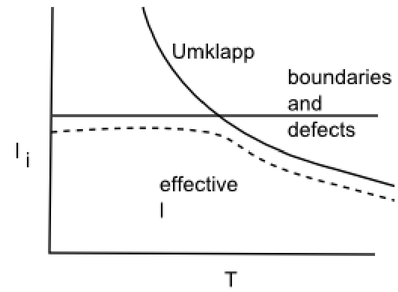
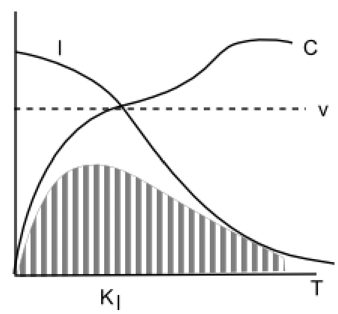
Topic 6-5: Thermal Conductivity and Temperature Dependence

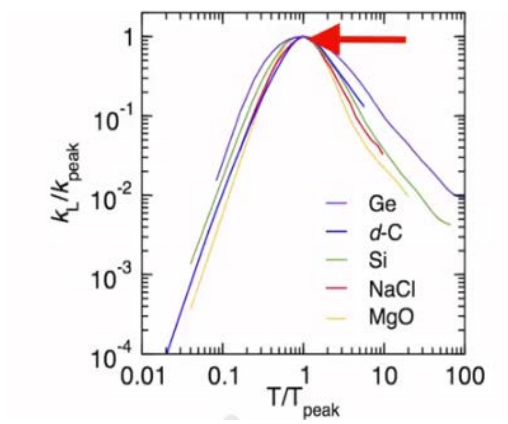
Summary: We begin by exploring the temperature dependence of the three factors in thermal conductivity: heat capacity, group velocity and mean free path. We then combine these to ascertain the temperature dependence of thermal conductivity. Finally, we explore the temperature dependence of the thermal conductivities of different varieties of silicon.

- $\kappa_L = \frac{1}{3} Cvl$
    - C is heat capacity
    - v is the group velocity of the phonons
    - l is the mean free path between collisions
- **Heat capacity:** Already explored temperature dependence of C
    - Constant $3k_bT$ at high temperature and decays to 0 at low temperature
- **Group velocity:** Bonds are approximately harmonic
    - No temperature dependence
    - Change in temperature changes amplitude but not spring constant or mass
    - Assume group velocity is independent of temperature
    - If group velocity changes with temperature we say the lattice stiffens or softens with temperature
- **Mean free path**: phonons limited by boundaries, defects and Umklapp scattering
    - Get net mean free path by $\frac{1}{l} = \sum_i \frac{1}{l_i}$ where each i is a different scattering mechanism
    - Umklapp scattering is dominant effect at high temperatures ($l \propto \frac{1}{T}$)
    - At low temperatures the phonon population is low but boundaries and defects still exist
        - Mean free path is roughly constant with T at low T



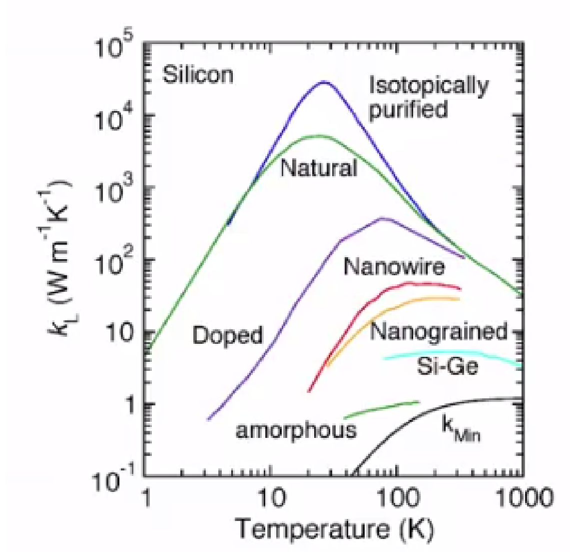
- Bringing it all together: mean free path l decays w/ T, heat capacity rises and flattens, and group velocity is relatively constant:





- Each material has a peak in thermal conductivity
  - Axis is normalized to peak temperature and thermal conductivity to facilitate comparison
- What we have done thus far is a good approximation of reality!

Thermal conductivity of silicon



- Natural silicon
  - Cold side: T^3 dependence from heat capacity
  - Hot side: heat capacity constant, mean free path decays from Umklapp scattering so 1/T dependence
- Isotopically purified: removing isotopes lessens impurities and therefore less defects which increases mean free path and in turn increases thermal conductivity
  - As temperature increases, Umklapp scattering takes over and the purified silicon curve joins the natural silicon curve
  - Purified and natural silicon are similar at low temperatures because impurities don't affect *long wavelengths found at low T.* Recall at low T, the Planck distribution has only activated low frequency, long wavelength modes.
  - Impurities don't start acting like scattering sources until about 50 Kelvin
- Doped Si: adding impurities leads to a decrease in mean free path and therefore a decrease in thermal conductivity
- Si-Ge alloy: similar to doped Si with more impurities
- Nanowires: very close boundaries which increases boundary scattering
- Nanograins: same as nanowires except boundaries are between grains instead of a surface and the atmosphere

- Amorphous silicon: now completely non-crystalline, description of phonons falls apart and we have a very low thermal conductivity

Questions to Ponder

1. There is a minimum κ at the bottom of the graph on the previous page. What is this? If you were to develop an expression for minimum κ what would you put in it?