

2.57 Nano-to-Macro Transport Processes

Fall 2004

Lecture 1

1. Overview for nano sciences
 - 1.1 Length scale
 - 1.2 Examples in microtechnology
 - 1.3 Examples in nanotechnology
 - 1.4 Nano for energy (phonon, phonon, electron; wavelength, mean free path)
 - 1.5 Nanoscale heat transfer in devices (e.g., CMOS)
 - 1.6 Nano and microfabrication
 - 1.7 Transport regimes
 - 1.8 Overview of the book chapters and chapters to be covered

2. Classical Laws related to transport
 - 2.1 Heat transfer
 - 2.1.1 Conduction

Fourier's law:

$$q = -k \nabla T \text{ or } q = -k \frac{dT}{dx} \text{ in one dimension}$$

where:

q [W/m²] is heat flux,
 k [W/m-K] is thermal conductivity.

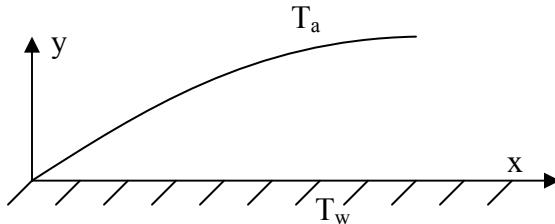
2.1.2 Convection

Newton's law of cooling:

$$q = h(T_w - T_a)$$

where:

h [W/m²K] is heat transfer coefficient.



Nonslip boundary condition is assumed at the wall, i.e.,

$$u_x(y=0) = u_y(y=0) = 0, \quad T(y=0) = T_w.$$

Note: this assumption is NOT accurate for small scales.

2.1.3 Radiation

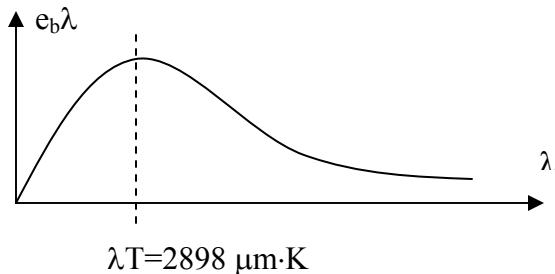
Planck's law:

$$e_{b,\lambda} = \frac{c_1}{\lambda^5 (e^{c_2/\lambda T} - 1)}$$

where:

c_1 and c_2 are constants,
 λ is wavelength, and the subscript b denotes black body.

The curve for block-body radiation is drawn as following:



Integrating the Planck's law leads to the Stefan-Boltzmann law:

$$e_b = \sigma T^4$$

where:

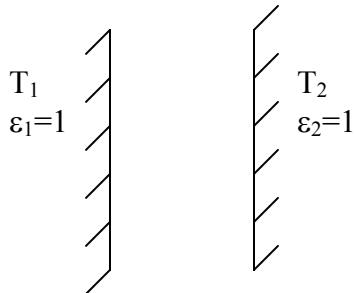
$$\sigma = 5.67 \times 10^{-8} \text{ W/m}^2 \text{ K}^4$$

For real surface, we define "emissivity" as

$$\varepsilon = \frac{e}{e_b}$$

For the two planar walls shown below, the heat flux of radiation is evaluated as

$$q = \sigma(T_1^4 - T_2^4)$$



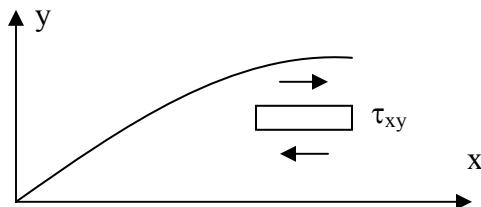
2.2 Newton shear stress law

The shear stress for the sketched one-dimensional flow is:

$$\tau_{xy} = \mu \frac{\partial u}{\partial y}$$

where:

μ [N-s/m²] is dynamic viscosity.



2.3 Fick's diffusion law

$$j_i = -\rho D \frac{dm_i}{dx}$$

where:

D [m^2/s] is mass diffusivity,
 m_i is the mass fraction for the i th species.

2.4 Ohm's law

$$R = \frac{V}{I}$$

or

$$J = \sigma \epsilon = \sigma \left(-\frac{1}{e} \frac{d\Phi}{dx} \right) = -\sigma \frac{d\varphi_e}{dx}$$

where:

J [A/m^2] is electric current density,
 σ [$\Omega^{-1}\text{m}^{-1}$] is electrical conductivity,
 ϵ [V/m] is electric field,
 Φ is potential energy,
 φ is electrostatic potential.

2.5 Questions

- a) What are the similarities among above equations?
- b) Are these laws still valid at nanoscale?

2.6 Note:

All above are constitutive equations with two unknown variables.

Another equation (e.g. mass, momentum conservation) is needed to solve problems.

3. Scaling trend

For a sphere, the volume-to-surface ratio is

$$\frac{V}{S} = \frac{4\pi r^3 / 3}{4\pi r^2} = \frac{r}{3}.$$

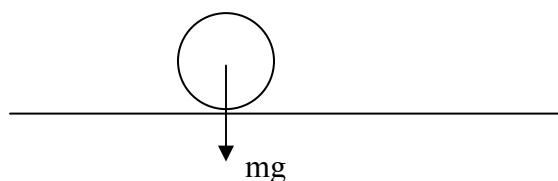
The volumetric effect decreases with the reducing length scale. Surface effect becomes dominant at smaller scales.

For a spherical fluid drop, we have

$$\gamma = \frac{\text{Gravitational force}}{\text{Surface force}} = \frac{\rho g (4\pi r^3 / 3)}{\sigma (2\pi r)} = \frac{2\rho gr^2}{3\sigma}.$$

Substituting $\rho = 10^3 \text{ kg/m}^3$, $\sigma = 78 \text{ mN/m}$ into this equation, we get

$$r = 1 \text{ m}, \gamma = 8.4 \times 10^4; r = 1 \text{ mm}, \gamma = 8.4 \times 10^{-2}.$$

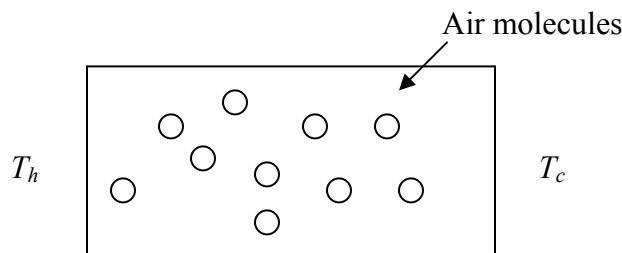


4. Microscopic pictures of energy carriers

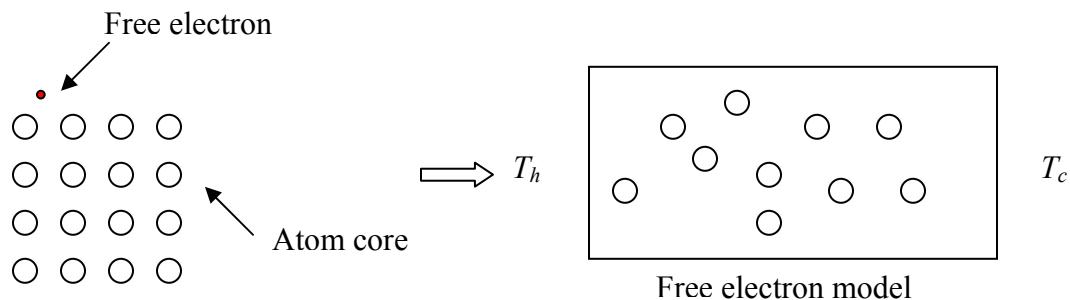
4.1 Heat

4.1.1 Heat conduction

Gases: hotter air molecules (with larger kinetic energy) randomly pass their excess energy to cooler molecules. Heat is transported to the cold side by such a process. Note the average velocity of a molecule can be as large as 500 m/s.



Dielectric solids: heat is conducted through the vibration of atoms. The atom cores are spaced by 2-5 Å in the lattice. Under the free electron approximation, the electrons are viewed as free electron gas.

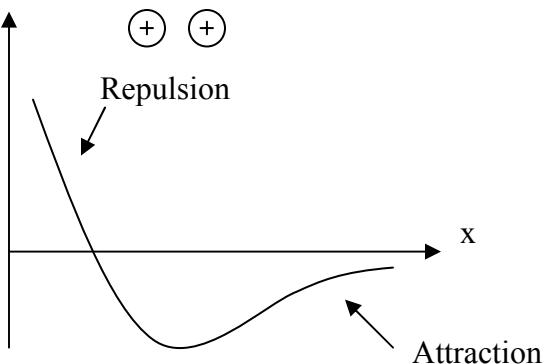


Consider two atoms with a parabolic interatomic potential. The interatomic force is

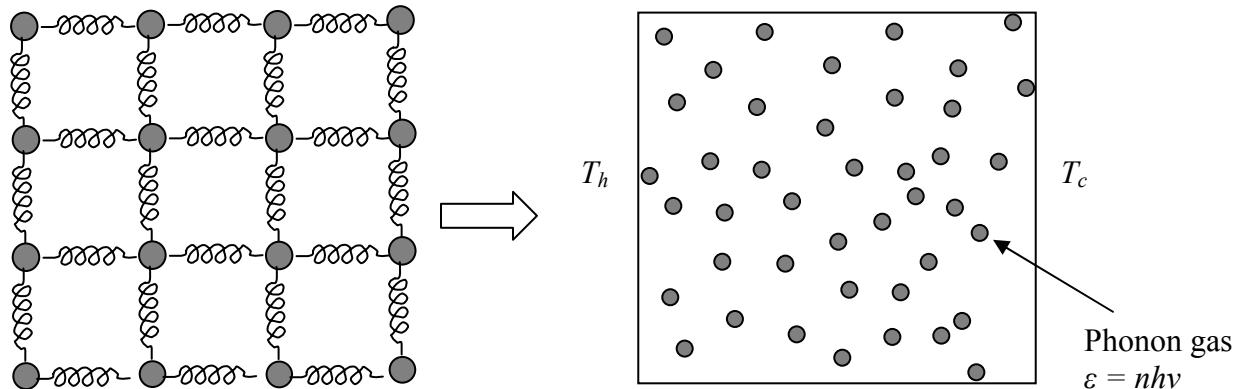
$$F = -\nabla\Phi \approx K\Delta x$$

where Δx is the displacement from the minimum potential position (equilibrium position), K is constant.

Interatomic potential Φ



A simplified picture of the interatomic interactions in crystals can be represented by the mass-spring system. The propagation of sound in a solid is due to long wavelength lattice waves. Quantum mechanics states that the energy of each lattice wave is discrete and must be multiples of $h\nu$. Based on argument we will discuss in chapter 5, the spring system can be further simplified as a box of phonon particles.



Now, molecules, electrons, and phonons are all gases in a box. You can see similarities and why I said we can describe them in parallel.