# Transport in Metals: Review



- Transport Review
- Material strength
- ~~[illegible]~~

Recall began discussion of transport with: neutral gas, where:

$$d < \bar{r} < l_{mfp} < L.$$

Now, for metal: ($T=0$ Fermi gas)

$$\boxed{T < \hbar^2 k^2/2m \sim \frac{\hbar^2}{2m_e r_e^2}} \qquad r_e \sim \left(\frac{L^3}{N}\right)^{1/3}$$

- basic picture is quantum mechanical
  Only surface of Fermi sphere interacts
- scales:

$$\boxed{T < \frac{\hbar^2 n^{2/3}}{m_e}}$$

$\bar{r} \rightarrow r_e \quad , \quad r_e \cong \left(L^3/N\right)^{1/3}$

electron scale / particle scale

$l_{mfp} \rightarrow v_F \tau_{rlx}$.

interaction scale

$v_F \cong \frac{\hbar k_F}{m_e}$ → characteristic velocity → set by Pauli prin.

$N \cong k_F^3 L^3$

$E_F = \frac{m_e v_F^2}{2}$ → defines Fermi energy

$\tau_{rlx}$ → relaxation time $\sim \tau_{e,i}$ e.g.

i.e.

$$\boxed{r_e < v_F \tau_{rlx} < L}$$

$L \rightarrow L$ system size

- activity ⇒ at Fermi surface layer: $\delta N/N \sim \Delta k/k$

N.B. – free electron model ultimately deficient
– must address crystalline structure effects

# Strength of Materials

→ Here, review some elementary properties of material strength, failure

→ continues in spirit of transport discussion (micro ↔ macro).

→ focus on
- metals
- dielectrics

} [redacted]

[redacted] . . .

## A.) Metals

- To discuss elastic properties, need physical picture of metal structure

i.e. what is arrangement of electrons, ions in space, and how does it respond to distortion?

Clue: metals resist compression, extension

⇒ have both repulsive, attractive forces/potentials at work, microscopically.

- analogy is with lattice, in case of crystal.

- so will look for basic $\begin{bmatrix} \text{element} \\ \text{unit size} \end{bmatrix}$ with scale $R$, and $\mathcal{E}(R)$

→ Model of "Cohesion" in Metal.

i.e. what holds it together, and how?

- Fermi gas model + static ion background over-simplified. Role of ions is more fundamental.

- now, take $\boxed{\text{metal} = \text{ensemble of atomic spheres}}$

{monovalent metal i.e. 1 electron + "ion"}

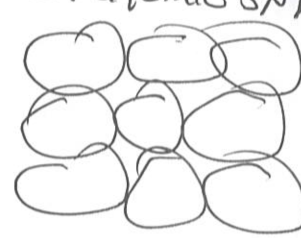
- each atomic sphere net neutral (ions + free electrons)

- $N_{atm} \frac{4\pi R^3}{3} = V$

  $N_{atm}$ → # atoms; $V$ → volume.

  $R \equiv$ atomic radius

  ⇒ metal ensemble of atomic spheres.



  defines scale $R$ of atomic sphere. {packing of spheres

- each sphere does not interact with neighbors
- monovalent metal ⟺ $R \Leftrightarrow r_s$
- so, electrostatic energy of atomic sphere due ⊕ ion, ⊖ electron cloud

i.e. $E(R) \cong -\frac{9}{10}\, e^2/R \rightarrow -\frac{9}{10R}$ (cal)

Then: for total energy

~ attraction energy
+
~ non-uniformity correction
+ cloud-cloud
~ repulsion correction (electron)
+
~ exchange term

+ ↳ just corrects Coulombic $U<0$.

K.E → $>0$, repulsive! $\sim /R^2$.

$$\boxed{E(R) = \frac{1.1}{R^2} - \frac{1.36}{R}} \quad (\text{au})$$

energy of atomic cell

$\sim \frac{\hbar^2 k^2}{2m}$ (Coulomb corrected)

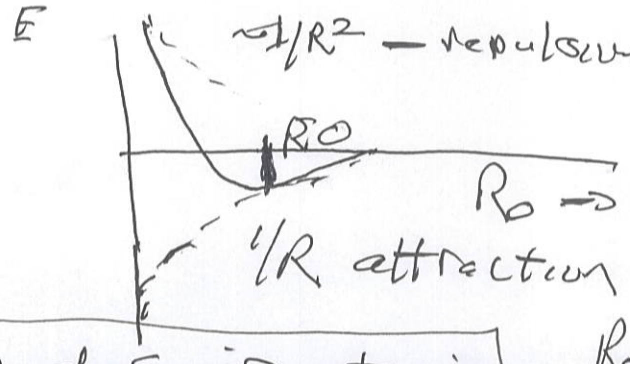
$\sim \hbar^2/2mR^2$ → kinetic repulsion

$\sim \frac{q_1}{R^2} - \frac{q_2}{R}$, $q_1, q_2 \sim O(1)$

Metal:
- ensemble of atomic cells
- each cell: coulombic attraction + Pauli repulsion.

The point:

- kinetic repulsion + coulomb attraction
  ⇒ minimum in energy!, assured
- i.e.




$R_0 \sim 1.62$ 94
$\sim .9$ Å.

$R_0$ → min. eqbm radius.

$R_0$ = eqbm radius

- but, model is deficient, quantitatively, and in variation with atomic #

- need electron repulsive core, i.e.

i.e.

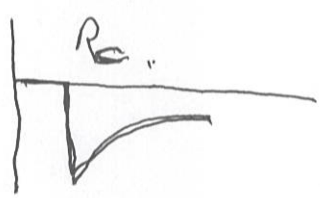
i.e. Core = nucleus + closed shell electron cloud → finite radius.

⇒ attraction of ions for electrons will create a repulsive core, a la' screening against other electrons.

so

$$\boxed{E(R) \cong \frac{1.1}{R^2} - \frac{1.36}{R} + 1.5\frac{R_c^2}{R^3}}$$ a.u. eV

i.e. from:




and re-computing contributions

typically: $R_c \sim 1 \to 2$ a.u.

still guarantees minimum in E, i.e. an $R_o$.

This brings us to strength!

i.e. have shown cell energy has

Strength $\to$ Single $\left\{\begin{matrix}\text{Cloud}\\ \text{Atom}\end{matrix}\right\}$ Energy is key!

$E(R) \to$ elastic response to stress.

i.e. $\left\{\begin{array}{l}\text{resistance compression} \Rightarrow \text{Pauli term}\\ \text{resistance expansion} \Rightarrow \text{Coulomb}\\ \text{cell response} \Leftrightarrow \text{media response}\end{array}\right.$

Define:

$$\boxed{\underbrace{\chi}_{\text{compressibility}} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T}$$

$\Rightarrow$ [change in volume with pressure.]

$$\boxed{K = 1/\chi \to \text{rigidity, or bulk modulus}}$$

$\to \sim P$, dimensionally $\to$ energy density

$c_s^2 \sim P/\rho$.

Consider atomic volume: $\underbrace{R_0}_{\text{scale}}$

Then: $V \sim (4/3)\pi R_0^3$

$$P \sim \left(\frac{1}{S_{atm}}\right)\left(-\frac{\partial E}{\partial R}\right)\Bigg|_{R_0}$$

[surface area of atom]

i.e. $F \sim P \underbrace{S_{atm}}_{\text{atomic surface area}} \sim \left(-\partial E/\partial R\right)\Big|_{R_0}$

$S_A = 4\pi R_0^2$

$$\boxed{P \cong \left(1/4\pi R_0^2\right)\left(-\frac{\partial E}{\partial R}\right)\Bigg|_{R_0}} \to \text{pressure.}$$

$$\boxed{\chi = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)}$$ compr.

$$\simeq \frac{-1}{\frac{4\pi}{3}R_0^3}\;\frac{\partial\left(\frac{4\pi}{3}R_0^3\right)}{\partial\left(1/4\pi R_0^2\left(-\frac{\partial E}{\partial R}\right)\right)}$$

$$\simeq \frac{-1}{\left(\frac{4\pi R_0^3}{3}\right)}\;\frac{\left[4\pi R_0^2\, dR\right]}{\left[\frac{1}{4\pi R_0^2}\left(-\frac{\partial^2 E}{\partial R^2}\right)_{R_0} dR\right]}$$

$$\left[\text{n.b. } \partial E/\partial R\big|_{R_{min}} \simeq 0\right]$$

$$\boxed{\chi \simeq 12\pi R_0 \Big/ \left(\partial^2 E/\partial R^2\big|_{R_0}\right)}$$ compressibility

$\Rightarrow$ Bulk modulus: $\boxed{K \simeq E''(R)\big|_{R_0} / R_0 \simeq \left\{\text{curvature of energy graph at minimum}\right\}}$

N.B. $\rightarrow$ stiff metal $\rightarrow$ $\cup$ tight well

$E''$ big

$\rightarrow$ pliable metal $\rightarrow$ $\smile$ loose well

F.O.M.: $R_0^2 \mathcal{E}'' / \mathcal{E}$

Some #'s for compressibilities:

$10^3$ a.u. ↔ $3.42 \times 10^{-12}$ $cm^2/dyne$

$10^3$ a.u.

| $\chi$ | Li | Na | K | Rb | Cs |
|---|---|---|---|---|---|
| calc. | 1.6 | 4.1 | 14.1 | 20.6 | 30.9 |
| exp | 2.5 | 4.6 | 10.2 | 15.2 | 20.5 |

a.u.

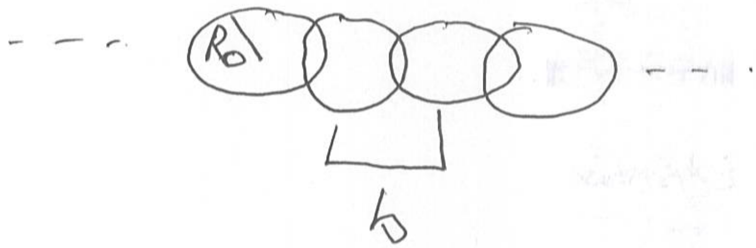
| | | | | | |
|---|---|---|---|---|---|
| $R_0$ | 3.02 | 4.16 | 5.44 | 5.95 | 6.66 |

## Material / Metal Vibrations, Extension

- Now, much like crystal, can ask two questions:
  - → what are thermal fluctuation levels in size / length of metal
    i.e. fluctns. in rod.
  - → how does metal expand with heating / contract with cooling

i.e. what is coefficient of thermal

eg, have model of:




linear chain of atomic spheres, spaced by b.

$\Rightarrow N \sim L/b$ cells., each cell $\sim R_0$.

→ Need sho approx.

$$\mathcal{E}(R) \cong \mathcal{E}(R_0) + (R-R_0)\left.\frac{\partial \mathcal{E}}{\partial R}\right|_{R_0}$$

$\mathcal{E}(R_0)$: irrel.; $\left.\frac{\partial \mathcal{E}}{\partial R}\right|_{R_0}$: 0

$$+ \frac{(R-R_0)^2}{2}\mathcal{E}''\Big|_{R_0} + \frac{(R-R_0)^3}{6}\mathcal{E}'''\Big|_{R_0}$$

$$\cong \alpha\,\rho^2 - \beta\,\rho^3$$

$\beta$: anharmonic term.

$\alpha = 1/2\,\mathcal{E}''\big|_{R_0}$ → ~ spring const.

$\beta = -1/6\,\mathcal{E}'''\big|_{R_0}$.

so

a.) for thermal fluctuation level of length,

$k_B T \sim \cancel{1/2}\,\alpha\,(\delta R)^2$

$(\delta R)_{RMS} \sim (k_B T/\alpha)^{1/2}$.

so

$\frac{\delta L}{L} \sim \frac{\delta R}{b}$

$\boxed{\delta L \sim (L/b)\,\delta R.}$

b.) for coefficient of thermal expansion

$\langle \delta R \rangle = \langle \rho \rangle = \int d\rho\; \rho\, \exp[-\mathcal{E}/T]$

and have familiar problem with parity

$$\langle \rho \rangle \cong \frac{\int d\rho\, \rho \left[ \exp\left(-\frac{(\alpha\rho^2 - \beta\rho^3)}{k_B T}\right)\right]}{\int d\rho \left[\exp\left(-\frac{\alpha\rho^2}{k_B T}\right)\right]}$$

for higher $T$.

$$\cong \frac{\int d\rho\, \rho \left(\cancel{1} + \frac{\beta\rho^3}{k_B T}\right) \exp\left(-\frac{\alpha\rho^2}{k_B T}\right)}{\int d\rho \left[\exp\left(-\alpha\rho^2/k_B T\right)\right]}$$

$$\cong \beta\alpha^{-3/2}T^{3/2} \Big/ \alpha^{-1/2}T^{1/2}$$

so

$$\boxed{\langle \rho \rangle \cong \beta T/\alpha^2}$$

and
$$\boxed{\frac{\Delta L}{L} \sim \frac{(\partial\langle\rho\rangle/\partial T)}{b} \Delta T}$$

coeff of anharmonicity

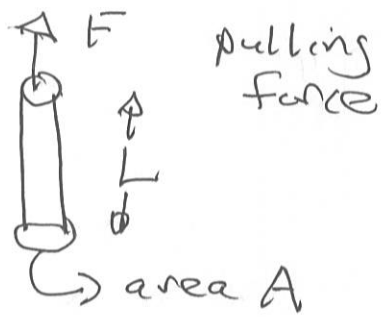
$\Delta L$ ...

$$\frac{\Delta L}{L} \sim \left(\beta / b\alpha^2\right) \Delta T$$

↳ coeff thermal expansion.

## Elastic Properties – General

(c.f. D. Tabor
"Gases, Liquids, Solids and other states of matter")




$\sigma = F/A$ ∞ Hooke's Law:

tensile stress

$$\sigma \sim \underset{\text{Young's modulus}}{E}\ \underbrace{\Delta L/L}_{\text{strain}}$$

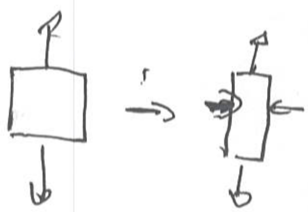
i.e.

$$\boxed{(F/A) \sim E\,(\Delta L/L) \qquad E \equiv \text{Young's Modulus (tensile)}}$$

as before, have:

$K = P/-\Delta V = (1\ \partial V)^{-1}$ → Bulk also:

$n = \frac{\tau}{\theta} \equiv$ rigidity modulus (stress/strain ratio for shearing)

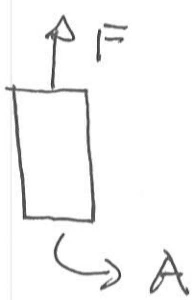


$\nu = \frac{\varepsilon_T}{\varepsilon_L} = \frac{\text{contractile strain}}{\text{linear strain}}$

$\nu$: poisson ratio

(ratio of thinning to extension)

Elastic Bar Fletnr (again) → General




$\sigma \sim F/A$

strain $\varepsilon$

$\therefore \quad F = EA\varepsilon$

so incremental extension $\Rightarrow d\varepsilon$

$$F L d\varepsilon = EA\varepsilon L d\varepsilon = EAL\,\varepsilon d\varepsilon$$

so, stretching to some final state

i.e. $\int dW = \underset{\substack{\downarrow \\ \text{work done}}}{W} = \int_0^{\varepsilon_0} F L \, d\varepsilon$

so

$$\boxed{W = \tfrac{1}{2} E A L \varepsilon_0^2}$$

so, for thermal flctns.

$$W \sim K_b T \quad \Rightarrow \langle \varepsilon_0^2 \rangle \sim K_b T / EAL.$$

$$\Rightarrow \boxed{\langle \delta L^2 \rangle \sim L^2 \frac{K_b T}{EAL} \sim \frac{K_b T L}{EA.}}$$

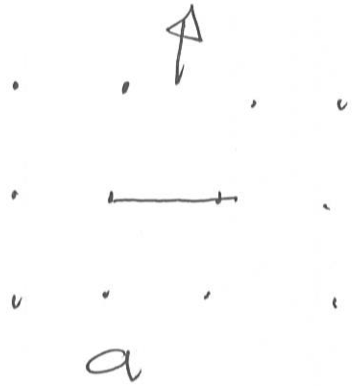
and: $\left\{ \begin{array}{l} A \sim 100\,mm^2 \qquad T \sim 300K \\ L \sim 1m \\ E \sim 10^{11}\,Nm^{-2} \text{ (brass)} \\ \\ \langle \delta L^2 \rangle \sim 10^{-28}\,m^2 \end{array} \right.$

Now, can generalize idea from metals

i.e. $\boxed{\text{Young's Modulus} - \text{Interatomic spring const.}}$

⇒ Consider generic lattice:

{ seek wave speed, etc.



$$\sigma = E\,\varepsilon$$

$$\underbrace{\frac{F}{a^2}}_{\text{face area}} = \underbrace{E}_{\text{Young's modulus}}\frac{x}{a}$$

but $F = -kx$, to fit ~~Hooke's~~ Hooke's Law, and from fit to potential.

$$\Rightarrow \boxed{\frac{k}{a} = E}$$

Generically, $E \sim$ (micro) spring const / (micro) scale.

Now, consider again the bar, ... at lattice level

$$m\ddot{x} + kx = 0 \qquad m \equiv \text{atomic mass}$$

$$\omega^2 = k/m = aE/m$$

$$= \frac{1}{a^2}\frac{a^3 E}{m} \qquad \rho \equiv m/a^3$$

$$\boxed{\omega^2 = \frac{1}{a^2}(E/\rho)}$$

$\Rightarrow$ speed of wave, i.e. (acoustic).

$$C_s^2 = E/\rho.$$

[recall lattice discussion].

N.B.: Can generally explain most solid elastic properties with:

h.o. = fit to attractive + repulsive (forces potential)

see Tabor, for detailed cases.