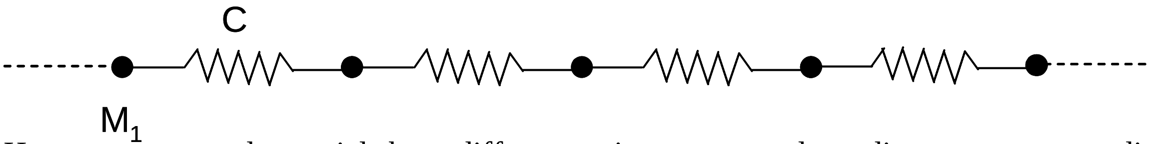
MATS 251A / MAE 265A: Electronic & Photonic properties of Materials

HOMEWORK 4

(Due Tuesday, November 21, 2007)

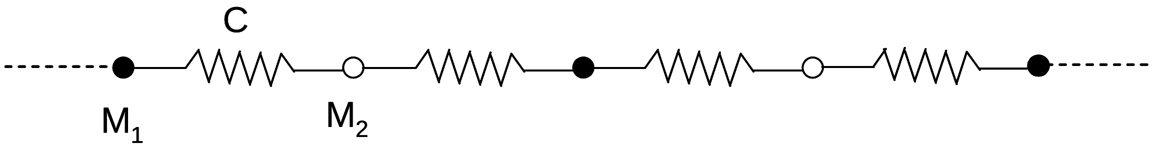
1. In class, we derived the dispersion relationship (ω *vs.* k) for phonons using the following model (equal masses $\mathbf{M_1}$ and same spring constants **C**):



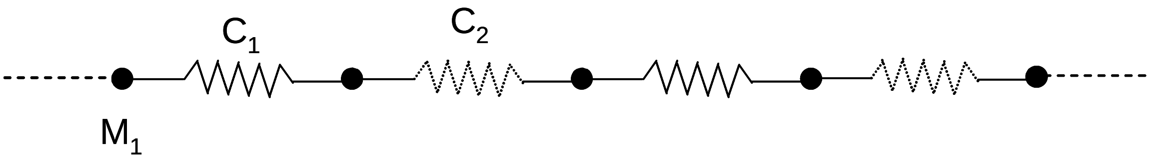
However, most real materials have different spring constants depending on atom-atom distances and for compound semiconductors, different masses (*e.g.,* GaAs)

Sketch qualitatively, with important points labeled, the dispersion relationships in the following cases:

(a) Unequal masses ($\mathbf{M_1 \neq M_2}$), but same spring constant (**C**)



(b) Same mass ($\mathbf{M_1}$), but different spring constant ($\mathbf{C_1}$ and $\mathbf{C_2}$)



(c) Same mass ($\mathbf{M_1}$), and different spring constants as in (b), where $\mathbf{C_1 >> C_2}$
This is the case for molecular crystals, *e.g.* C_{60} (buckminsterfullerene), solid O_2 etc. Why?

2. **Phonon engineering for reduced thermal conductivity**

Read the following paper: "Phonon Engineering in nanostructures for solid-state energy conversion", by G. Chen, T.Zeng, T. Borcia-Tasciuc and D.Song, Materials Science and Engineering A, vol. 292, p, 155-161, (2000) and answer the following questions:

(a) What is the lowest thermal conductivity (**k**) that can be obtained in materials? At approximately what length scales, in the specific case of Si, do size effects contribute to the thermal conductivity?

(b) What is a superlattice? Why is the **k** of superlattices lower than in the bulk? Explain the mechanisms of reduction with specific reference to (i) mini-Brillouin zones and (ii) Umklapp scattering.

The qualitative discussion in the paper" Thermal conductivity of superlattices", S.Y. Ren and J.D. Dow, Physical review B, vol. 25 (6), p. 3750-3755, (1982) could be useful.

(c) Suggest one possible application each of reduced and enhanced thermal conductivity.

3. Optical phonons limit the maximum electric fields that can be applied in semiconductors

Consider a semiconductor with an effective mass of $m^* = 0.26\ m_e$. The optical phonon energy is 50 meV. The carrier scattering relaxation time is 0.1 ps at 300 K. Calculate the electric field at which the electron can induce/emit optical phonons. (Beyond this limiting electric field, the device resistance is dramatically increased)

4. Basic semiconductor calculations

A semiconductor with a band gap energy (E_g) of 1 eV, with equal hole and electron effective masses, is p-doped with an acceptor concentration of $10^{18}/\mathrm{cm}^3$. The acceptor energy level is located 0.2 eV above the valence band edge.

(a) Show that intrinsic conduction in this material is negligible at 300K.

(b) Calculate the conductivity (σ) of the material at room temperature (~ 300K), given a hole mobility at 300K of $100\mathrm{cm}^2/\mathrm{Vs}$.

(c) Plot the logarithm of the hole concentration, *ln p*, vs. reciprocal temperature (1/T) for the temperature range 10 K-1000K. (*Make sure that the slopes in the different temperature ranges are correct*)

(d) If the effective mass of the electrons at the lower conduction band edge is three times higher than that of the holes at the valence band edge, how far is the Fermi energy (E_F) from the middle of the forbidden band?

(e) Prove that, in practice, the semiconductor GaAs can never be fabricated to be intrinsic at room temperature (~ 300 K) *i.e.,* it is always p-/n-type. Assume the following: $m^*_{hh} = 0.45\ m_e$, $m^*_{lh} = 0.082\ m_e$, $m^*_e = 0.067\ m_e$, where hh: heavy hole mass, lh: light hole mass, and m_e is the electron mass $\sim 10^{-30}$ kg. The bandgap is ~.142 eV)