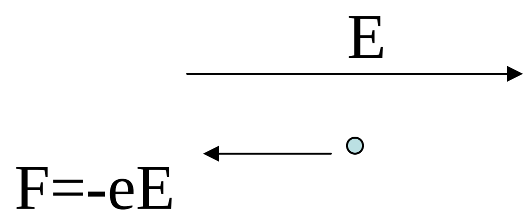
Therefore,

$\sigma=-nev/E$ and we define $v=-\mu E$

μ is mobility, since the electric field creates a force on the electron $F=-eE$

$$\boxed{\sigma = ne\mu}$$

Does this microscopic picture of metals give us Ohm's Law?



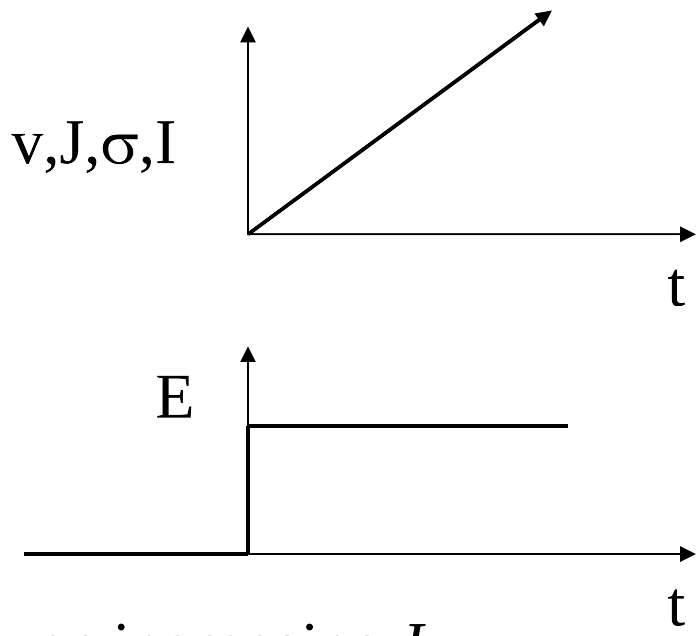
$F = ma$

$m(dv/dt) = -eE$

$v = -(eE/m)t$

$J = \sigma E = -nev = ne^2Et/m$

$\sigma = ne^2t/m$



Constant E gives ever-increasing J

No, Ohm's law can not be only from electric force on electron!

Hydrodynamic representation of e- motion

p=momentum=mv

$$\frac{dp(t)}{dt} = -\frac{p(t)}{\tau} + F_1(t) + F_2(t) + \ldots$$

Response (ma) Drag Driving Force Restoring Force...

$$\frac{dp(t)}{dt} \approx -\frac{p(t)}{\tau} - eE$$

Add a drag term, i.e. the electrons have many collisions during drift

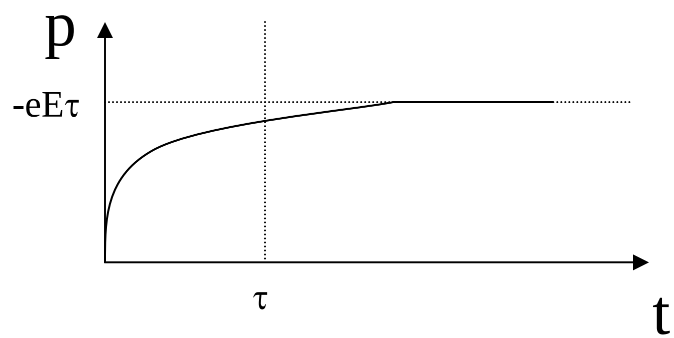
1/τ represents a ‘viscosity’ in mechanical terms

In steady state,

$$\frac{dp(t)}{dt} = 0$$

$$p(t) = p_{\infty}(1 - e^{\frac{-t}{\tau}})$$

$$p_{\infty} = -eE\tau$$



If the environment has a lot of collisions,

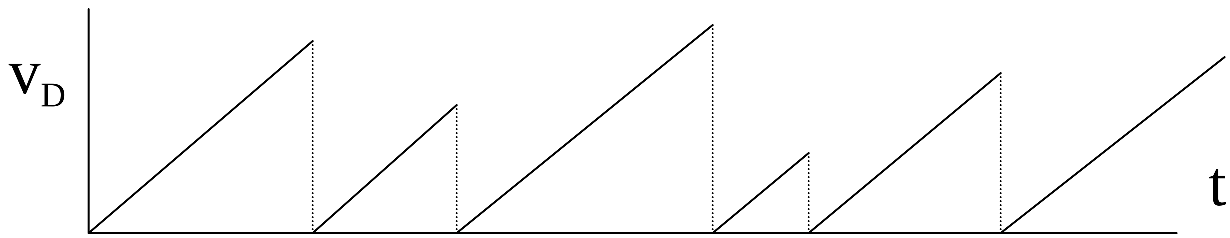
mv_{avg}=-eEτ $\quad$ v_{avg}=-eEτ/m

Now we have Ohm's law $\boxed{\sigma = \frac{ne^2\tau}{m}}$ $\boxed{\mu = \frac{e\tau}{m}}$

Mobility μ in Free-Electron Theory

Between collisions with the lattice atoms, each electron experiences a force from the electric field given by F = -eE
and therefore an acceleration given by a = F/m = -eE/m

Theory assumes that the energy picked up from the electric field by the electron between collisions is delivered to the lattice in each collision, so acceleration must start again.



If the average time between collisions is τ, the average velocity is

$$v_D = -(eE/m)\tau$$

$$\mu = -\frac{v_D}{E} = \frac{e\tau}{m}$$

Predicting conductivity using Drude

n_{theory} from the periodic table (# valence e- and the crystal structure)

$n_{theory}=A_V Z \rho_m / A$,

where AV is 6.023x10^{23} atoms/mole

ρ_m is the density

Z is the number of electrons per atom

A is the atomic weight

For metals, $n_{theory} \sim 10^{22}$ cm^{-3}

If we assume that this is correct, we can extract τ

Element	Z	n ($10^{22}/cm^3$)	r_s(Å)	r_s/a_0
Li (78 K)	1	4.70	1.72	3.25
Na (5 K)	1	2.65	2.08	3.93
K (5 K)	1	1.40	2.57	4.86
Rb (5 K)	1	1.15	2.75	5.20
Cs (5 K)	1	0.91	2.98	5.62
Cu	1	8.47	1.41	2.67
Ag	1	5.86	1.60	3.02
Au	1	5.90	1.59	3.01
Be	2	24.7	0.99	1.87
Mg	2	8.61	1.41	2.66
Ca	2	4.61	1.73	3.27
Sr	2	3.55	1.89	3.57
Ba	2	3.15	1.96	3.71
Nb	1	5.56	1.63	3.07
Fe	2	17.0	1.12	2.12
Mn (α)	2	16.5	1.13	2.14
Zn	2	13.2	1.22	2.30
Cd	2	9.27	1.37	2.59
Hg (78 K)	2	8.65	1.40	2.65
Al	3	18.1	1.10	2.07
Ga	3	15.4	1.16	2.19
In	3	11.5	1.27	2.41
Tl	3	10.5	1.31	2.48
Sn	4	14.8	1.17	2.22
Pb	4	13.2	1.22	2.30
Bi	5	14.1	1.19	2.25
Sb	5	16.5	1.13	2.14

Table by MIT OpenCourseWare.

Extracting Typical τ for Metals

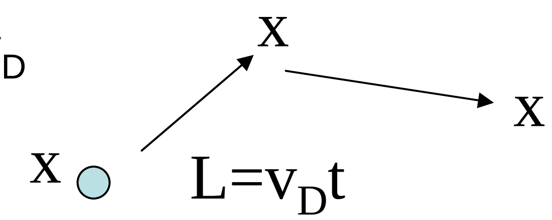
- $\tau \sim 10^{-14}$ sec for metals in Drude model

Element	77 K	273 K	373 K
Li	7.3	0.88	0.61
Na	17	3.2	
K	18	4.1	
Rb	14	2.8	
Cs	8.6	2.1	
Cu	21	2.7	1.9
Ag	20	4.0	2.8
Au	12	3.0	2.1
Be		0.51	0.27
Mg	6.7	1.1	0.74
Ca		2.2	1.5
Sr	1.4	0.44	
Ba	0.66	0.19	
Nb	2.1	0.42	0.33
Fe	3.2	0.24	0.14
Zn	2.4	0.49	0.34
Cd	2.4	0.56	
Hg	0.71		
Al	6.5	0.80	0.55
Ga	0.84	0.17	
In	1.7	0.38	0.25
Tl	0.91	0.22	0.15
Sn	1.1	0.23	0.15
Pb	0.57	0.14	0.099
Bi	0.072	0.023	0.016
Sb	0.27	0.055	0.036

Drude relaxation times in units of 10^{-14} second

Thermal Velocity

- So far we have discussed drift velocity v_D and scattering time τ related to the applied electric field
- Thermal velocity v_{th} is much greater than v_D



$$\frac{1}{2} m v_{th}^2 = \frac{3}{2} kT$$

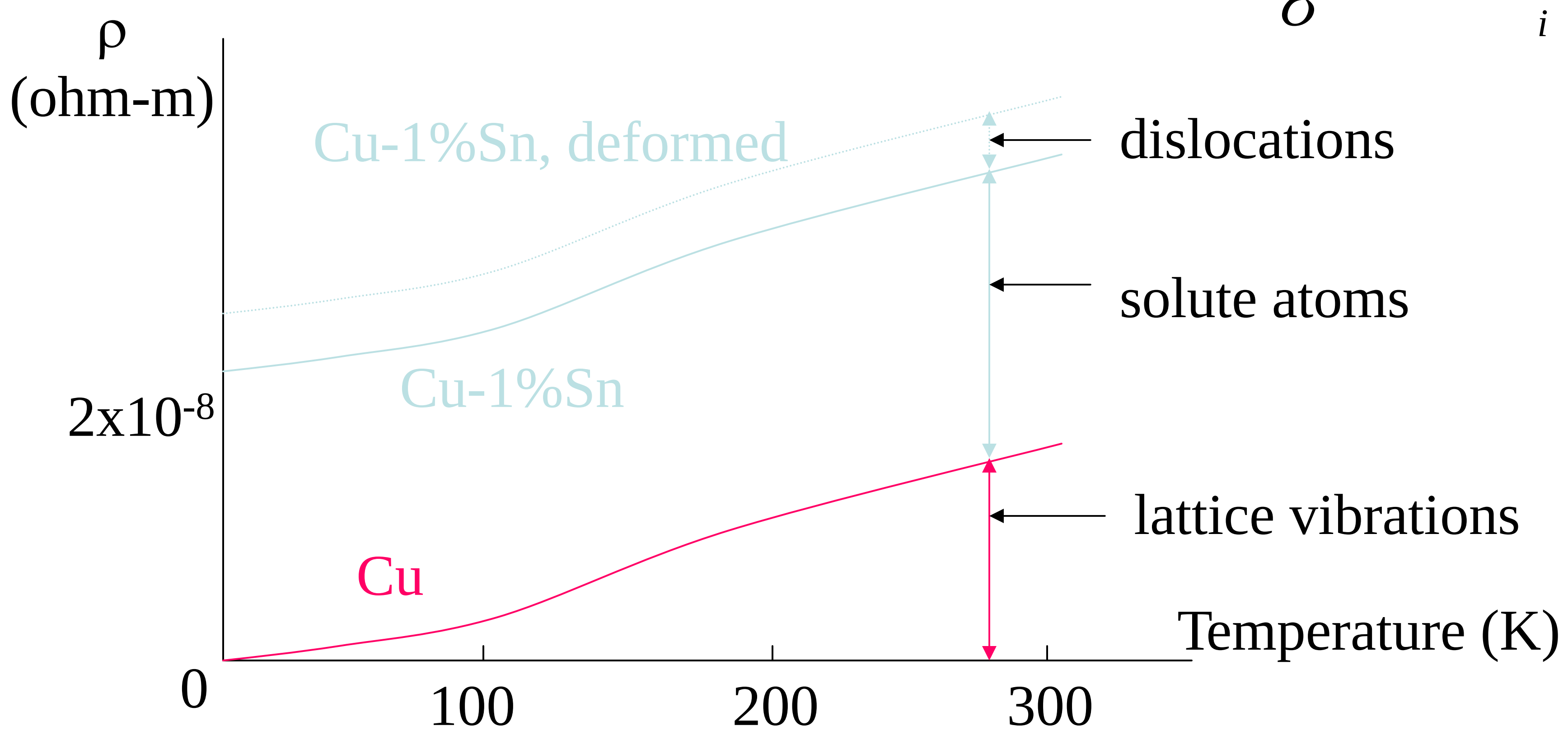
$$v_{th} = \sqrt{\frac{3kT}{m}}$$

Thermal velocity is much greater than drift velocity

Additivity of Resistivity

In metals & alloys, the various contributions to the scattering of free electrons, and therefore to resistivity, are approximately additive, i.e.,

$$\frac{1}{\sigma} = \rho \approx \sum_i \rho_i$$



Example: Conductivity Engineering

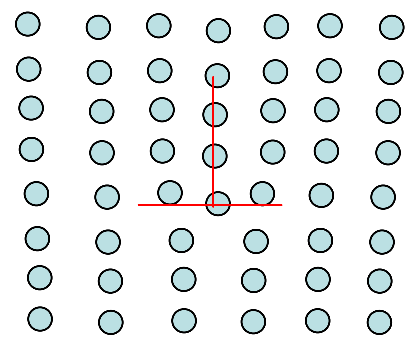
- Objective: increase strength of Cu but keep conductivity high

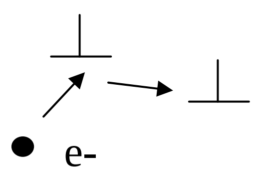
$$\sigma = \frac{ne^2\tau}{m} \qquad \mu = \frac{e\tau}{m}$$

$$\ell = v\tau$$

Scattering length connects scattering time to microstructure

Dislocation (edge)

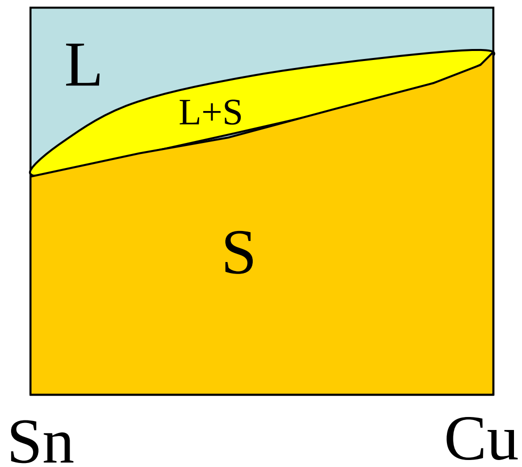


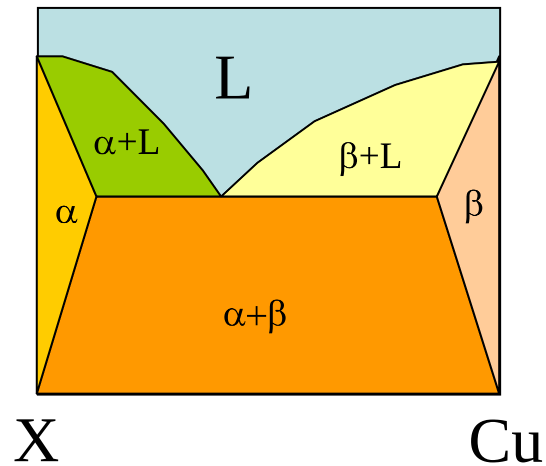


l decreases, τ decreases, σ decreases

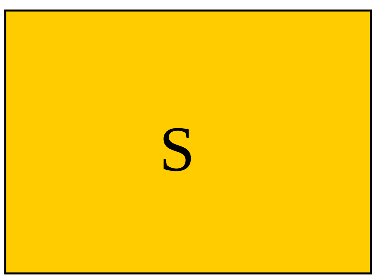
Example: Conductivity Engineering

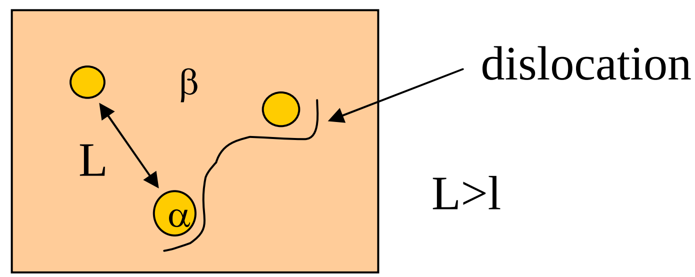
- Can increase strength with second phase particles
- As long as distance between second phase< l, conductivity marginally effected





microstructure





Material not strengthened, conductivity decreases

Dislocation motion inhibited by second phase; material strengthened; conductivity about the same

Example: Conductivity Engineering

- Scaling of Si CMOS includes conductivity engineering
- One example: as devices shrink…
  - vertical field increases
  - τ decreases due to increased scattering at SiO_2/Si interface
  - increased doping in channel need for electrostatic integrity: ionized impurity scattering
  - $\tau_{SiO2} < \tau_{impurity}$ if scaling continues 'properly'