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

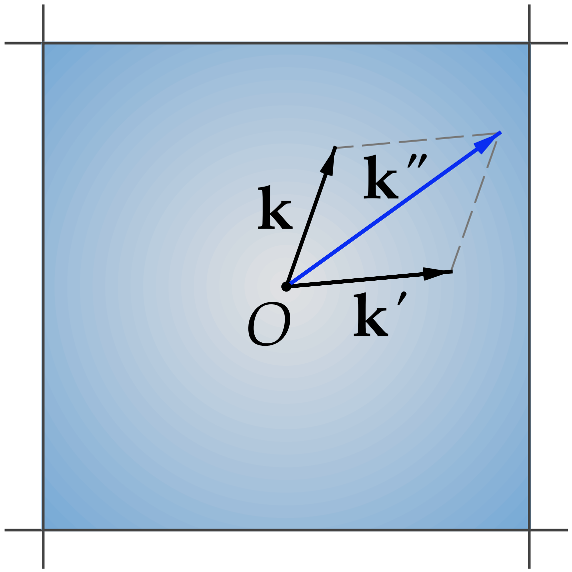
$$\mathbf{k}'' + \mathbf{G} = \mathbf{k} + \mathbf{k}' \ , \tag{6.12}$$

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

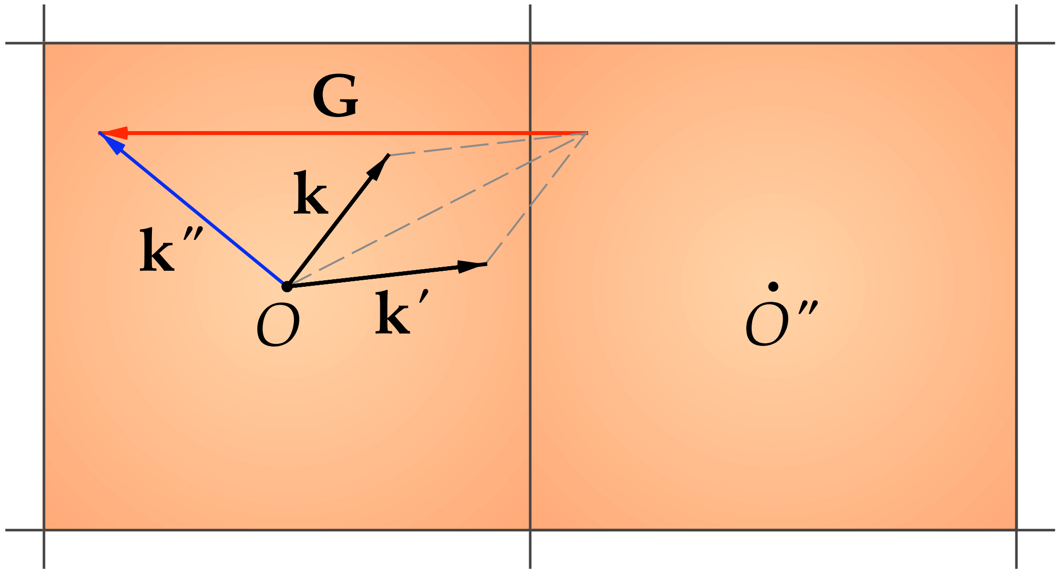
The quantity $\hbar\mathbf{k}$ is referred to as the *crystal momentum*.

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.



N-process



U-process

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).

Etymology of the word Umklapp

Klapp - clap (germ.)

um- 1. separable verb prefix (German) indicates
1) a turn, roundabout or reverse movement umdrehen

Lattice thermal conductivity

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

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

which relates the steady-state heat flux and a temperature gradient through the lattice thermal conductivity coefficient λ_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

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

where v_s is the average phonon velocity and Λ_{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 τ^{-1} is the phonon scattering rate.

We first discuss the temperature variation of the lattice thermal conductivity λ_l in terms of $\Lambda_{\text{ph}}(T)$ 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

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

In this temperature range the specific heat is only weakly temperature dependent, and λ_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

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

For $T \ll \theta_D$ we find

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

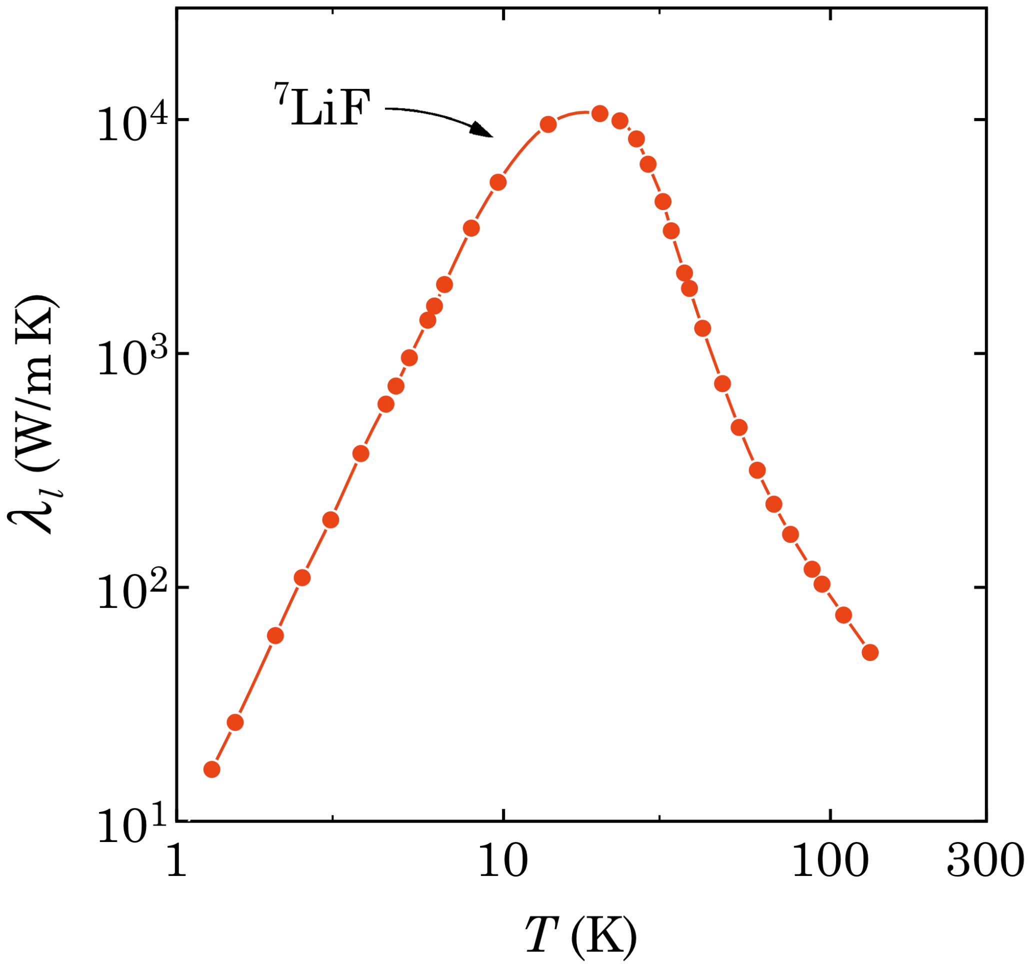
and

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

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 Λ_{ph} we expect

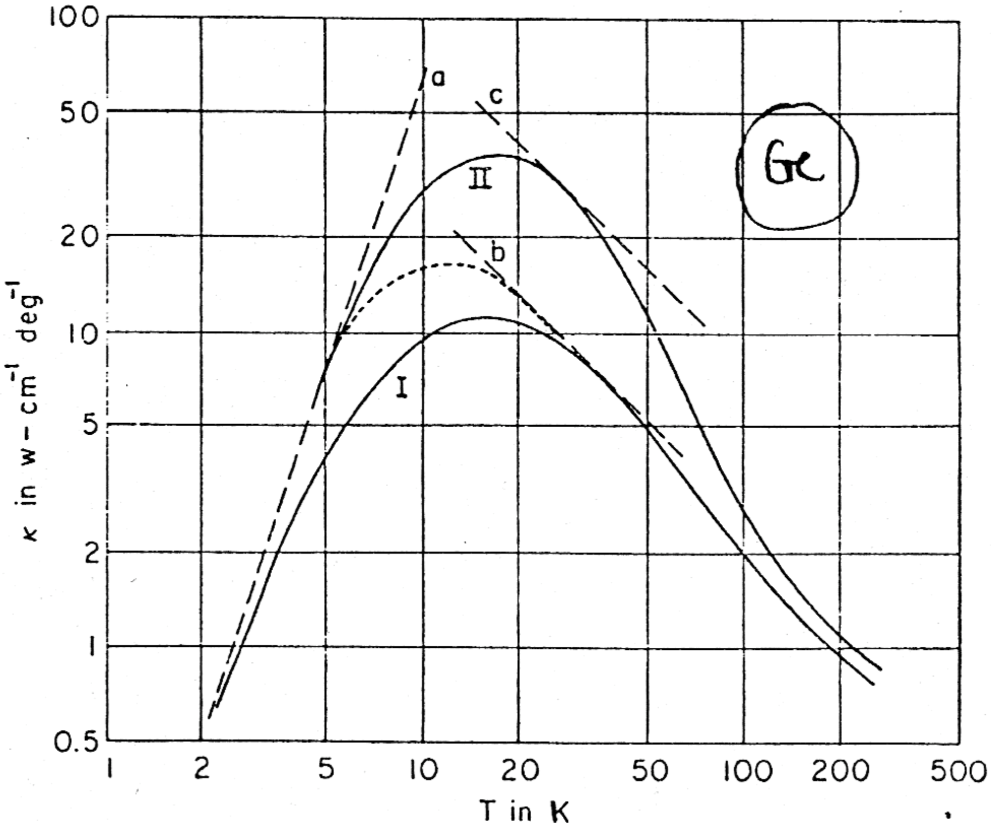
$$\lambda_l \propto T^3 \quad . \tag{6.20}$$

Thermal conductivity of ^{7}LiF



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

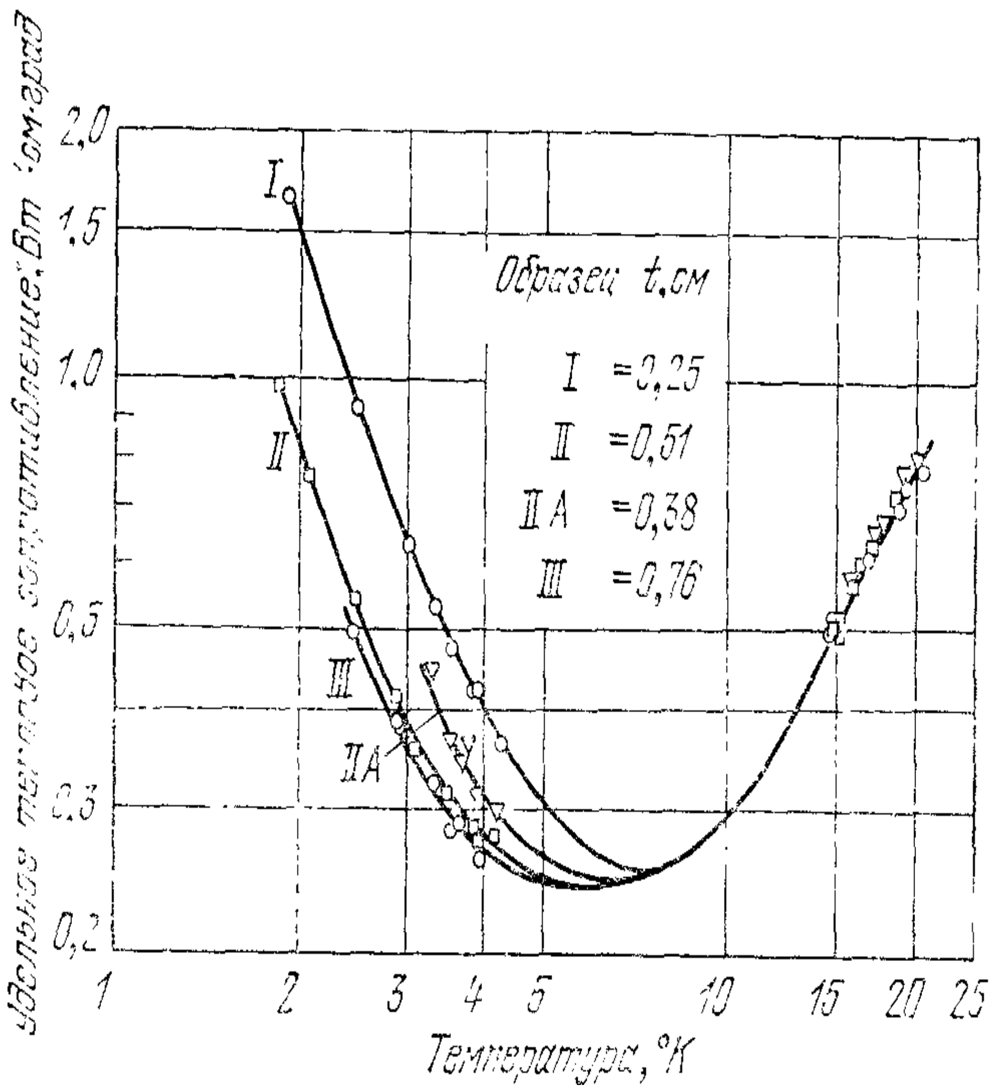
Thermal conductivity of naturally occurring germanium ($20\%\ ^{70}Ge$, $27\%\ ^{72}Ge$, $8\%\ ^{73}Ge$, $37\%\ ^{74}Ge$, $8\%\ ^{76}Ge$), curve I and enriched germanium ($96\%\ ^{74}Ge$), curve II



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

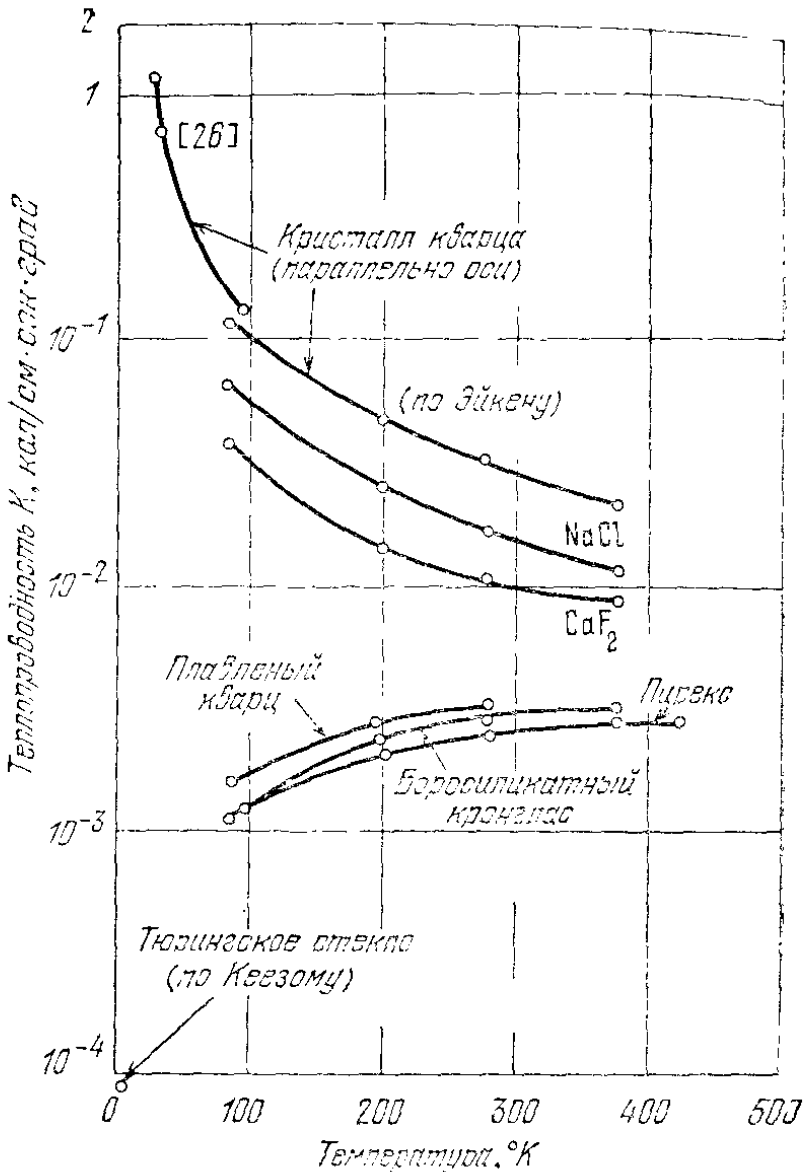
[from P. G. Klemens, Solid State Physics **7**, 1 (1958)]

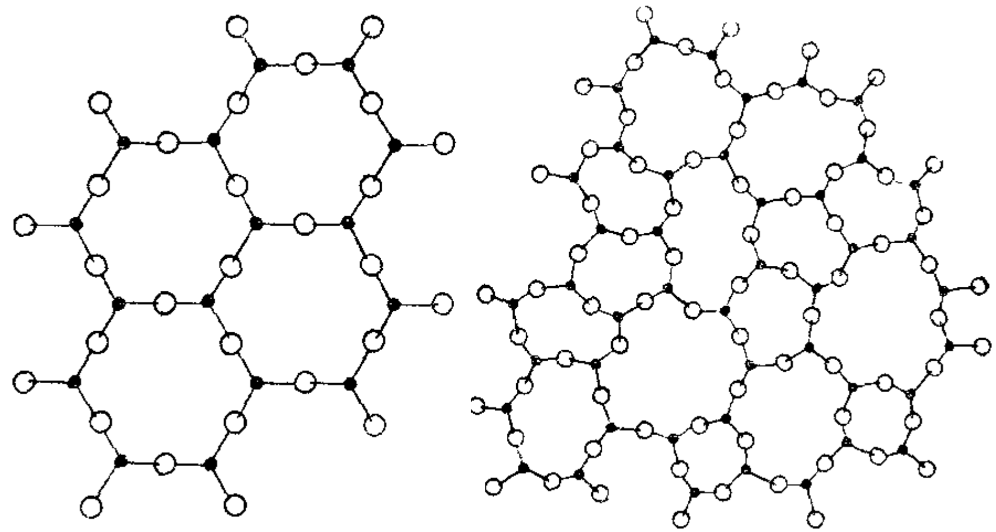
Thermal conductivity of KCl (experiment) as function of the sample size



Temperature dependence of the thermal resistance of potassium chloride (KCl) crystals of different thicknesses. Below 5°K, the thermal resistance depends on the crystal thickness t, since the mean free path of phonons is determined by the dimensions of the crystal. The increase in thermal resistance at low temperatures is caused by a decrease in the heat capacity of the lattice. The increase in thermal resistance above 10 °K is caused by an exponential increase in the number of transfer processes.

Temperature dependence of the thermal conductivity of some crystals and glasses.





а) б)

A two-dimensional diagram illustrating the difference between a crystal and glass: a - regularly repeating structure of atoms in a crystal, b - chaotic arrangement of atoms in glass. Material - quartz SiO_2, lines show directions of bonds; black circles are oxygen atoms.