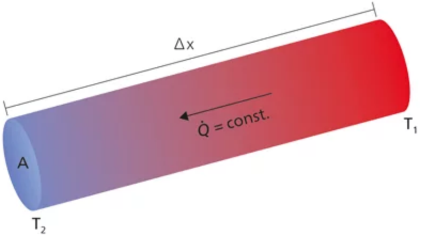
Lattice Thermal conductivity

analysis at “low” and “high” temperatures

July 1, 2021

Thermal Conductivity

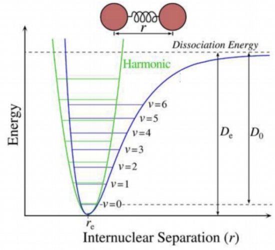
- Let's imagine to take a crystal and to apply a temperature gradient, for example heating one side of the crystal
- In this way the thermal energy propagates through a solid, it is carried by lattice waves or phonons.
- This create a flux of thermal energy through the crystal:
$$j_x = -K \frac{d}{dx} T$$
The coefficient K is called Thermal Conductivity



Thermal Conductivity

- A purely harmonic potential does not provide a coupling between phonons allowing them to travel trough the whole crystal without interaction, hence causing the conductivity to be infinite.
- Thermal resistance has its origins in anharmonic terms of the lattice energy.
- Hence the waves that carry the thermal energy scatter, this gives $K \neq \infty$:
$$K = \frac{1}{3} C_v v \Lambda$$
where v is the wave velocity and Λ is the mean free path of scattering

Armonic vs anarmonic potential



- For at harmonic energy $E(x) = cx^2$ we have
$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x e^{-cx^2/k_B T}}{\int_{-\infty}^{\infty} e^{-cx^2/k_B T}} = 0$$
In such a case we would have no expansion when temperature is changed, and thus we must consider an anharmonic oscillator.

Mean Free Path Λ

There are some mechanism that affect the mean free path in a solid:

- Interaction with impurities, defect, and/or isotopes
- Collision with sample boundaries (surfaces)
- Collision with other phonons

The first two mechanism come from deviation from translation symmetry, instead the last one is a deviation from the harmonic behaviour.

Temperature dependence of the thermal conductivity

- K depends on C_v and Λ that depend on the temperature. We can neglect the temperature dependence of sound velocity
- The C_v behaviour is: $\begin{cases} LowT & \propto T^3 \\ HighT & 3R \end{cases}$
- The Λ behaviour is $\propto \frac{1}{n_{ph}} = e^{\frac{\hbar\omega}{kT}} - 1$: $\begin{cases} LowT & \infty \\ HighT & \frac{\hbar\omega}{kT} \end{cases}$

Where n_{ph} indicates the phonon occupancy, whose frequency ranges from 0 to the debye frequency. However, already intuitively, we may anticipate that low energy phonons, i.e. those in the vicinity of the center of the 1st BZ may have quite different impacts comparing with those having bigger k-numbers close to the edges of the 1st BZ. Moreover, in real word the mean free path is upper bounded from the debey frequency ω_D, hence we put as constant $\Lambda(\omega_D) = D$

Temperature dependence of the thermal conductivity

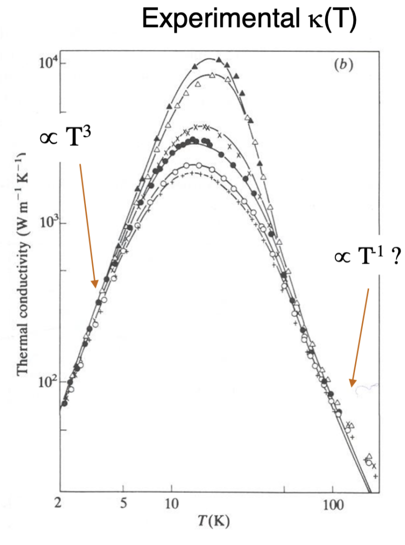


Figure 1: Caption

- Good data agreement in low temperature regime
- Problems in high temperatures description

Disagreement in high temperatures

- The disagreement is because when estimating Λ we have accounted for all excited phonons, while a more correct approximation would be to consider "high" energetic phonons only.
- For high energetic phonons it is meant those phonons that lie in the vicinity of the BZ edges.
- The low energy phonons do not participate relevantly in the energy transfer.
- In first approximation we can use the Boltzmann statistics to determine the probability to have a significant mode ($E = e^{\frac{\hbar\omega}{kT}} > E_{\frac{1}{2}}$)

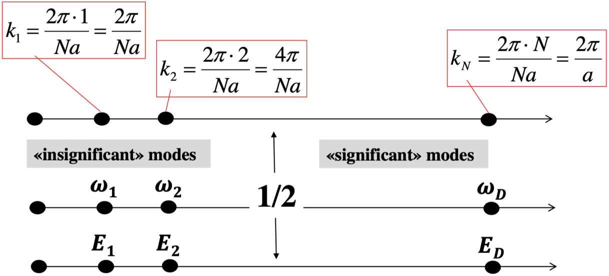


Figure 2: Caption

Temperature dependence of thermal conductivity

- To sum up if we have a space-limited sample, the thermal conductivity has the following behaviour: $\begin{cases} Low T & \propto T^3 \\ High T & \propto e^{\frac{\hbar\omega}{kT}} \end{cases}$

	C_V	Λ	κ
low T	$\propto T^3$	$n_{ph} \rightarrow 0$, so $\Lambda \rightarrow \infty$, but then $\Lambda \rightarrow D$ (size)	$\propto T^3$
high T	3R	$\propto \exp(\theta_D/2T)$	$\propto \exp(\theta_D/2T)$

Phonon collision N process

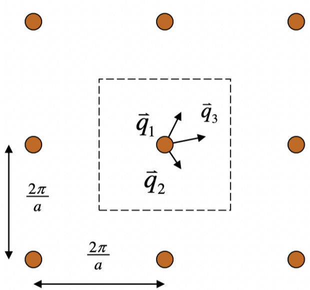


Figure 3: Caption

- The N-process is when two phonons collide and the new k-vector is still inside the first Brillouin zone.
- N-process does not create any resistance to heat flow, and this process is predominant at low temperature where phonons have lower momentum rather than at high temperatures
- $q_1 + q_2 = q_3$ and q_3 is still inside the 1st brillouin zone and they continue to carry the energy in the same direction

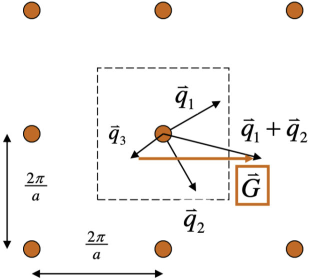
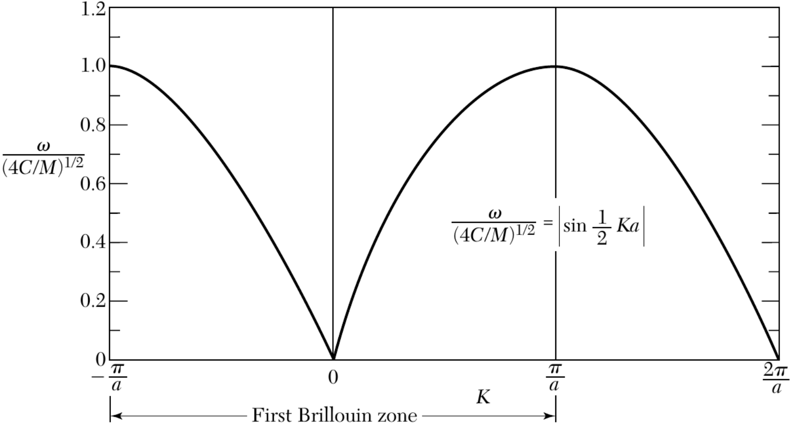


Figure 4: Caption

- Two phonons combine to give a net phonon with an opposite momentum! This causes resistance to heat flow.
- $q_1 + q_2 = q_3 + G$, where G is a reciprocal lattice vector. Hence, we can flip over the vector $q_1 + q_2$, subtracting G a reciprocal lattice vector, to get back into the Brillouin zone
- If the two initial wavevectors add to a new wavevector which is outside the Brillouin zone, they give a new wave with a group velocity in the opposite direction.

U-Process



1.2
1.0
0.8
0.6
0.4
0.2
0
$\frac{\omega}{(4C/M)^{1/2}}$
$\frac{\omega}{(4C/M)^{1/2}} = \left|\sin \frac{1}{2} Ka\right|$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
K
First Brillouin zone