# Lattice thermal conductivity

The transport of heat in a solid is phenomenologically described by the following equation

$$\dot{\mathbf{Q}} = -\lambda_l \, \mathrm{grad}\, T \quad , \qquad (6.13)$$

which relates the steady-state heat flux and a temperature gradient through the lattice thermal conductivity coefficient $\lambda_l$ .

The temperature gradient can occur only if the thermal conductivity is not infinitely high.

**We assume that the gas of phonons makes the main contribution to thermal conductivity.** Using an analogy with the kinetic theory of gases we can write

$$\lambda_l = \frac{1}{3} C_V v_s \Lambda_{ph} \ , \qquad (6.14)$$

where $v_s$ is the average phonon velocity and $\Lambda_{ph}$ is the phonon mean free path.

Equation (6.14) is often written as

$$\lambda_l = \tfrac{1}{3} C_V v_s^2 \tau \ , \qquad (6.15)$$

where $\tau^{-1}$ is the phonon scattering rate.

# Derivation of thermal conductivity of an ideal gas

The thermal conductivity coefficient $K$ **is the coefficient between heat flux and temperature gradient:**

$$j_U = -K \frac{dT}{dx}$$

If $c$ is the heat capacity of a particle, then in moving from a region at local temperature $T + \Delta T$ to a region at local temperature $T$ a particle will give up energy $c\,\Delta T$. Now $\Delta T$ between the ends of a free path of the particle is

$$\Delta T = \frac{dT}{dx}\ell_x = \frac{dT}{dx}v_x\tau \;,$$

where $\tau$ is the average time between collisions.

The net flux of energy

$$j_U = -n\langle v_x^2\rangle c\tau \frac{dT}{dx} = -\tfrac{1}{3}n\langle v^2\rangle\, c\tau \frac{dT}{dx}$$

for phonons, $v$ is constant,

$$j_U = -\tfrac{1}{3}Cv\ell \frac{dT}{dx}$$

**where** $\ell \equiv v\tau$ and $C \equiv nc$. Thus

$$K = \tfrac{1}{3}Cv\ell$$

## Umklapp processes

The cubic term in (6.2) is the first anharmonic term and is often assumed to be the most significant.

The physics of the phonon interaction can be described as follows. A phonon of wave vector $\mathbf{k}$ causes an elastic strain that modulates, due to the anharmonic interaction, the acoustic impedance of a crystal. Another phonon of wave vector $\mathbf{k}'$ is reflected from this acoustic-impedance modulation, as if from a moving diffraction grating, creating a third phonon of wave vector

$$\mathbf{k}'' = \mathbf{k} + \mathbf{k}' \ . \tag{6.10}$$

Conservation of energy requires that

$$\omega'' = \omega + \omega' \ . \tag{6.11}$$

Since in a periodic lattice a wave vector lies inside the first Brillouin zone, (6.10) is interpreted as

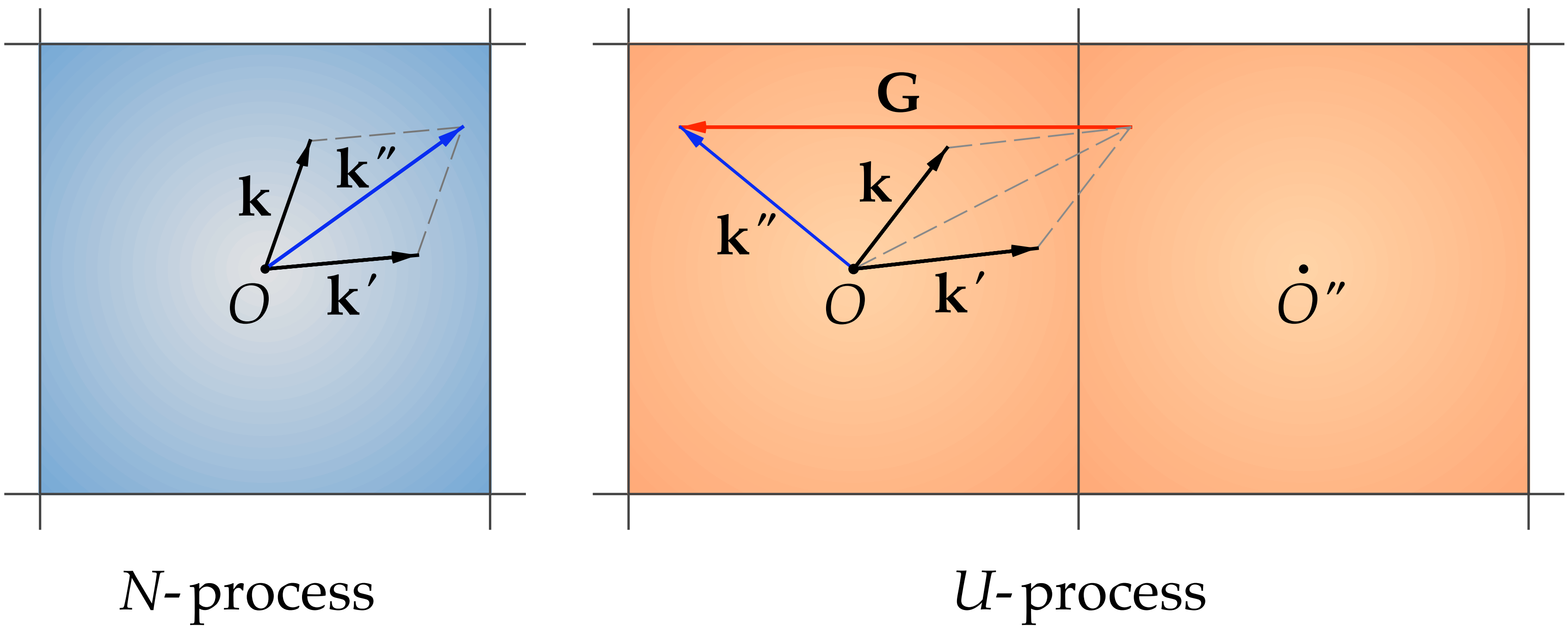
$$\mathbf{k}'' + \mathbf{G} = \mathbf{k} + \mathbf{k}' \ , \tag{6.12}$$

where $\mathbf{G}$ is the reciprocal lattice vector that brings $\mathbf{k}''$ inside the first Brillouin zone.

The quantity $\hbar\mathbf{k}$ is referred to as the *crystal momentum*.

Processes in which there is a change $\mathbf{G} \neq 0$ in the wave vectors of the phonons are known as *Umklapp prozesse* *(German)* or *U*-processes.

Processes in which wave vector is conserved are known as normal processes or *N*-processes.



Normal processes only redistribute the energy into different phonon modes without altering its total flow and do not contribute to the thermal resistivity.

On the contrary, **Umklapp** processes, for which there is a large change of crystal momentum at each scattering event, alter the total flow of energy and contribute to the thermal resistivity (because determine the phonon mean free path).

**Этимология слова Umklapp (моя версия)** Klapp - хлопок (нем.)

um- 1. отделяемая глагольная приставка (нем.) указывает
1) на поворот, окольное или обратное движение umdrehen поворачивать, umfahren — делать крюк, ехать в объезд sich umblicken — осматриваться, озираться (вокруг), оглядеться

We first discuss the temperature variation of the lattice thermal conductivity $\lambda_l$ in terms of $\Lambda_{\mathrm{ph}}(T)$ and $C_V(T)$.

a) High temperatures $\left(T \gg \theta_D\right)$:

The occupation number of the phonon mode $i$ is

$$n_i = \frac{1}{e^{\hbar\omega_i/k_B T} - 1} \quad . \tag{6.16}$$

When $T \gg \theta_D$ we have $n_i = T/\theta_D$ and find that

$$\Lambda_{\mathrm{ph}} \propto T^{-1} \quad . \tag{6.17}$$

In this temperature range the specific heat is only weakly temperature dependent, and $\lambda_l$ is expected to decrease with increasing temperature.

b) Low temperatures $(T \ll \theta_D)$:

Temperature dependence of the probability of the U-processes.

The wave vector $k''$ of the phonon created in a three-phonon U-process must be greater than $G/2$; consequently, its energy $\hbar\omega''$ must be greater than $k_B\theta_D/b$, where $b \approx 2$.

The occupation number of the phonon mode becomes

$$n_i \propto \frac{1}{e^{\theta_D/bT} - 1} \quad . \qquad (6.18)$$

For $T \ll \theta_D$ we find

$$n_i \propto e^{-\theta_D/bT}$$

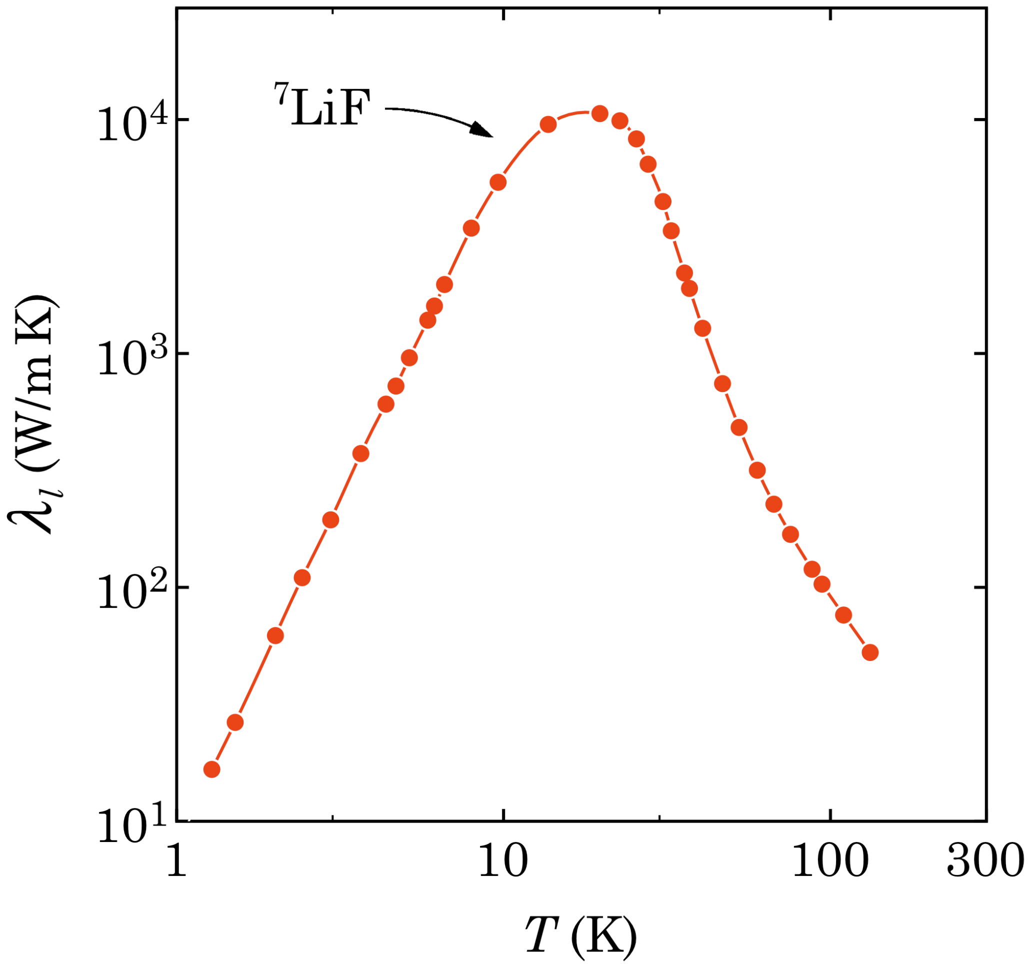
and

$$\lambda_l \propto e^{\theta_D/bT} \quad . \tag{6.19}$$

With decreasing temperature the regime is reached in which the mean free path of the phonons is limited either by the sample boundaries or defects and becomes temperature-independent. In this temperature range the lattice specific heat is proportional to $T^3$, so that in the regime of constant $\Lambda_{\mathrm{ph}}$ we expect

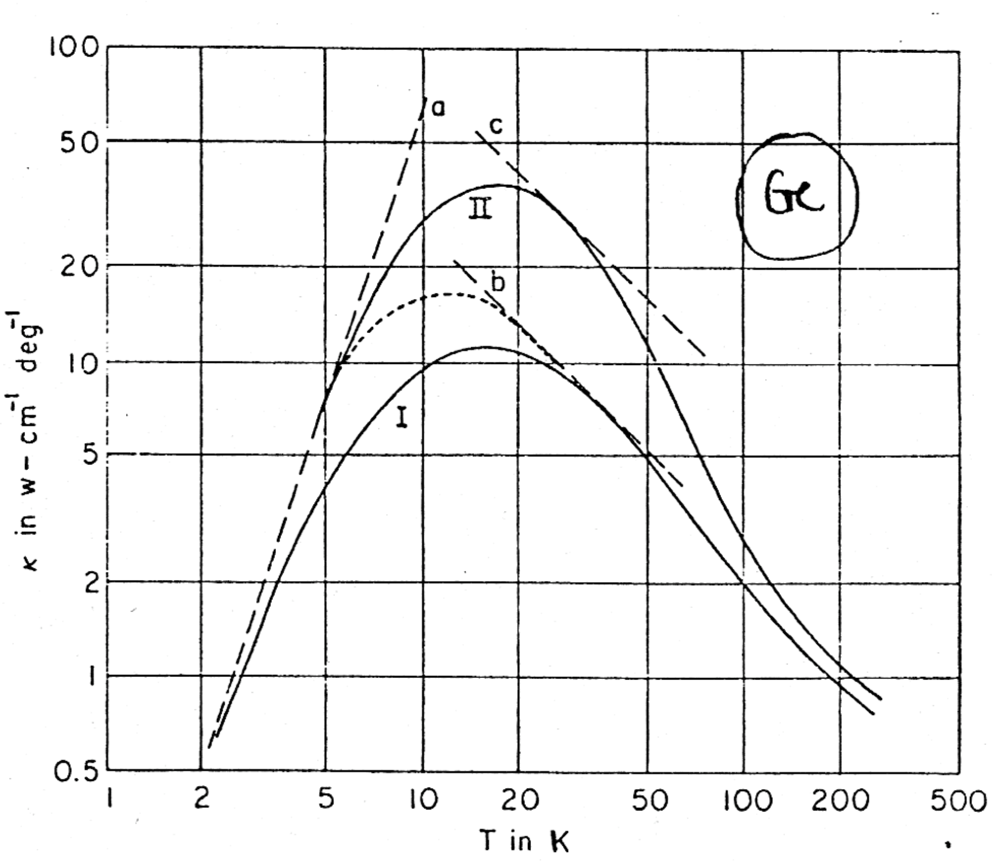
$$\lambda_l \propto T^3 \quad . \tag{6.20}$$

# Thermal conductivity of $^7$LiF




[data from R. Berman and J. C. F. Brock, Proc. Roy. Soc. A **289**, 46 (1965)]

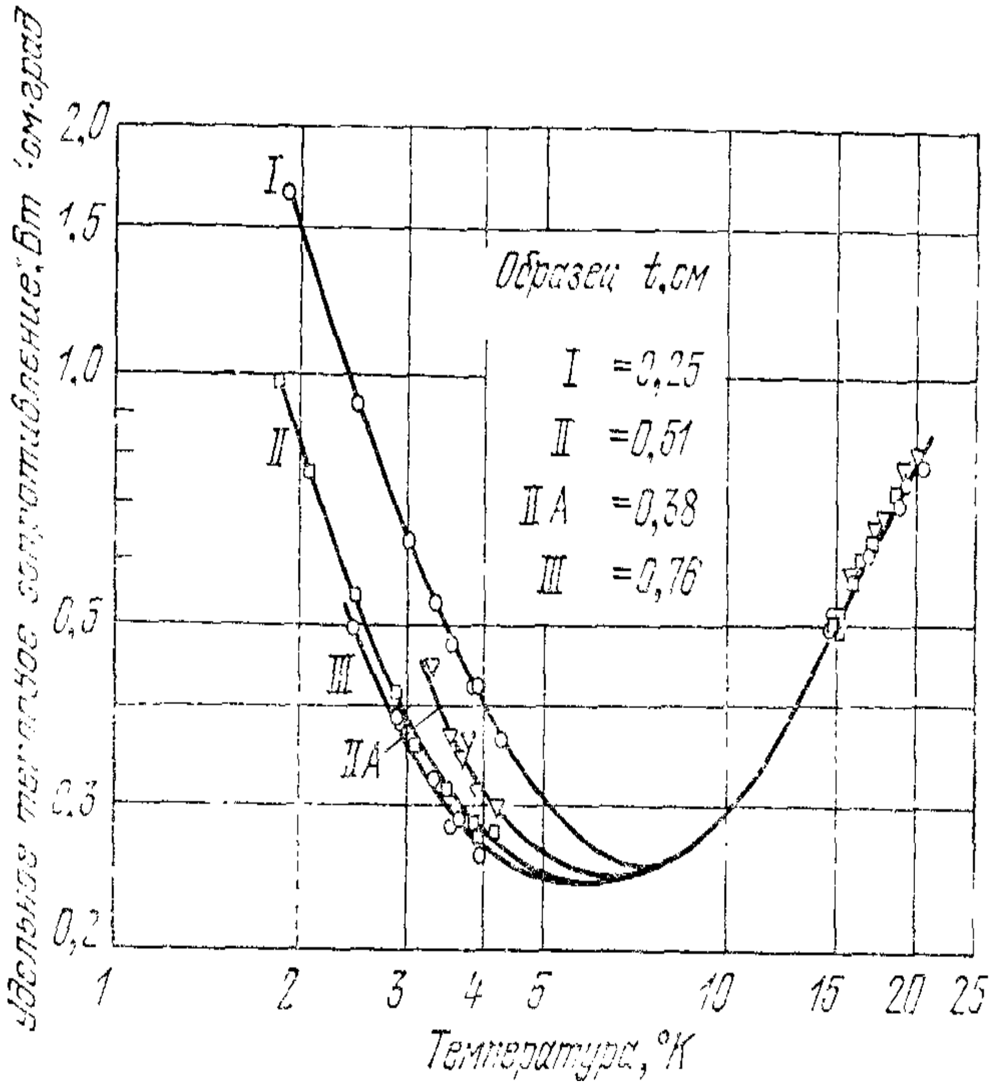
# Thermal conductivity of naturally occurring germanium ($20\%\ ^{70}Ge$, $27\%\ ^{72}Ge$, $8\%\ ^{73}Ge$, $37\%\ ^{74}Ge$, $8\%\ ^{76}Ge$), curve I and enriched germanium ($96\%\ ^{74}Ge$), curve II




**Influence of isotope composition on the temperature dependence of thermal conductivity (scattering of phonons by isotope impurities)**

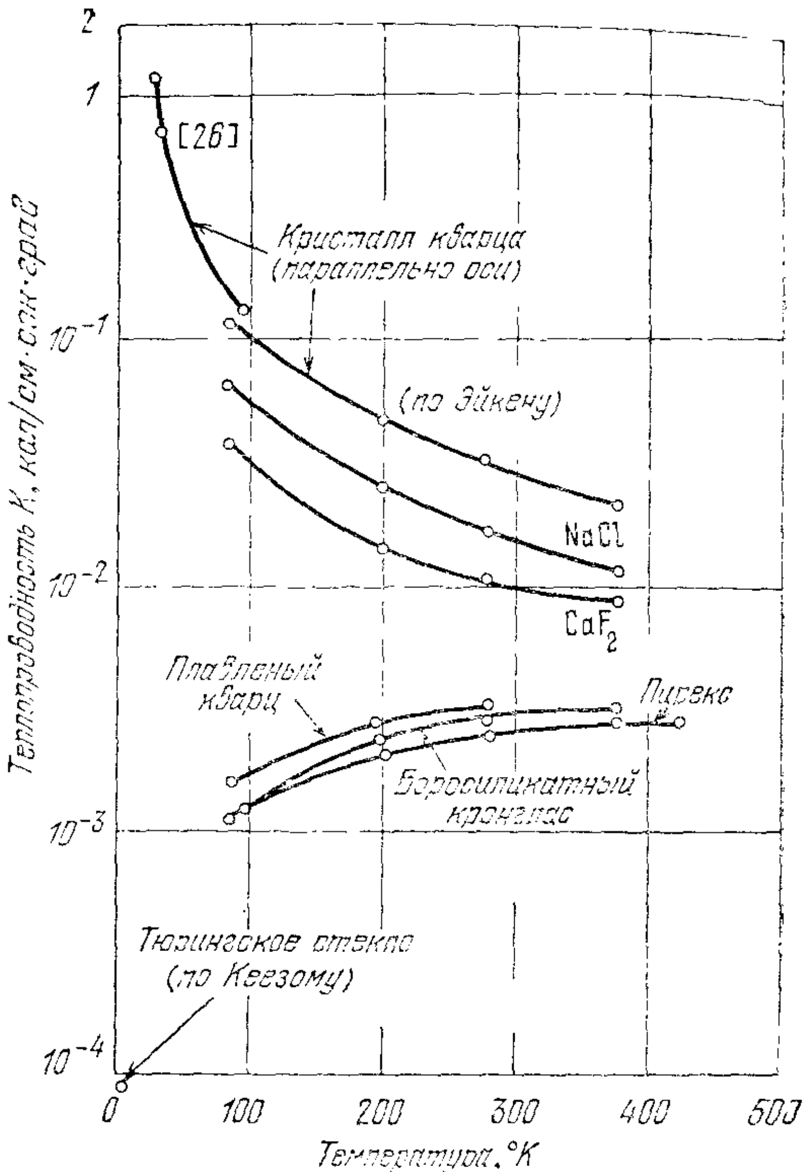
[from P. G. Klemens, Solid State Physics **7**, 1 (1958)]

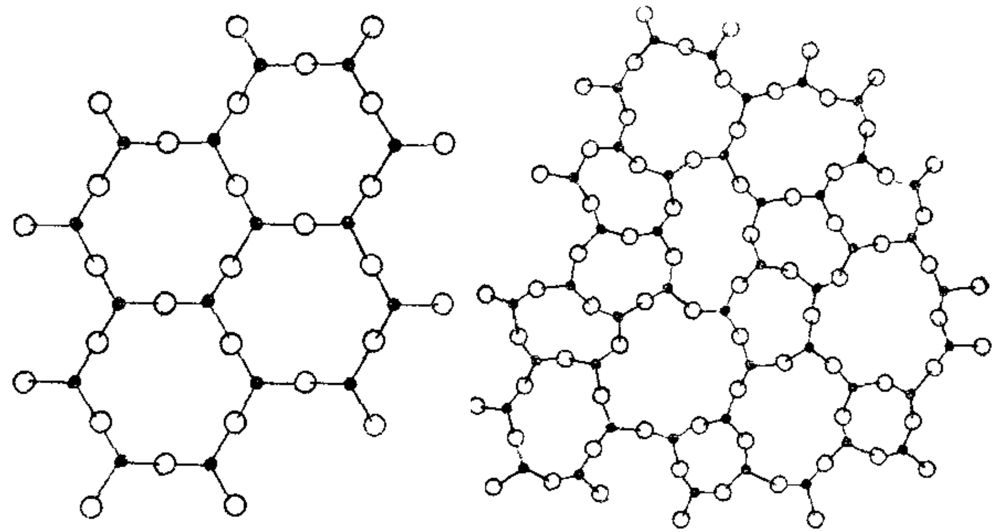
# Thermal conductivity of KCl (experiment) as function of the sample size




Температурная зависимость теплового сопротивления кристаллов хлорида калия (КСl) разной толщины. Ниже 5°К, тепловое сопротивление зависит от толщины кристалла t, поскольку средняя длина свободного пробега фононов определяется размерами кристалла Возрастание теплового сопротив1епия при низких температурах вызвано  уменьшением теплоемкости решетки, Увеличение теплового сопротивления выше 10 °К. вызвано экспоненциальным возрастанием числа процессов переброса.

# Температурная зависимость теплопроводности некоторых кристаллов и стекол.



а) б)

**Двумерная схема, иллюстрирующая различие между кристаллом и стеклом: а — регулярно повторяющаяся структура атомов в кристалле, б — хаотическое расположение атомов в стекле. Материал — кварц** $SiO_2$**, линии показывают направления связей; черные кружки — атомы кислорода.**