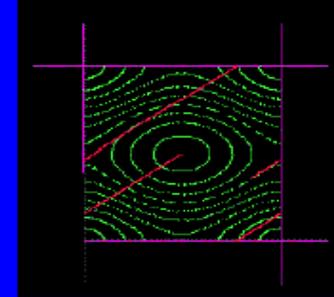
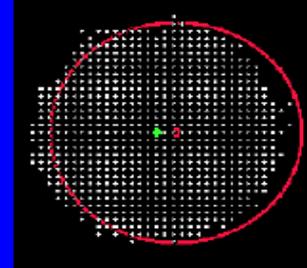
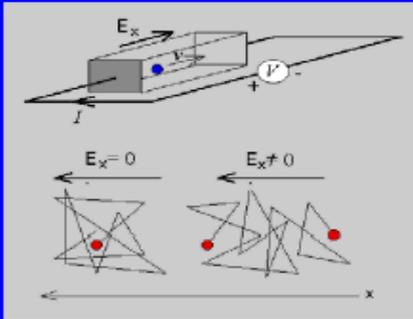


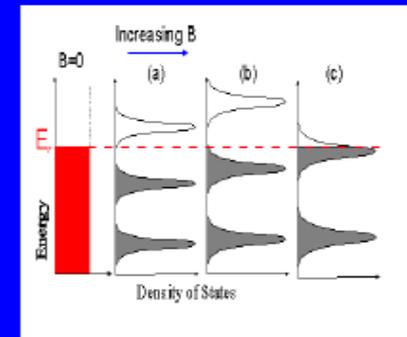
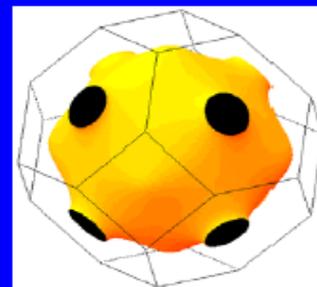
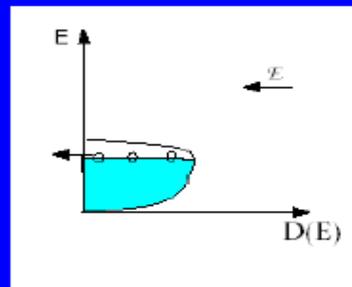
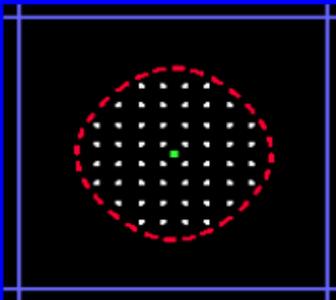
# Transport Phenomena in Solids

## Motions of electrons and transport phenomena

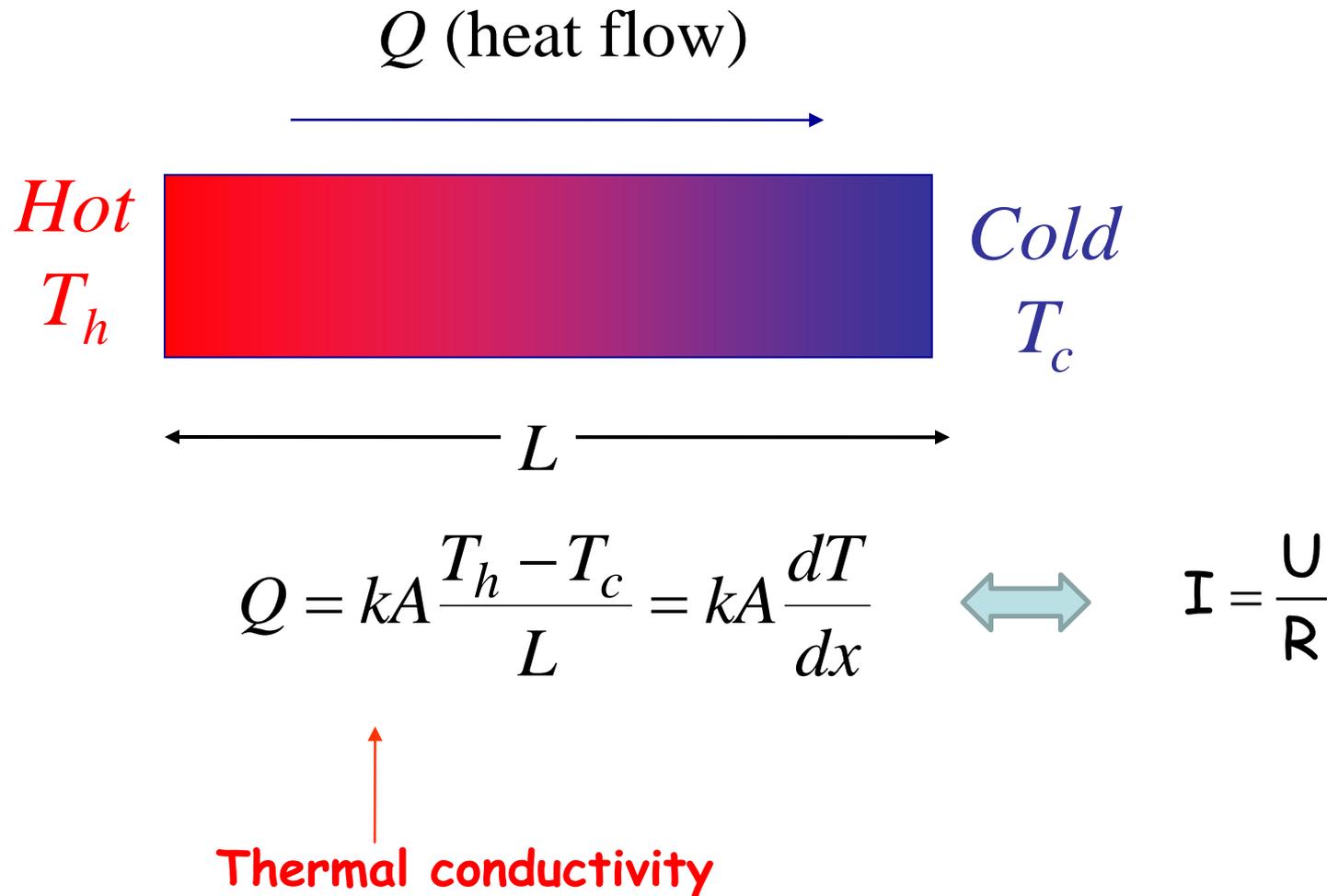


$$\sigma = \frac{ne^2\tau}{m}$$

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 E(\bar{k})}{\partial k_i \partial k_j}$$



# Thermal conductivity



$$U = \kappa(-\nabla T)$$

## Thermal conductivity in metals

the thermal current in a metal is conveyed by both **electrons** and **phonons**

$$\kappa = \kappa_{\text{el}} + \kappa_{\text{ph}},$$

## Matthiessen rule

the total electronic thermal resistivity  $W_{\text{el}}$  or  $1/k_{\text{el}}$  is given by

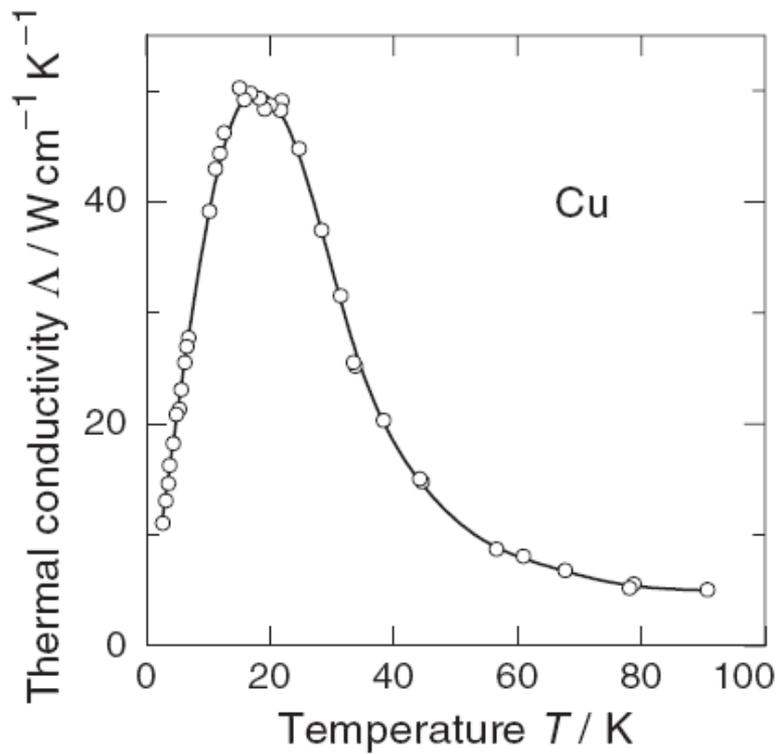
$$W_{\text{el}} = W_{\text{el}}^{\text{imp}} + W_{\text{el}}^{\text{lattice}}$$

the phonon thermal resistivity  $W_{\text{ph}}$  or  $1/k_{\text{ph}}$  consists of contributions due to **imperfections**, **phonon–electron** and **Umklapp phonon–phonon** interactions

Table 11.1. *Thermal conductivity data for metals, alloys and insulators*

substance	maximum thermal conductivity $\kappa_{\max}$ (watt/cm·K)	temperature at $\kappa_{\max}$ (K)
Cu	20–40	20–30
$\text{Cu}_{99.9}\text{Zn}_{0.1}$	8.7	30
$\text{Cu}_{99}\text{Zn}_1$	3	40
$\text{Cu}_{90}\text{Zn}_{10}$	1	60
$\text{Cu}_{74.5}\text{Zn}_{25.5}$	0.7	100
graphite	0.1	60
stainless steel	0.1–0.2	100–300
sapphire	60	30–40
nylon	0.001	20

from Mizutani



**Fig. 7.14.** Thermal conductivity of copper. As in dielectric crystals, a pronounced maximum is observed [314]

# kinetic theory of gases

$$\kappa = \frac{1}{3} C_V \Lambda$$

• the temperature dependence of the electronic thermal conductivity in metals

two different scattering sources in electronic thermal conduction:

- I. Impurities
- II. lattice vibrations

• The **mean free path**  $\Lambda$  of the conduction electron due to impurity scattering is obviously **temperature independent**.

•  $C_{el}$  is proportional to the absolute temperature  $T$

• the Fermi velocity  $v_F$  is independent of  $T$ .

$k_{el}$  **proportional** to the **absolute temperature**



$$W_{el}^{imp} = \beta/T$$

$$W_{\text{el}}^{\text{imp}} = \beta/T$$

The more impure the sample, the shorter the mean free path and, hence, the larger the coefficient  $\beta$ .

- the electronic thermal resistivity due to lattice vibrations

In the Debye model, the number of phonons decreases in proportion to  $T^3$  with decreasing temperature in the range  $T \ll \Theta_D$ .

$$n = \int_0^{\omega_D} D(\omega) n(\omega, T) d\omega$$

$$D(\omega) \propto \omega^2$$

$n(\omega, T)$  is the Planck distribution

$$n \propto T^3 \int_0^{\omega_D} x^2 dx / (e^x - 1)$$

Mean free path:

$$\Lambda = \frac{1}{\sqrt{2} \cdot \sigma \cdot n} \quad \Rightarrow \quad \Lambda \propto T^{-3}$$

$$C_{el} \propto T$$

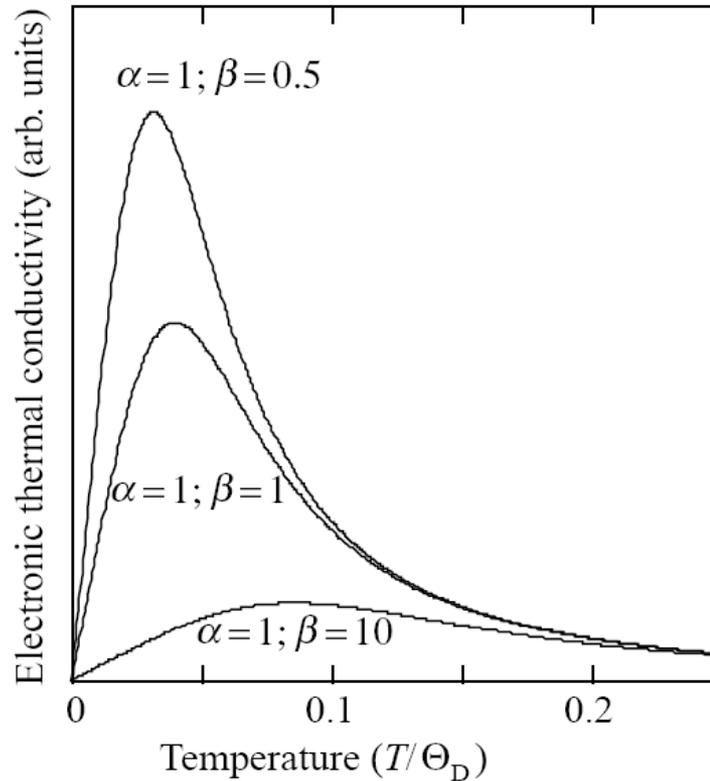


$$W_{el}^{\text{lattice}} = \alpha T^2$$

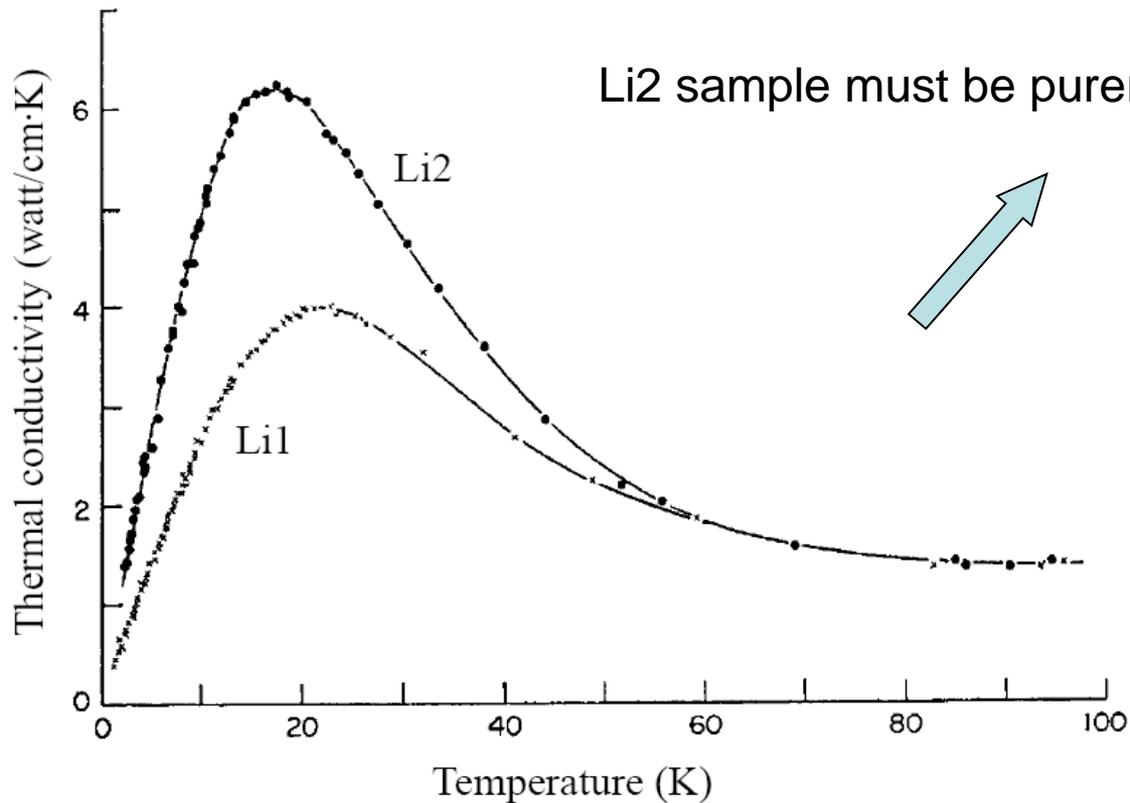
$$W_{el} = \alpha T^2 + (\beta/T)$$

The total thermal conductivity  $k$  at low temperatures in a metal is

$$K = \kappa_{el} + \kappa_{ph} = (1/W_{el}) + \kappa_{ph} = \frac{1}{\alpha T^2 + (\beta/T)} + \kappa_{ph}$$



Temperature dependence of the electronic thermal conductivity in a metal. A decrease in  $\beta$  indicates an increase in the purity of a specimen.



Temperature dependence of the thermal conductivity of two lithium metal samples. [Reproduced from K. Mendelssohn and H. M. Rosenberg, *Solid State Physics*, edited by F. Seitz and D. Turnbull, (Academic Press, New York, 1961) vol.12]

- the **electronic** thermal conductivity rapidly decreases with increasing solute concentration in an alloy
- the **phonon** thermal conductivity also decreases but its rate of decrease is much slower than that of  $k_{el}$
- the ratio  $k_{ph}/k$  at about 10 K is only 0.002 for pure Cu
- it becomes 0.3 for the  $\text{Cu}_{80}\text{Zn}_{20}$  alloy

## Electronic thermal conductivity

Mizutani

we formulate the electronic thermal conductivity by using the **linearized Boltzmann transport equation** in combination with **the relaxation time approximation**.

Both the electrical current density  $\mathbf{J}$  and thermal current density  $\mathbf{U}$  are expressed as linear functions of the electric field  $\mathbf{E}$  and temperature gradient in the following forms:

$$\mathbf{J} = L_{EE}\mathbf{E} + L_{ET}\nabla T$$

$$\mathbf{U} = L_{TE}\mathbf{E} + L_{TT}\nabla T,$$

$L_{EE}$  is the electrical conductivity,

$$L_{ET} = -L_{TE}/T$$

thermal conductivity is measured under the condition  $\mathbf{J}=0$

$$\kappa = -(L_{TT} - L_{TE} \cdot L_{ET} / L_{EE})$$

from the analogy with the expression for the electrical current density the **thermal current density** is

$$\mathbf{U} = (1/4\pi^3) \int \mathbf{v}_{\mathbf{k}} \varepsilon(\mathbf{k}) f(\mathbf{r}, \mathbf{k}) d\mathbf{k} \quad \longleftrightarrow \quad \mathbf{J} = ((-e)/4\pi^3) \int \mathbf{v}_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}) d\mathbf{k}$$

- both heat and electrical charge are carried simultaneously.
- electrons at the Fermi level  $\varepsilon_F (\equiv \zeta)$  convey the **current density  $\mathbf{J}$** .

energy flow  $[\mathbf{J}/(-e)]\zeta$

**This must be subtracted from the energy current to derive the flow of heat.**

$$\mathbf{U} = \frac{1}{4\pi^3} \int \mathbf{v}_{\mathbf{k}} \varepsilon(\mathbf{k}) f(\mathbf{r}, \mathbf{k}) d\mathbf{k} - \left( \frac{\mathbf{J}}{(-e)} \right) \zeta = \frac{1}{4\pi^3} \int [\varepsilon(\mathbf{k}) - \zeta] \mathbf{v}_{\mathbf{k}} [f(\mathbf{r}, \mathbf{k}) - f_0(\mathbf{k})] d\mathbf{k}$$

$$\mathbf{J} = ((-e)/4\pi^3) \int \mathbf{v}_{\mathbf{k}} f(\mathbf{r}, \mathbf{k}) d\mathbf{k}$$

$$\int \mathbf{v}_{\mathbf{k}} f_0(\mathbf{k}) d\mathbf{k} = 0 \quad \text{and} \quad \int \boldsymbol{\varepsilon}(\mathbf{k}) \mathbf{v}_{\mathbf{k}} f_0(\mathbf{k}) d\mathbf{k} = 0.$$

$$-\mathbf{v}_{\mathbf{k}} \cdot \nabla f(\mathbf{r}, \mathbf{k}) - \frac{(-e)}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}} = - \left( \frac{\partial f}{\partial t} \right)_{\text{scatter}}$$



We try to solve the **linearized Boltzmann transport equation** under the condition that only the **temperature gradient** exists in a metal.

$$-\left( \frac{\partial f}{\partial t} \right)_{\text{scatter}} = \frac{f(\mathbf{r}, \mathbf{k}) - f_0(\boldsymbol{\varepsilon}_{\mathbf{k}}, T)}{\tau} = \frac{\phi(\mathbf{r}, \mathbf{k})}{\tau}$$

$$-\mathbf{v}_{\mathbf{k}} \cdot \frac{\partial f_0}{\partial T} \nabla T - \frac{(-e)}{\hbar} (\mathbf{E} + \mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial f_0}{\partial \mathbf{k}}$$

$$f_0(\boldsymbol{\varepsilon}_{\mathbf{k}}, T) = 1 / \{ \exp[(\boldsymbol{\varepsilon}_{\mathbf{k}} - \zeta) / k_B T] + 1 \}$$



$$\frac{\partial f_0}{\partial T} = - \left( \frac{\partial f_0}{\partial \boldsymbol{\varepsilon}} \right) \left[ \left( \frac{\boldsymbol{\varepsilon} - \zeta}{T} \right) + \frac{\partial \zeta}{\partial T} \right]$$

$$f(\mathbf{r}, \mathbf{k}) - f_0(\varepsilon_{\mathbf{k}}, T) = \left( -\frac{\partial f_0}{\partial \varepsilon} \right) \tau \mathbf{v}_{\mathbf{k}} \cdot \left[ -\left( \frac{\varepsilon(\mathbf{k}) - \zeta}{T} \right) \nabla T + (-e) \left( \mathbf{E} - \frac{\nabla \zeta}{(-e)} \right) \right],$$

$\nabla \zeta / (-e)$  implies that the chemical potential gradient gives rise to an additional field to induce a diffusional current.

$\{\mathbf{E} - [\nabla \zeta / (-e)]\}$  serve as an effective electric field.

$\rightarrow 0$

$$\mathbf{U} = -\frac{1}{4\pi^3} \int [\varepsilon(\mathbf{k}) - \zeta]^2 \tau(\mathbf{k}) \mathbf{v}_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \left( -\frac{\partial f_0}{\partial \varepsilon} \right) d\mathbf{k} \cdot \left( \frac{\nabla T}{T} \right),$$

$$\iiint d\mathbf{k} = \iint dS \int dk_{\perp} = \iint dS \int \frac{d\varepsilon}{|\partial \varepsilon / \partial k_{\perp}|} = \iint dS \int \frac{d\varepsilon}{|\nabla_{k_{\perp}} \varepsilon|},$$

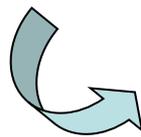
$$\mathbf{U} = -\frac{1}{4\pi^3} \int \int \mathbf{v}_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \tau(\mathbf{k}) [\varepsilon(\mathbf{k}) - \zeta]^2 \frac{dS}{\hbar v_{\perp}} \left( -\frac{\partial f_0}{\partial \varepsilon} \right) d\varepsilon \cdot \left( \frac{\nabla T}{T} \right).$$

using

$$I = \int_0^{\infty} f(E, T) \left( \frac{dF(E)}{dE} \right) dE, \quad I = F[E_F(T)] + \left( \frac{\pi^2}{6} \right) (k_B T)^2 \left[ \frac{d^2 F(E)}{dE^2} \right]_{E=E_F(T)} + \dots$$

$$\mathbf{U} = - \left[ \frac{[\varepsilon(\mathbf{k}) - \zeta]^2 \sigma(\varepsilon)}{(-e)^2} + \frac{\pi^2 (k_B T)^2}{6} \frac{\partial^2}{\partial \varepsilon^2} \left\{ [\varepsilon(\mathbf{k}) - \zeta]^2 \frac{\sigma(\varepsilon)}{(-e)^2} \right\} + \dots \right]_{\varepsilon=\zeta} \cdot \left( \frac{\nabla T}{T} \right),$$

Insertion of  $\varepsilon = \zeta$



$$\mathbf{U} = - \left( \frac{\pi^2 k_B^2 T \sigma}{3(-e)^2} \right) \nabla T.$$

we have calculated the coefficient  $L_{TT}$

$$\kappa = -L_{TT}(1 - L_{TE} \cdot L_{ET} / L_{EE} \cdot L_{TT})$$

the correction term  $L_{TE} \cdot L_{ET} / L_{EE} \cdot L_{TT}$  to be of the order of  $(T/T_F)^2$ , if the free electron model is applied to a metal having the Fermi temperature  $T_F$

Since  $(T/T_F)^2$  is negligibly small in ordinary metals, the electronic thermal conductivity is well represented by

$$\kappa_{\text{el}} = \frac{\pi^2 k_B^2 T}{3(-e)^2} \sigma(T)$$

This leads to the Wiedemann–Franz law

A more rigorous treatment can prove that this is valid when the scattering of electrons is elastic and the relaxation time is independent of energy.

## Wiedemann–Franz law and Lorenz number

the ratio of the electronic thermal conductivity over the electrical conductivity, say, at room temperature becomes constant, regardless of the metal concerned.

$$L_0 \equiv \frac{\kappa_{\text{el}}}{\sigma T} = \frac{\pi^2}{3} \frac{k_{\text{B}}^2}{(-e)^2}$$

where  $L_0$  is called the limiting **Lorenz number** and is a universal constant

$$L_0 = 2.45 \cdot 10^8 \text{ volt}^2/\text{K}^2$$

element	$\kappa$ (W/m·K)	$L$ ( $10^{-8}$ V <sup>2</sup> /K <sup>2</sup> )
Ag	436	2.34
Al	236	2.10
Au	318	2.39
Ca	186	2.13
Cs	37	2.5
Cu	404	2.27
Fe	80	2.57
K	98	2.24
Li	65	2.05
Mg	151	2.29
Na	142	2.23
Ni	93	2.19
Pb	36	2.50
Pd	72	2.57
Pt	72	2.59
Rb	56	2.30
Ru	131	2.52
Sn	62	2.5
Zn	127	2.60

*Thermal conductivity  $\kappa$  and  
measured Lorenz number  $L$   
for typical metals at 273 K*

from Mizutani

The **Wiedemann–Franz** law **would fail** when the temperature is lowered below 273 K, since the **inelastic scattering** effect becomes substantial

inelastic scattering contributes to the electrical and thermal conduction in a different way so that its role can be qualitatively extracted by studying the temperature dependence of the measured Lorenz number over a wide temperature range.

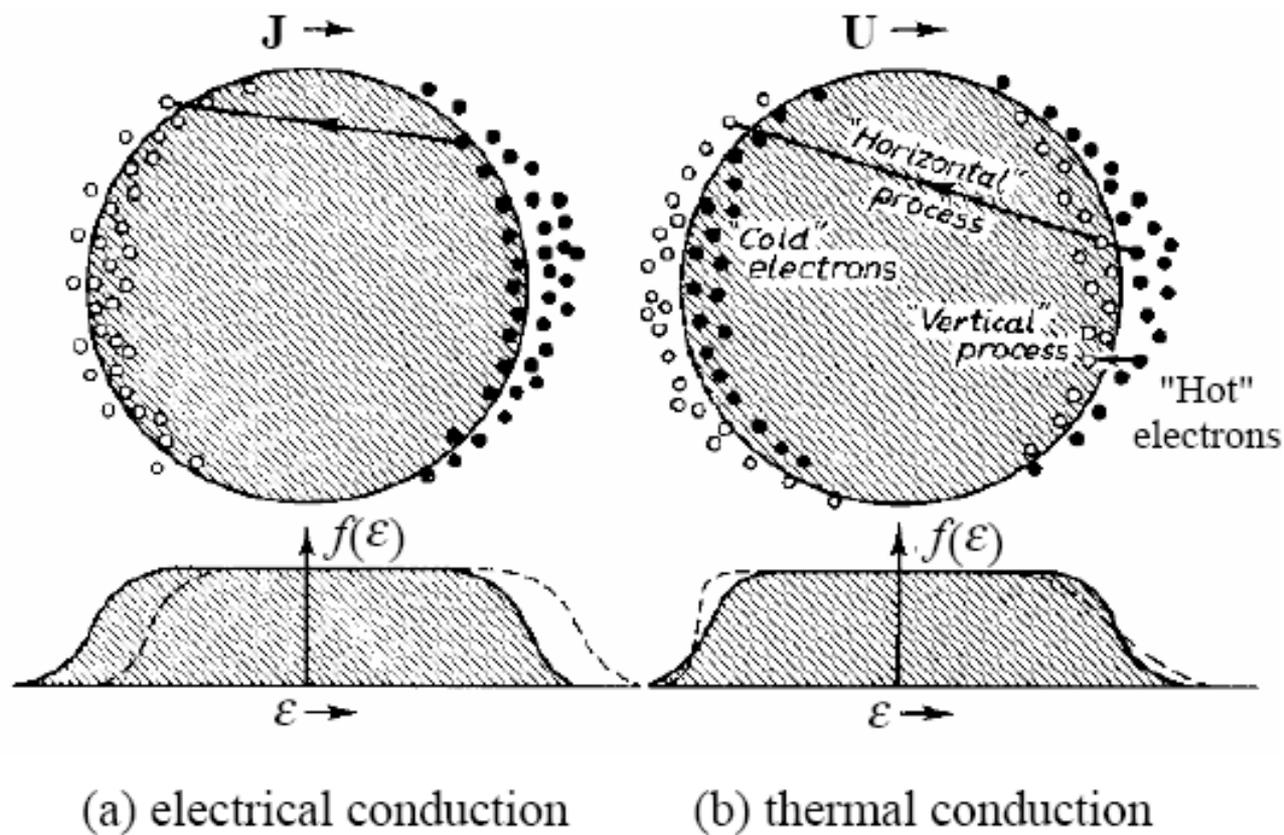
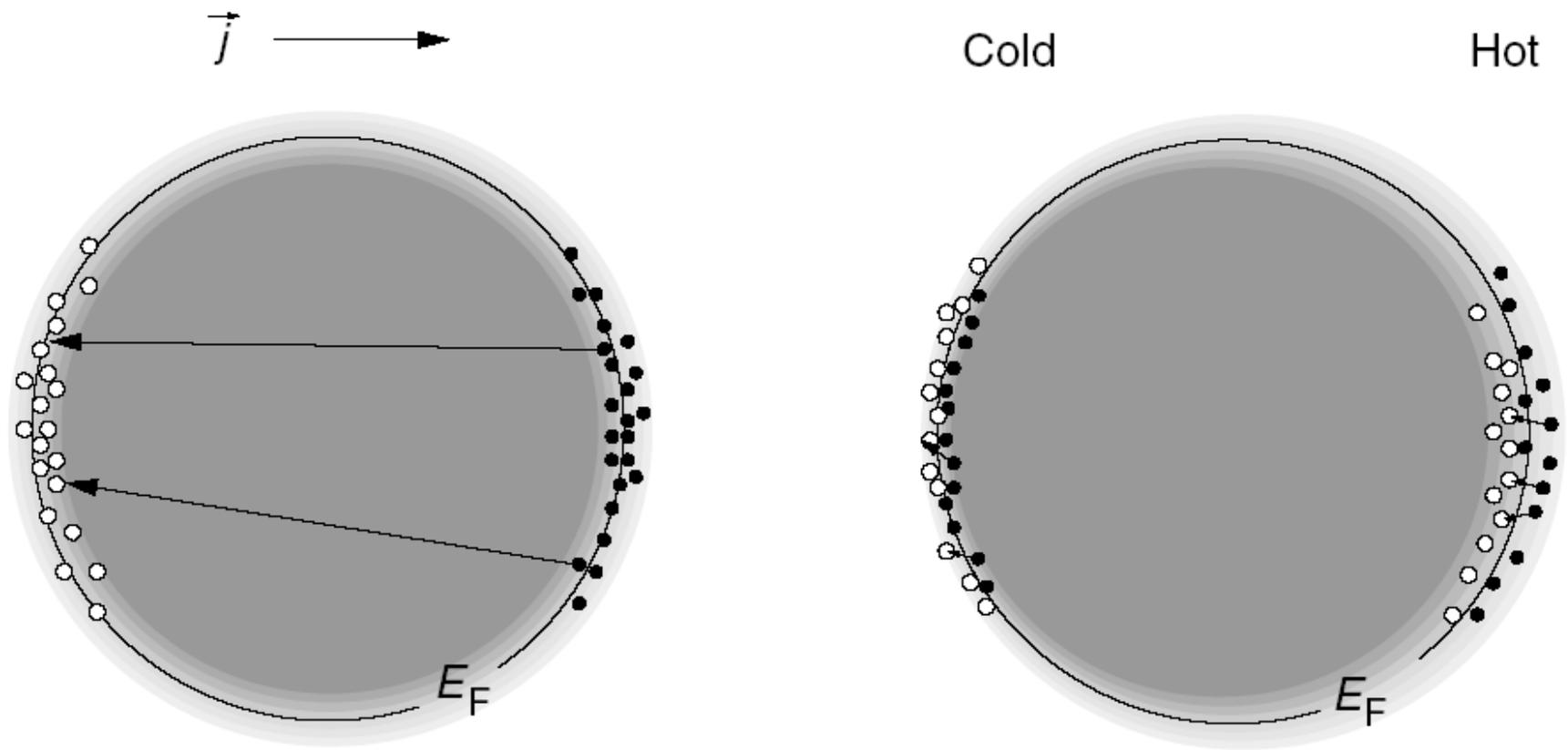


Figure 11.3. Electron distributions and scattering process in (a) electrical conduction and (b) thermal conduction. The dashed curve in each represents the electron distribution in the presence of external fields: (a)  $\mathbf{E}$  and (b)  $\nabla T$ . [Reproduced from J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, 1964)]



**Fig. 7.12.** Fermi sphere and scattering processes. The *tinted areas* represent the Fermi spheres, the *circles* the Fermi levels in equilibrium. Charge carriers exceeding the equilibrium occupation are represented by *dots* (electrons), and by *open circles* (holes or empty states). (a) Scattering processes stabilizing the position of the Fermi sphere in an electric field. (b) Scattering processes leading to a stationary state in the presence of a thermal gradient

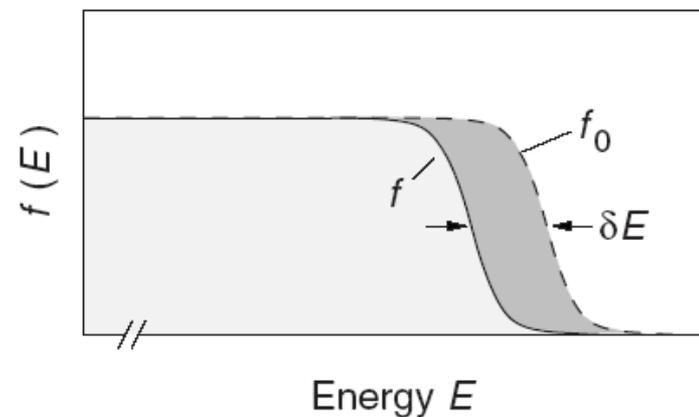
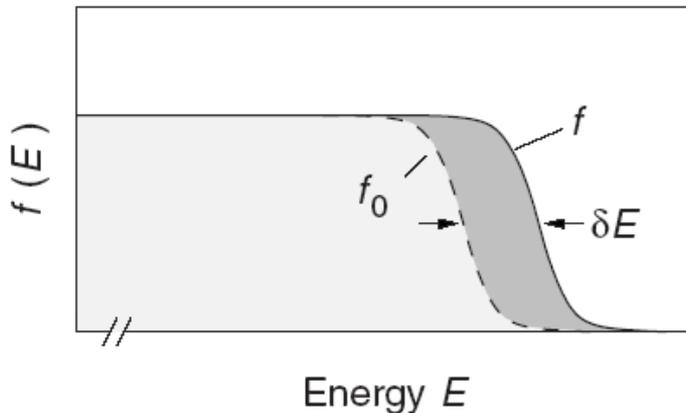
Electric field



$$\delta k = -e\tau \mathcal{E} / \hbar, \\ \delta E \approx -e\tau v(k) \cdot \mathcal{E}.$$

Enss

$$f(\mathbf{k}) = f_0 \left( \mathbf{k} + \frac{e\tau \mathcal{E}}{\hbar} \right) = f_0 \left( E(\mathbf{k}) + e\tau v(\mathbf{k}) \cdot \mathcal{E} \right).$$



**Fig. 7.10.** Fermi–Dirac distribution  $f(E)$  in a dc electric field. The equilibrium distribution  $f_0(E)$  is represented by *dashed lines*, the distribution  $f(E)$  in the electric field by *full lines*. The *dark areas* indicate the difference between the two distributions. The energy of the electrons on the front (a) of the Fermi sphere is increased by  $\delta E$ , on the back (b) the energy is reduced by the same amount

from Enss

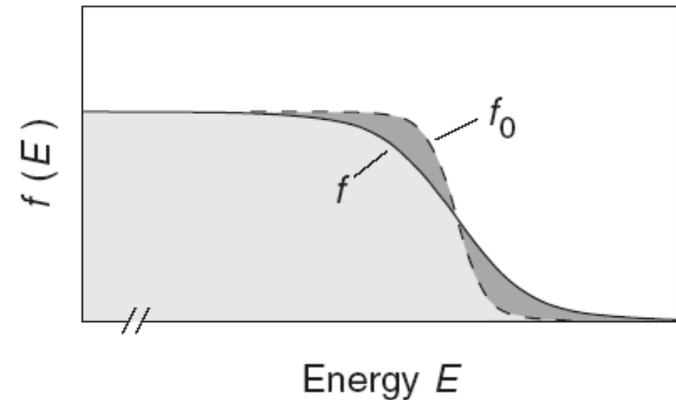
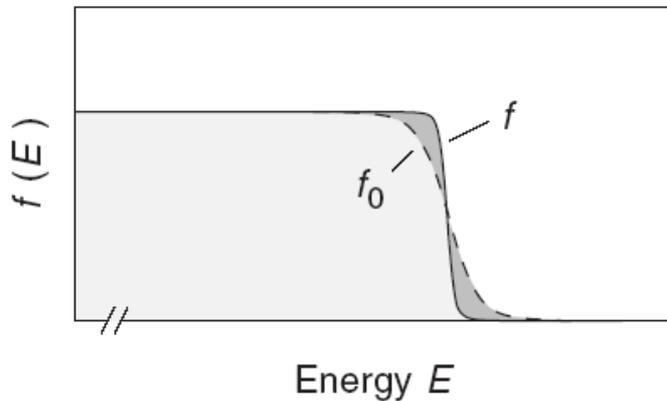
Heat transport



$$\delta T = -\tau \mathbf{v}(\mathbf{k}) \cdot \nabla T.$$

$$f(T) = f_0\left(T - \tau \mathbf{v}(\mathbf{k}) \cdot \nabla T\right)$$

While an electric field causes a change of the wave vector, a temperature gradient leads to a temperature difference



**Fig. 7.11.** Fermi–Dirac distribution  $f(E)$  in the presence of a temperature gradient. The distribution function  $f(E)$  is represented by *full lines*, the equilibrium distribution  $f_0(E)$  by *dashed lines*. The *dark areas* indicate the difference between the two distributions. The flank of the distribution function of the electrons coming from the cold end (**a**) is steeper than  $f_0(E)$ , the distribution function of the electrons from the warm end (**b**) is flatter

- In **electrical conduction** the Fermi surface of a metal specimen is shifted as a whole when an electric field is applied. This implies that more electrons travel to the right than to the left.
- Scattering processes are needed to establish a steady state.
- the **scattering angle** involved becomes smaller and smaller with **decreasing temperature** due to the fact that phonons of only small wave vectors remain active. At low temperatures, therefore, electrons cannot be transferred from one side of the Fermi surface to the other in a single jump. This leads to the well-known  $T^5$ -law for the electrical resistivity at low temperatures.

## in the thermal conduction process

- More electrons to be distributed above the Fermi level on the right and more electrons below it on the left
- we have more “hot” electrons on the right-hand side of the Fermi surface and more “cold” electrons on the left-hand side, resulting in the flow of heat.
- the horizontal process favors large-angle scattering, which is abundant at high temperatures but becomes scarce at low temperatures in both electrical and thermal conduction.
- The vertical process requires a single jump with a small scattering angle but the energy must be exchanged with phonons so that the scattering involved must be inelastic.

At **high temperatures**  $T > \Theta_D$ , the vertical process is no longer well defined, since region  $k_B T$  across the Fermi sphere exceeds the maximum phonon energy of  $k_B \Theta_D$ .  $\rightarrow$  *quasi-elastic scattering*  $\rightarrow$  the vertical process is ineffective and the ratio  $L/L_0$  tends to unity, leading to the validity of the Wiedemann–Franz law.

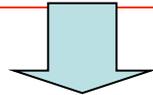
With **decreasing temperature** below  $\Theta_D$ , the vertical process begins to play its role in thermal conduction and **the thermal current** is more substantially **reduced** than expected from the Wiedemann–Franz law. This results in a lowering of the ratio  $L/L_0$  **below unity** and the Wiedemann-Franz law gradually breaks down with decreasing temperature.

the dependence of the ratio  $L/L_0$  on the purity of a specimen in the temperature range well below  $\Theta_D$ .

an ideally **pure metal** free from impurity scattering at low temperatures

→ the number of phonons decreases with decreasing temperature and eventually vanishes at absolute zero.

- the electronic thermal resistivity due to lattice vibrations decreases as  $T^2$
- the electrical resistivity  $\rho_{\text{lattice}}$  decreases as  $T^5$  with decreasing temperature.

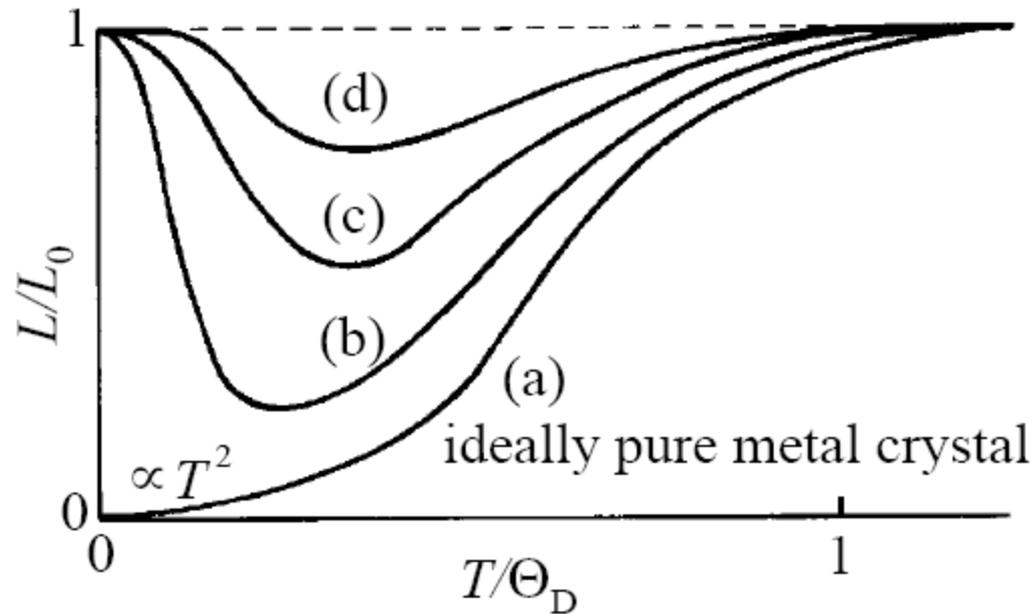


$L/L_0$  tends towards zero as  $T^2$  in a pure metal

**If a specimen is impure**

impurity scattering dominates at low temperatures  $T \ll \Theta_D$ .

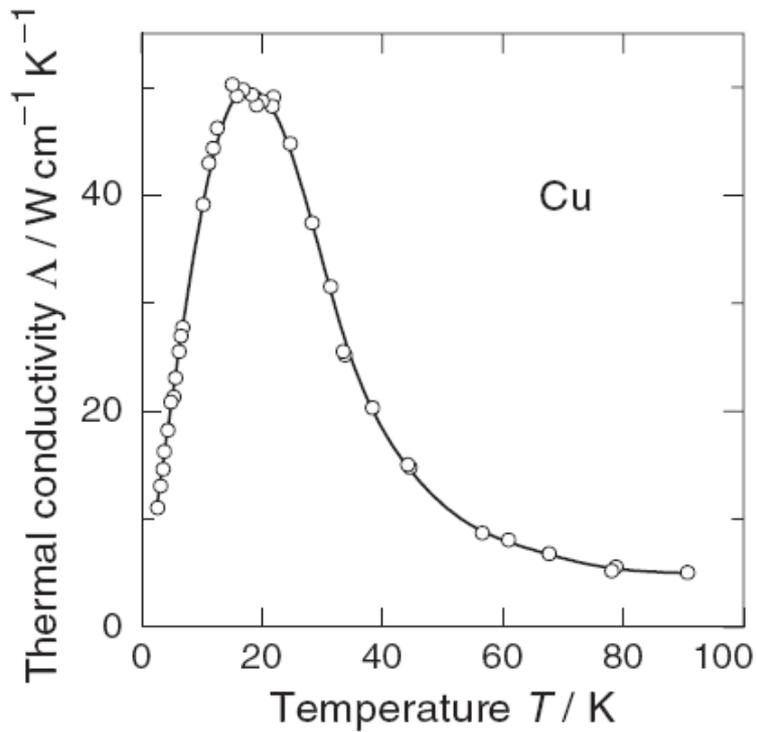
Since the impurity scattering is elastic, the ratio approaches unity again and the Wiedemann–Franz law revives in the range where the temperature-independent residual resistivity is observed.



Temperature dependence of  $L/L_0$ . Curve (a) refers to an ideally perfect crystal metal with zero residual resistivity. The residual resistivity increases in the sequence (b) to (d). [Reproduced from H. M. Rosenberg, *Low Temperature Solid State Physics*, (Clarendon Press, Oxford 1963)]

the conditions for the Wiedemann–Franz law to be valid

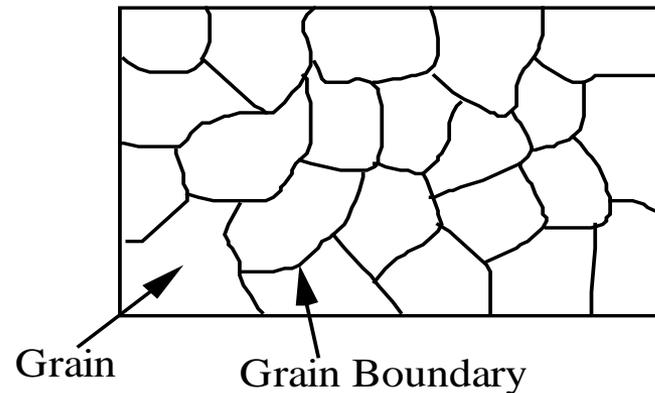
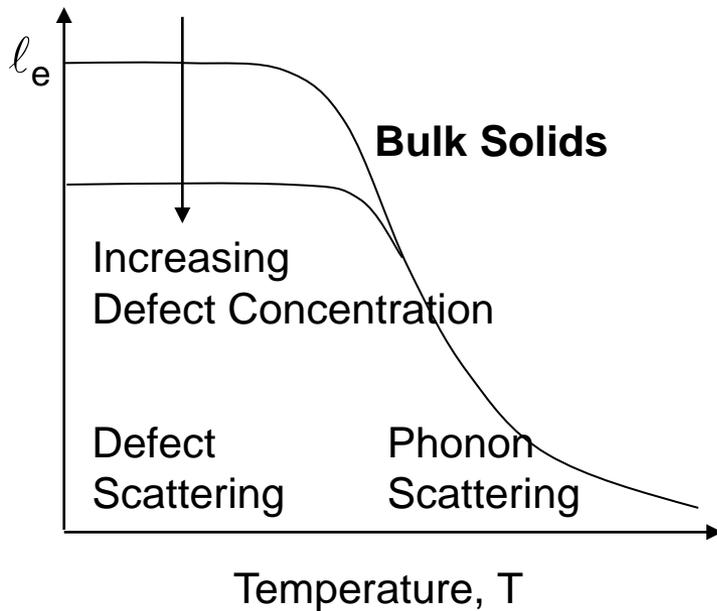
- (1) The **phonon thermal conductivity** can be ignored relative to the electronic thermal conductivity
- (2) The **elastic scattering** should dominate. This is realized either at high temperatures  $T > \Theta_D$  or at low temperatures where only the residual resistivity is observed.
- (3) The **relaxation time** involved in the electronic thermal conductivity **is the same** as that in the electrical conductivity so that the same scattering mechanism must be responsible for both of them.



**Fig. 7.14.** Thermal conductivity of copper. As in dielectric crystals, a pronounced maximum is observed [314]

## Electron Scattering Mechanisms

- Defect Scattering
- Phonon Scattering
- Boundary Scattering (Film Thickness, Grain Boundary)



from Solid State Course by Mark Jarrel (Louisiana Univ.),

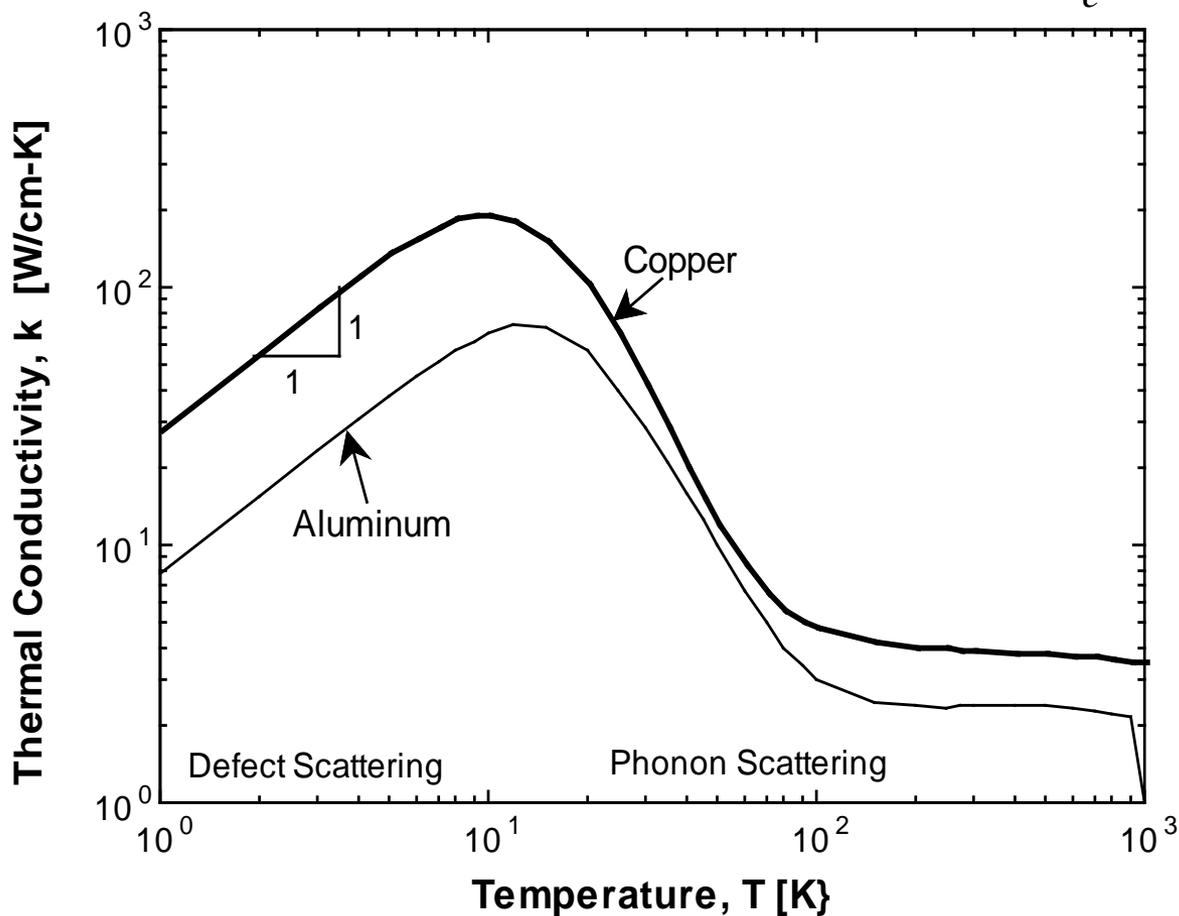
# Thermal Conductivity of Cu and Al

$$k_e = \frac{1}{3} C_e v_F \ell_e = \frac{1}{3} C_e v_F^2 \tau_e$$

Matthiessen Rule:

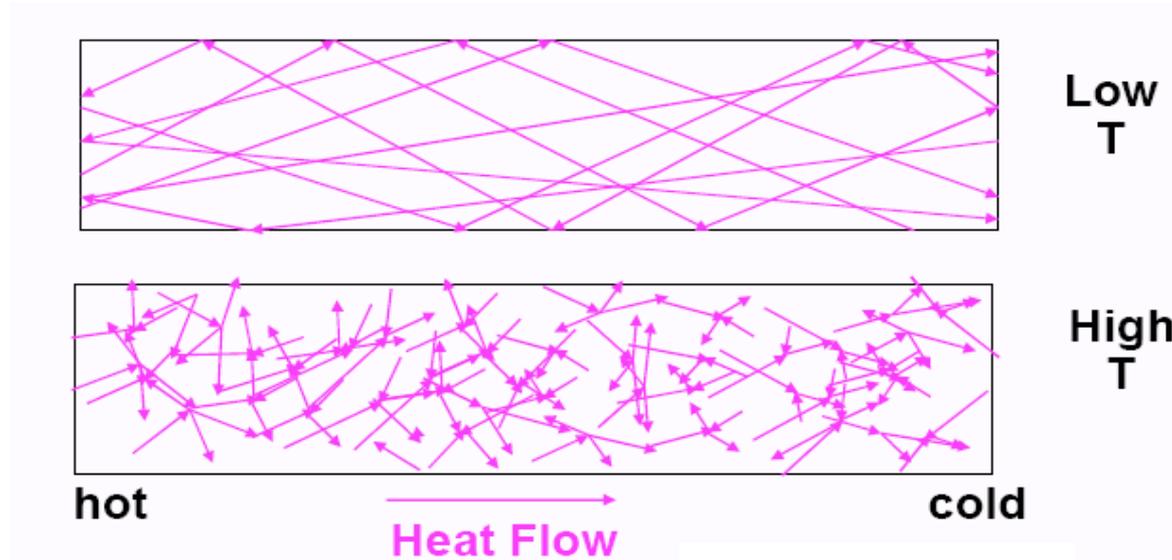
$$\frac{1}{\tau_e} = \frac{1}{\tau_{defect}} + \frac{1}{\tau_{boundary}} + \frac{1}{\tau_{phonon}}$$

$$\frac{1}{\ell_e} = \frac{1}{\ell_{defect}} + \frac{1}{\ell_{boundary}} + \frac{1}{\ell_{phonon}}$$



Electrons dominate  $k$  in metals

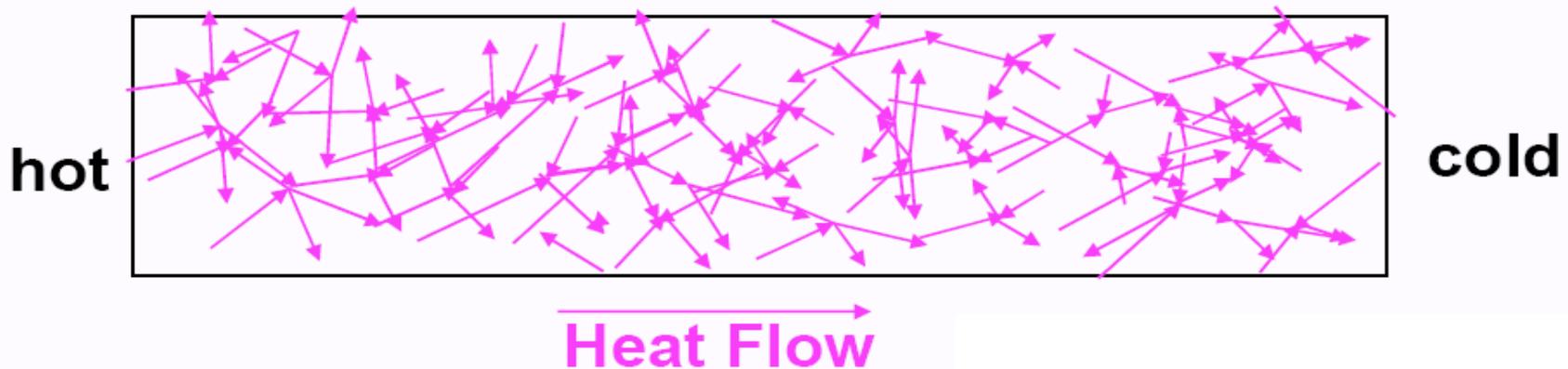
# The **Phonon** Thermal Conductivity in insulators



# Phonons also act like a gas

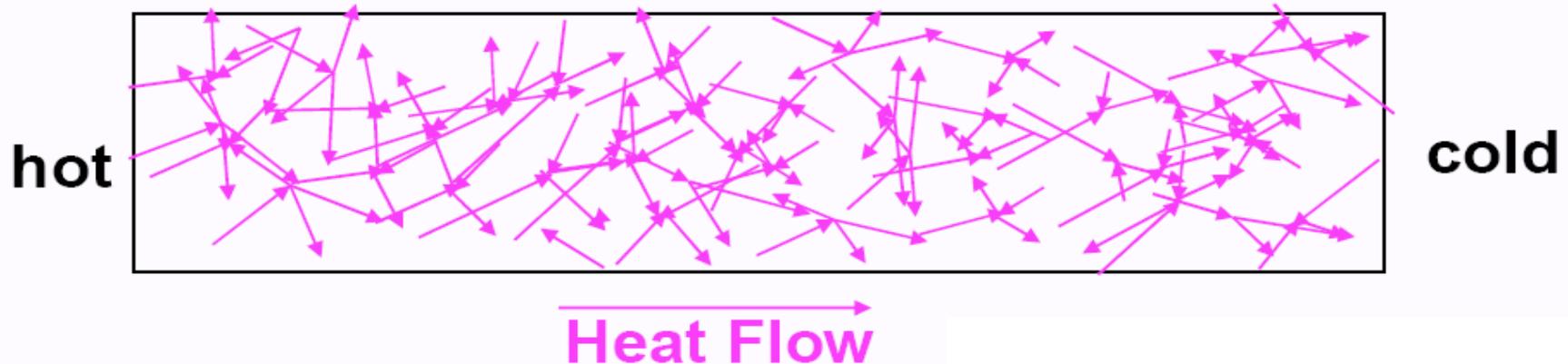
- A phonon is a particle - a quantum of vibration
- It carries energy just like a molecule.
- Phonon can come to equilibrium by scattering just like molecules
- Scattering is due to defects and anharmonicity.
- Leads to heat transport just as for molecules

$$K = (1/3) C v L = \text{thermal conductivity}$$



# Phonons also act like a gas

- What is different about phonons and gas molecules?
- Speed =  $v_{\text{group}}$  is largest for low energy ( $v_{\text{sound}}$ ) and smaller for high energy
- The heat capacity  $\sim T^3$  at low  $T$ ,  $\sim 3Nk_B$  at high  $T$
- The density of phonons  $\langle n \rangle$  increases with  $T$ . Scattering increases  $\sim \langle n \rangle$  since each phonon has scatters from other phonons. Therefore we expect the mean free path to decrease with  $T$



## Phonon–Phonon Scattering

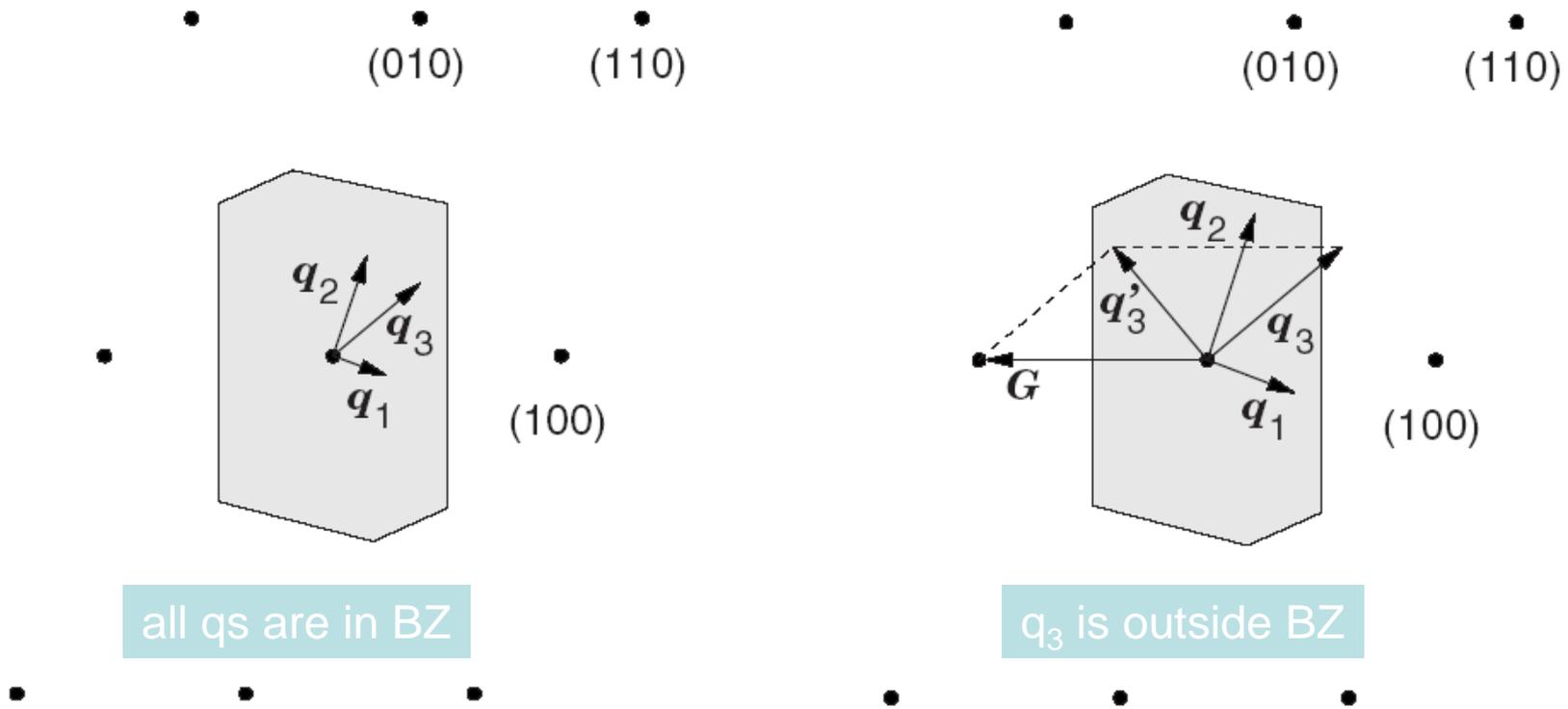
The most important interaction process between phonons is the *three-phonon process* in which two phonons merge into a single phonon, or a single phonon decays into two phonons. Conservation of energy and quasimomentum requires:

$$\hbar\omega_1 \pm \hbar\omega_2 = \hbar\omega_3 \quad \text{and} \quad \hbar\mathbf{q}_1 \pm \hbar\mathbf{q}_2 = \hbar\mathbf{q}_3 + \hbar\mathbf{G} .$$

Depending on the signs, these equations reflect the *creation* or *annihilation* of a phonon in the collision process. A characteristic feature of quasimomentum conservation is the occurrence of a reciprocal lattice vector  $\mathbf{G}$  in this equation. Processes that do not involve a reciprocal lattice vector are called *normal processes*, whereas those that do, are called *umklapp processes*.

crystal momentum is conserved

crystal momentum is not conserved



**Fig. 6.9.** Three-phonon processes. *Full circles* represent the reciprocal lattice. (a) Normal process: the wave vectors of all phonons lie within the *grey tinted* first Brillouin zone. (b) Umklapp process: the resulting vector  $q_3$  ends outside the first Brillouin zone. Addition of the reciprocal lattice vector  $G$  leads to the vector  $q'_3$  inside the zone

## Normal Processes

As already mentioned, the sum of the quasimomenta of the colliding phonons is conserved in N-processes, and consequently the total quasimomentum  $\mathbf{P}$  of all phonons is also conserved.

$$\mathbf{P} = \sum_{\mathbf{q}} n_{\mathbf{q}} \hbar \mathbf{q} = \text{const.}$$

$n_{\mathbf{q}}$  represents the number density of the phonons with the wave vector  $\mathbf{q}$ .

Since N-processes influence neither the flux of momentum nor the transport of energy they do not degrade the thermal current.

Because these processes also conserve the total quasimomentum  $\mathbf{P}$ , they do not give rise to heat resistance

## Umklapp Processes

It is possible for  $q_3$  to lie outside the first Brillouin zone even if three phonons take part, as in the N-process. In this case, the addition of a reciprocal lattice vector brings the wave vector of the generated phonon back into the first zone. However, the total quasimomentum  $P$  is changed by these umklapp processes and consequently the heat flow is degraded.

At high temperatures, the overwhelming number of excited phonons are phonons with a **frequency close to the Debye frequency  $\omega_D$**  and a wave vector comparable with that of the zone boundary. As a consequence, virtually **every collision** leads to a final state **outside the Brillouin zone** and is therefore an **umklapp process**. At  $T > \Theta$  the number of thermally excited phonons and hence the density of scattering centers  $n$  rises **proportional to  $T$** . Since the **frequency** of the **dominant** phonons is  $\omega_D$  that **does not change** with temperature, the cross section  $\Sigma$  for the phonon-phonon collisions is **constant**.

$$T > \Theta$$

$$\Lambda \propto T^{-1}$$

$$k = \frac{1}{3} C \cdot v \cdot \Lambda \quad \longrightarrow$$

$$k \propto T^{-1}$$

At low temperatures,

in the defect scattering range

$$C_v \sim T^3$$

$$\Lambda = \text{constant}$$

$$V_q = \text{constant}$$

$$k = \frac{1}{3} C \cdot v \cdot \Lambda$$

$$k \sim T^3$$

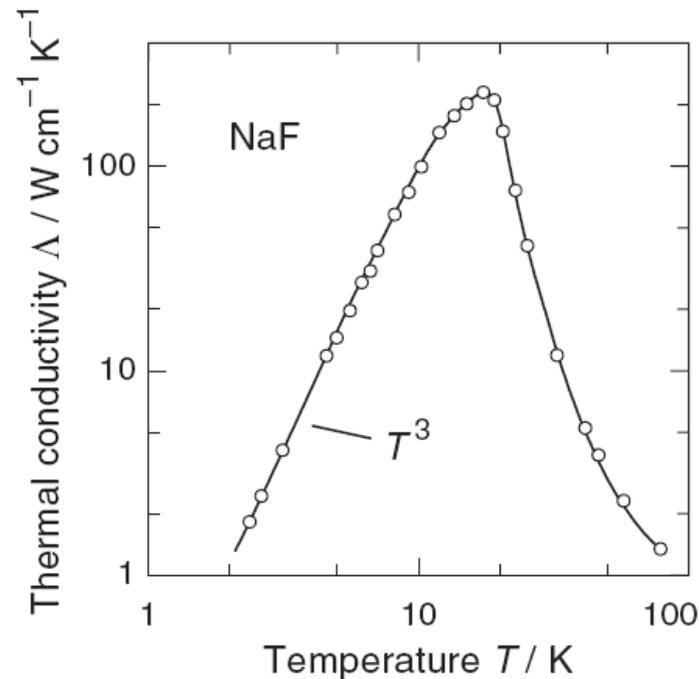
## Intermediate temperature

Umklapp processes are only possible if the colliding phonons carry high enough momenta. Roughly speaking, this condition is fulfilled for phonons with the frequency  $\omega > \omega_D/2$ . At intermediate temperatures, i.e., below the Debye temperature, the number of phonons with energy  $\hbar\omega_D/2$  decreases

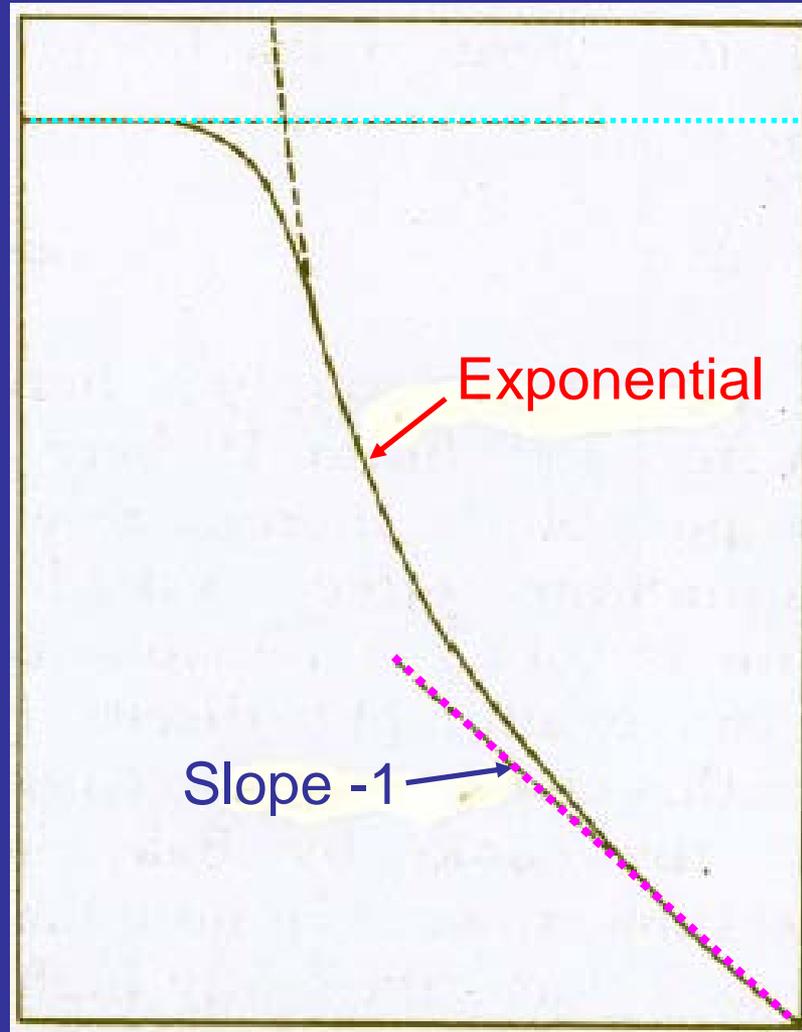
$$f(\omega, T) = [\exp(\hbar\omega_D/2k_B T) - 1]^{-1} \approx \exp(-\hbar\omega_D/2k_B T) = \exp(-\Theta/2T)$$

$$k \propto \Lambda \propto e^{\Theta/2T}$$

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Enss



## Log-log plot



Phonon mean  
free path  $\Lambda$   
(  $\propto \tau$  )

Very low  $T$  ,  
 $\Lambda = v_g \tau = \text{constant}$

Intermediate  $T$  ,  
 $\Lambda = v_g \tau \propto (1/T) \exp(1/T)$   
dominated by U process

High  $T$  ,  
 $\Lambda = v_g \tau \propto T^{-1}$

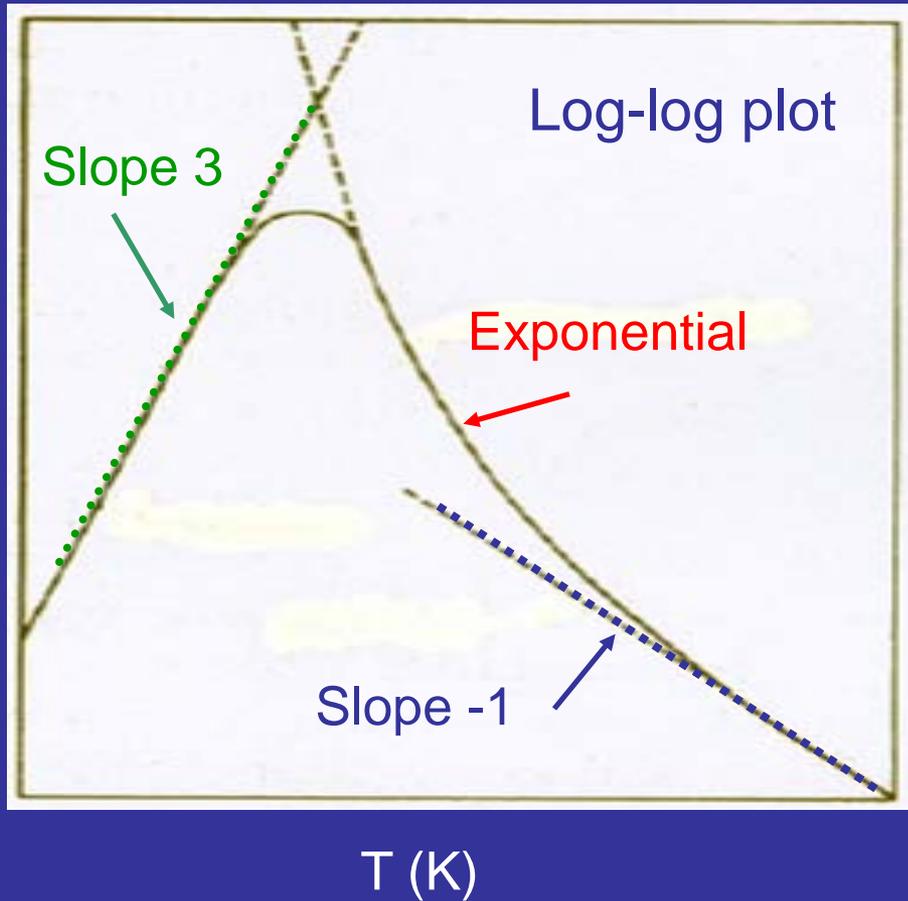
$T$  (K)

Other effects

Impurity scatterings

Defect scatterings

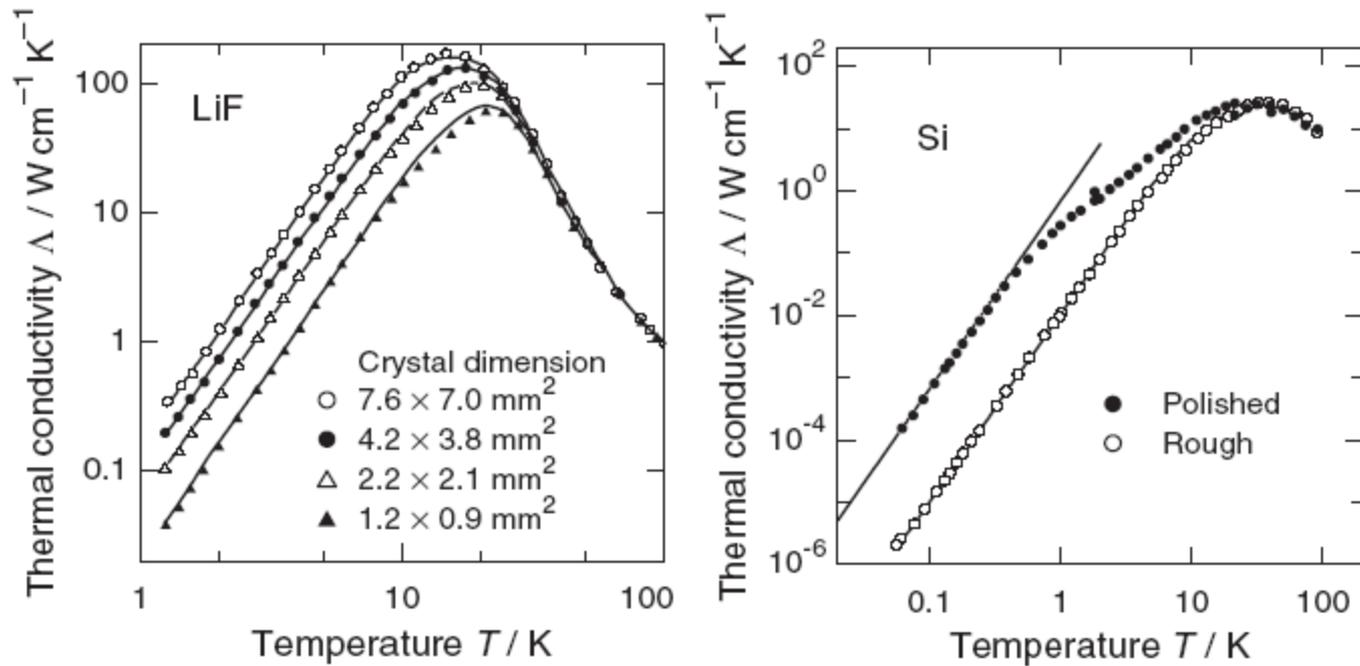
break periodicity



## Defect Scattering

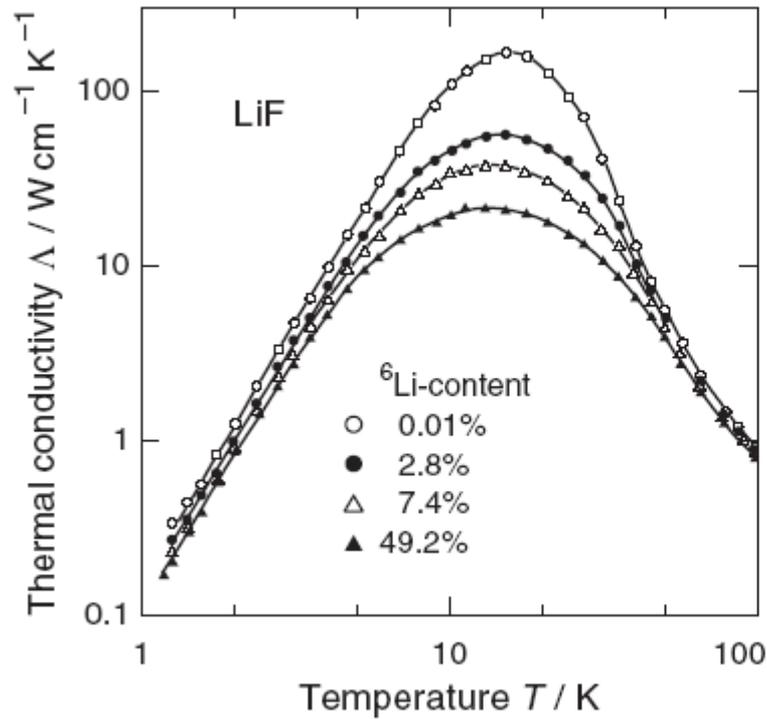
If the temperature decreases further, the rate of umklapp processes becomes vanishingly small and only N-processes remain. Nevertheless, the thermal conductivity does not continue to increase on cooling because the phonon mean free path is finally limited by defect scattering.

- **Surfaces**
- **Point Defects**
- **Dislocations**
- **Grain Boundaries**



**Fig. 6.10.** (a) Thermal conductivity versus temperature of LiF crystals with different cross-sectional areas [272]. (b) Thermal conductivity of silicon crystals with polished ( $\bullet$ ) and rough ( $\circ$ ) surface, respectively [273]

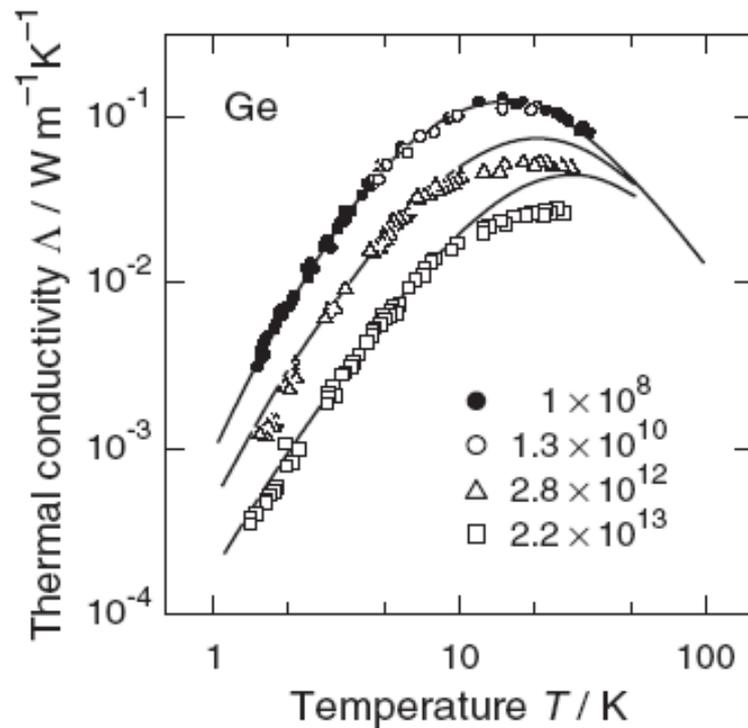
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$\text{Li}^7 - 96.25\%$

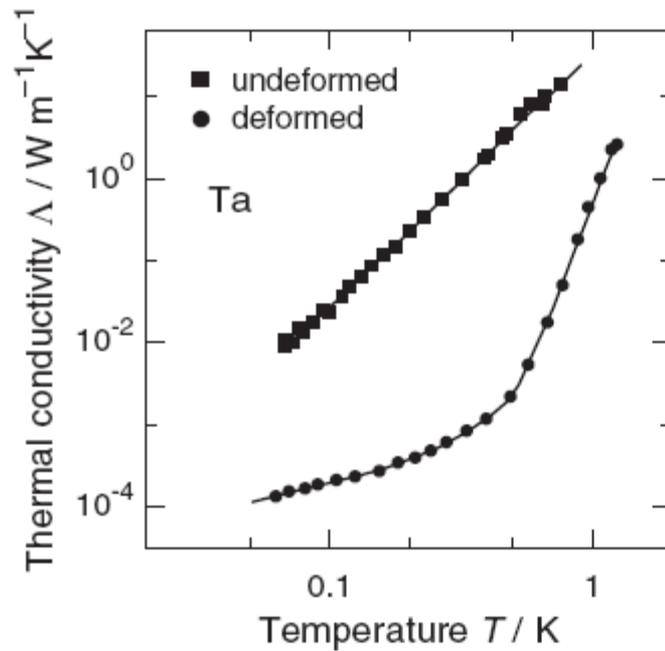
**Fig. 6.11.** Temperature variation of the thermal conductivity of LiF crystals with different  ${}^6\text{Li}$  concentration [274]

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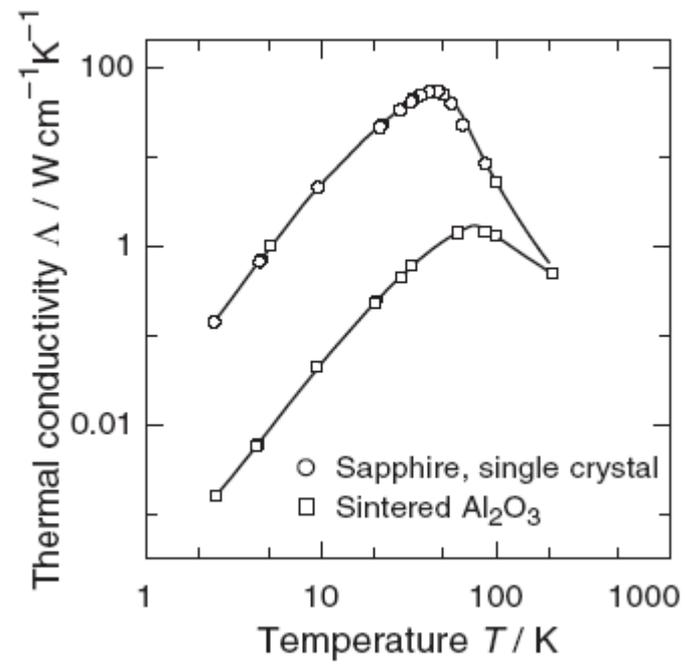
**Fig. 6.12.** Thermal conductivity of germanium crystals with a dislocation density ranging from  $10^8 \text{ m}^{-2}$  to  $2.2 \times 10^{13} \text{ m}^{-2}$ . *Solid lines* represent theoretical curves, as described in the text [276]

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**Fig. 6.13.** Thermal conductivity of high-purity tantalum single crystals. The conductivity of the undeformed specimen (*full squares*) is much higher than that of the deformed sample (*full circles*) with a dislocation density of  $4 \times 10^{14} \text{ m}^{-2}$  [279]

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**Grain Boundaries**

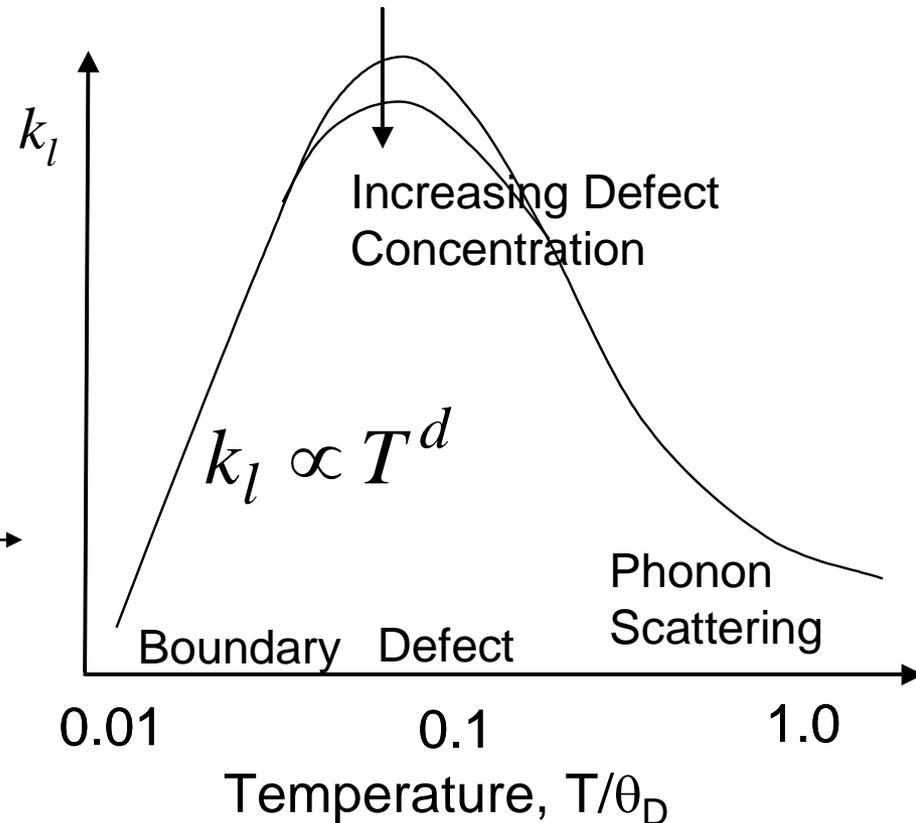
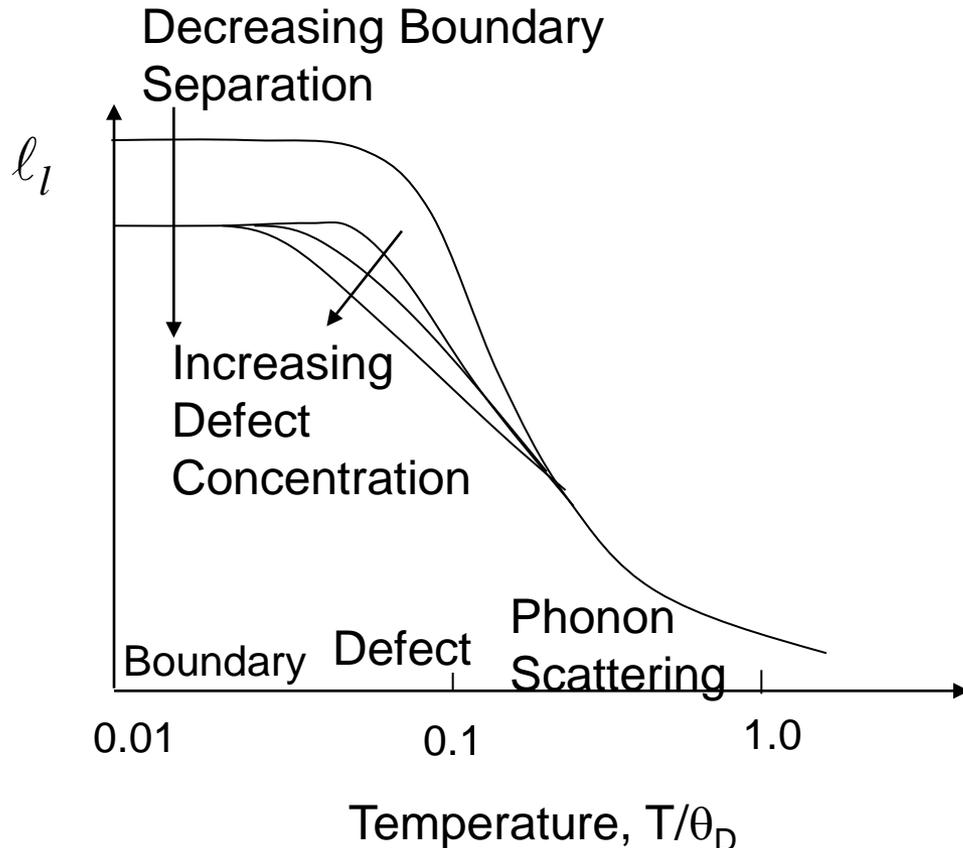
# Phonon Thermal Conductivity

## DIELECTRICS

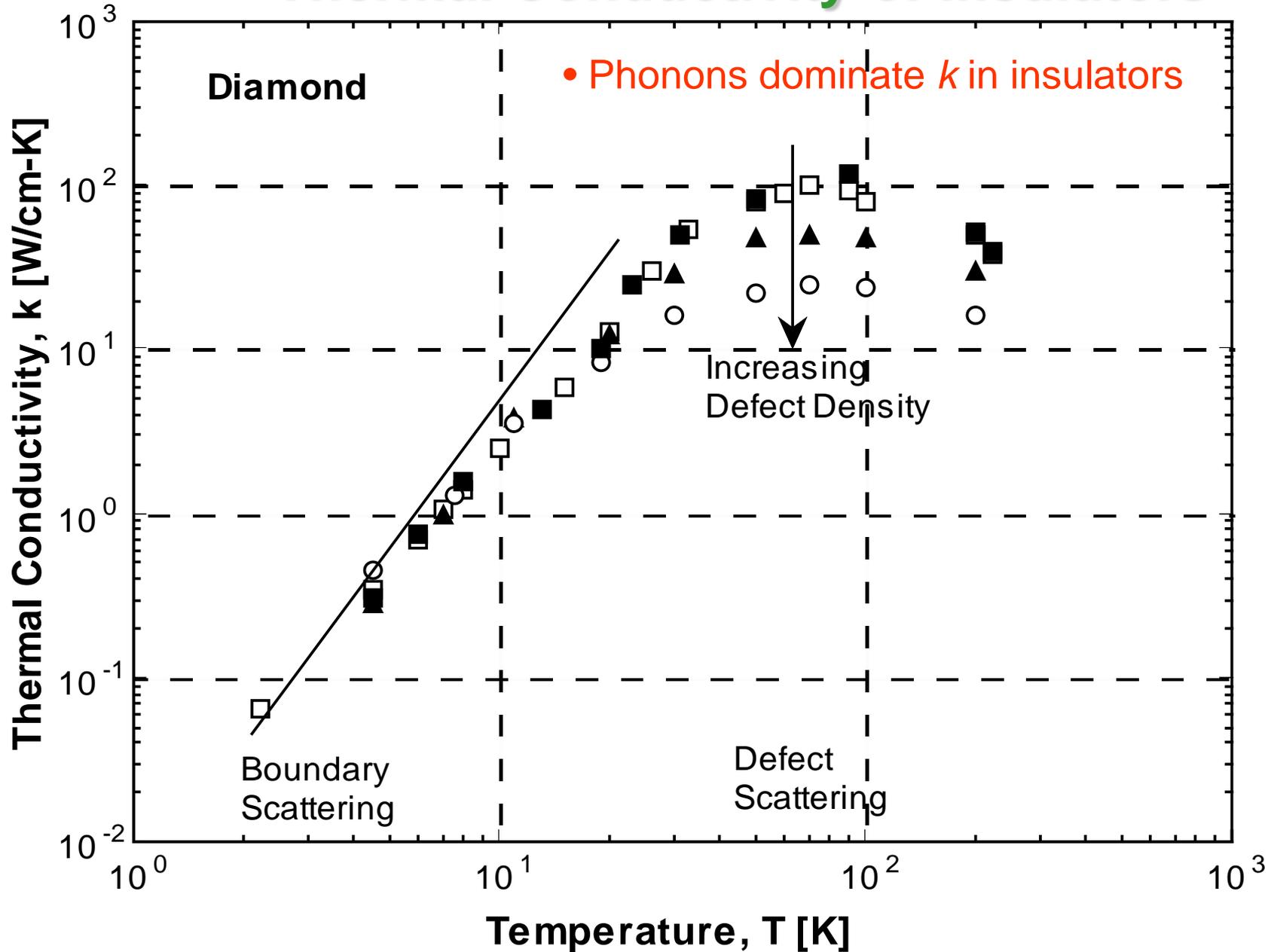
Kinetic Theory  $k_l = \frac{1}{3} C_l v_s \ell_l = \frac{1}{3} C_l v_s^2 \tau_l$

### Phonon Scattering Mechanisms

- Boundary Scattering
- Defect & Dislocation Scattering
- Phonon-Phonon Scattering



# Thermal Conductivity of Insulators



# Experimental Determination of the Thermal Conductivity

the equation for heat conduction

$$\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T(x,t)}{\partial t}$$

$$\alpha = k / C$$

$\alpha$  –thermal diffusivity

C represents the heat capacity per unit volume.

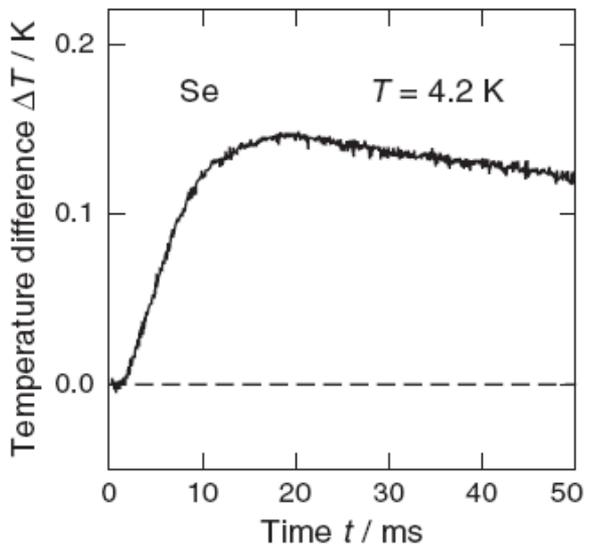
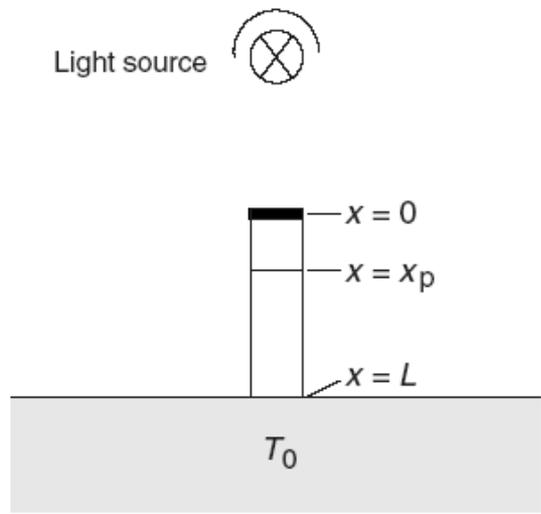


Fig. 6.7. (a) Schematic drawing of a setup to determine thermal conductivity and specific heat simultaneously. (b) Temporal variation of the temperature increase  $\Delta T$  at  $x = x_p$  for selenium at  $T_0 = 4.2$  K [268]

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$$\Delta T(x, t) = [T(x, t) - T_0]$$

$$\Delta T(x, t) \approx \frac{Q_{\text{pulse}}}{A \sqrt{\pi k C t}} \exp\left(-\frac{x^2}{4\alpha t}\right)$$

$$C = \frac{1}{A x_p \sqrt{\pi e/2}} \frac{Q_{\text{pulse}}}{\Delta T_{\text{max}}}$$

$$\alpha = \frac{x_p^2}{2t_{\text{max}}}$$

$$\alpha = k / C$$