

Beyond the Harmonic Approximation

Expectations within the harmonic approximation:

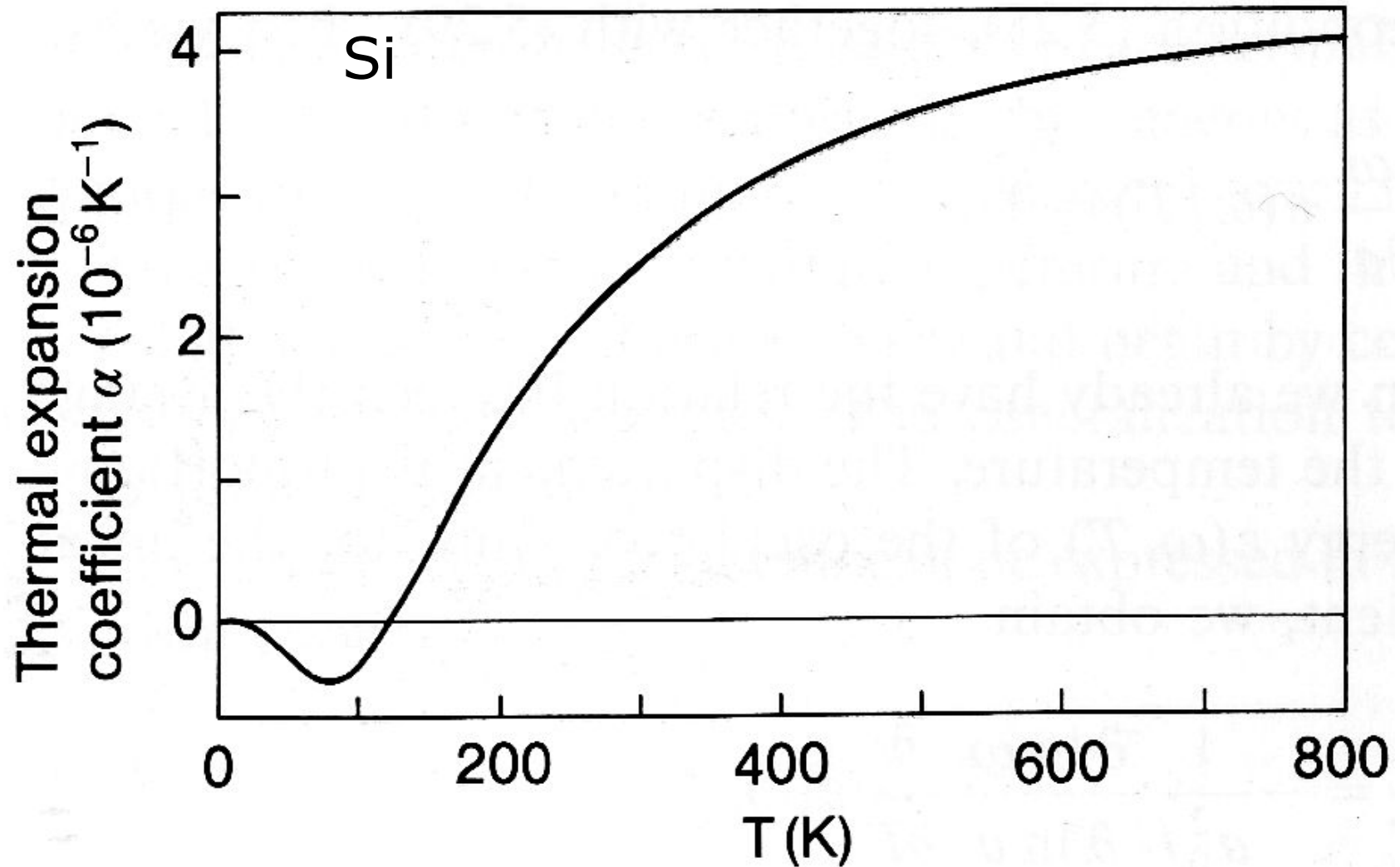
- modes independent (superposition)
- no damping, infinite phonon lifetime, sharp lines
- no thermal expansion
- elastic constants independent of T
- c_v constant at high T

Some findings from real crystals:

- phonon mixing (3-phonon processes)
- non-zero line widths
- thermal expansion
- elastic constants depend on T

Tafel: Ausdehnung

Thermal expansion need not be $\sim T$



Thermal conductivity vs. Temperature

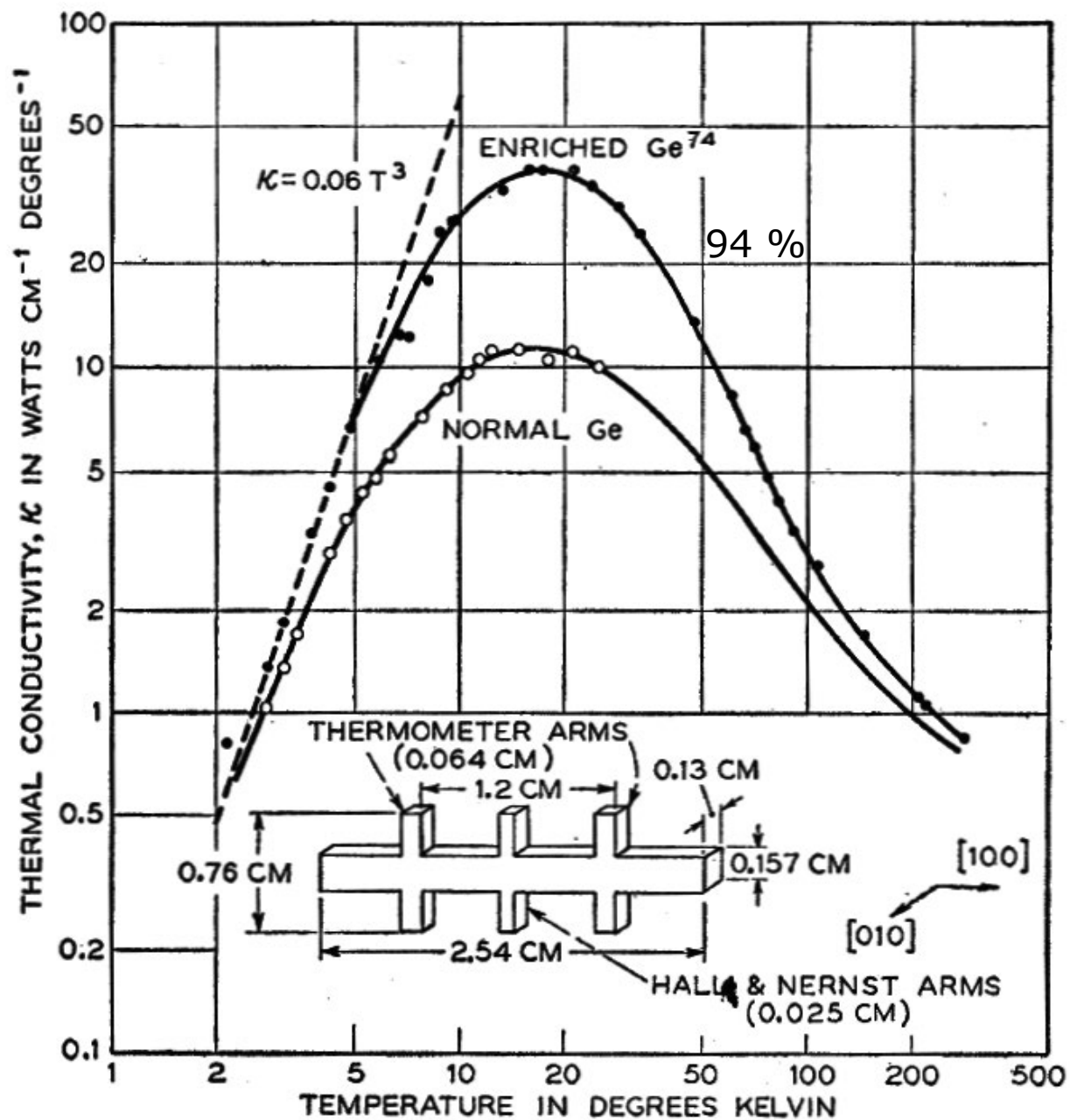


FIG. 1. Isotope effect on thermal conduction in Ge.

T. H. Geballe & G. W. Hull,
Phys. Rev. 110, 773 (1958)

Tafel: Wärmeleitung

Miniexkurs: Frequenzmischung

Eingangssignale: $x = \sin(\omega t)$, $y = \sin(\omega' t)$

lineares System, z. B. $x + y$

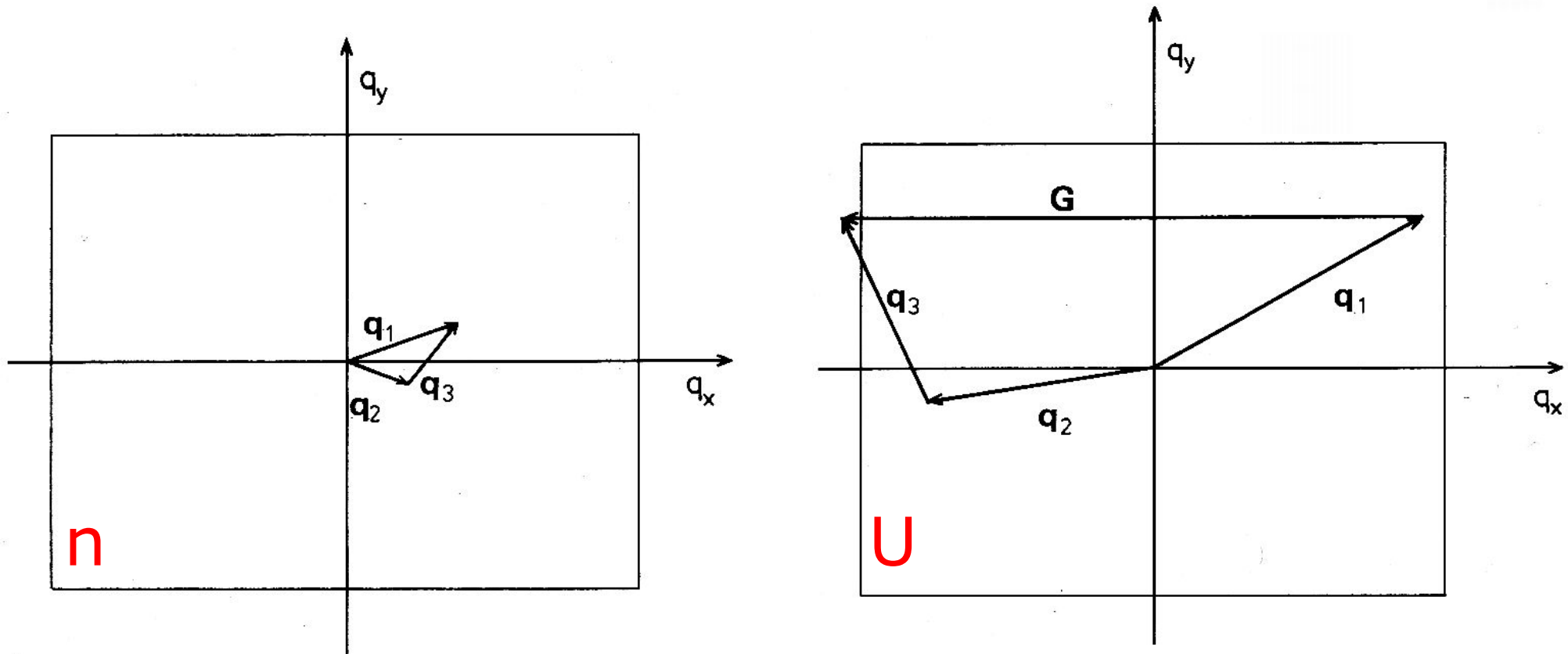
Spektrum des Ausgangssignals enthält nur ω und ω'

nichtlineares System, z. B. $x \cdot y$

Spektrum des Ausgangssignals enthält auch $\omega + \omega'$, $\omega - \omega'$

(falls $\omega = \omega'$ also 2ω)

denn $\sin(a) \sin(b) = \frac{1}{2} (\cos(a-b) - \cos(a+b))$



n-process: q_1 is split into two vectors q_2 and q_3 .

The sign of the x-component of the group velocity v_x remains unchanged.

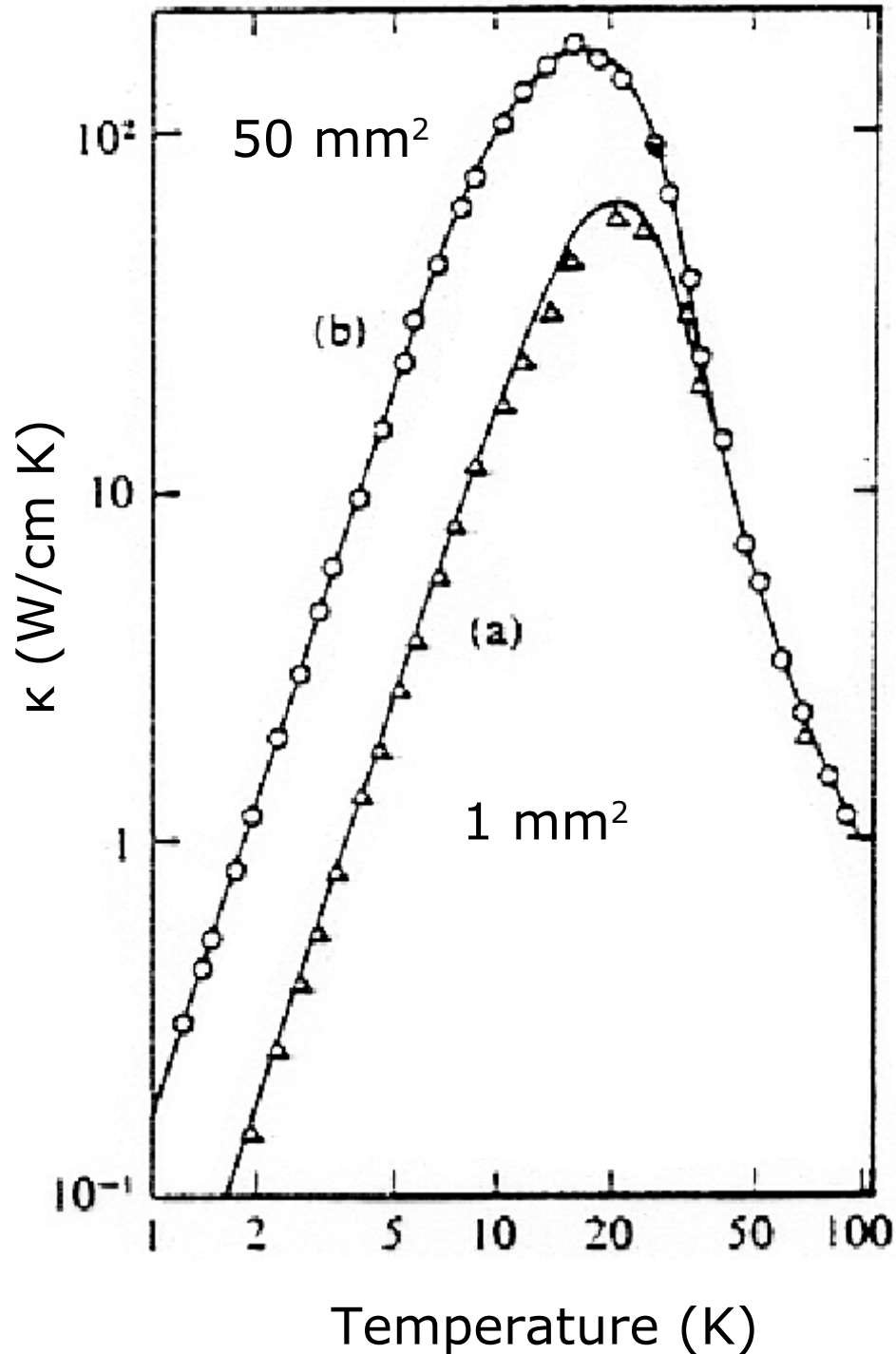
The direction of energy flow is not affected.

U-process: q_1 is split with the help of G .

For q_2 and q_3 , sign of v_x is inverted.

This reverses the direction of energy flow.

Low $T \rightarrow$ low $\omega \rightarrow$ low $q \rightarrow$ No U



Lattice thermal conductivity vs. T

LiF single crystal bars

(Li enriched to 99.9 % ^7Li to minimize isotope scattering)

cross-sections:

(a) $1.23 \times 0.91 \text{ mm}^2$

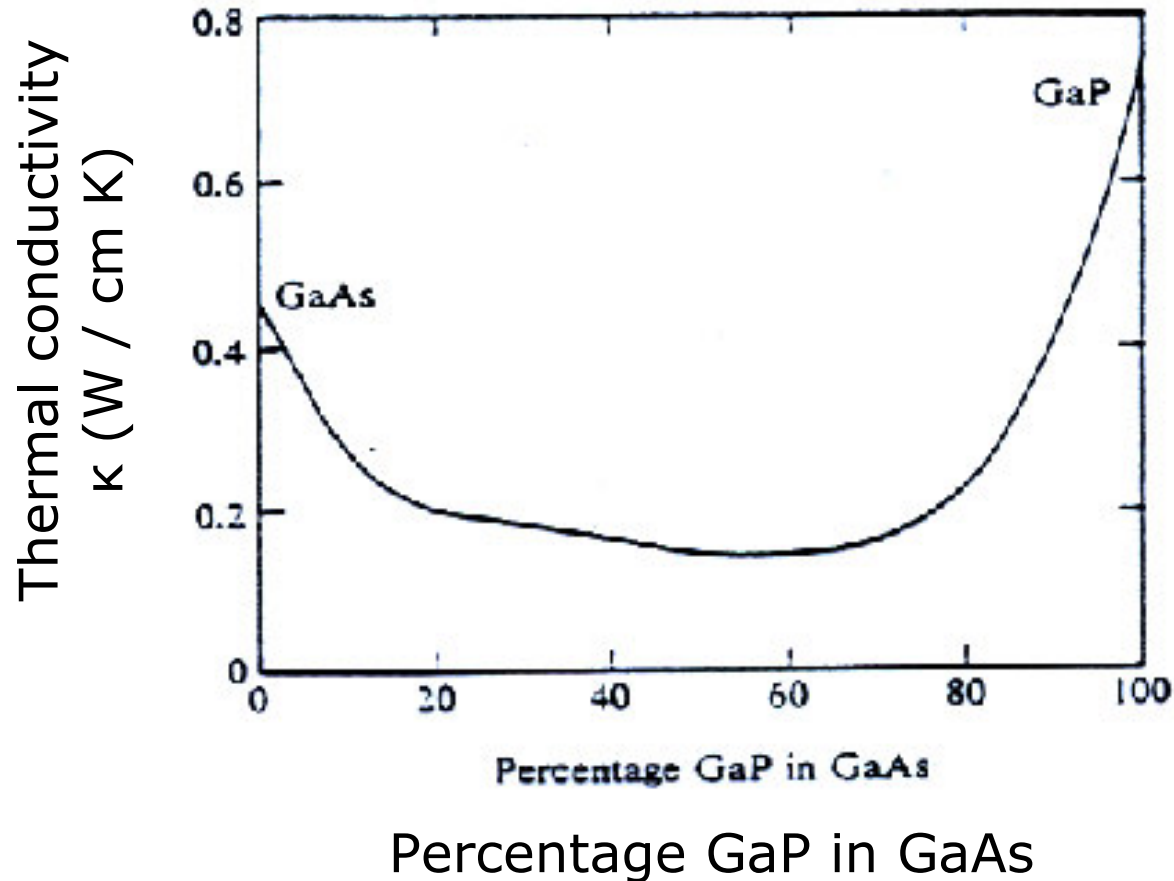
(b) $7.55 \times 6.97 \text{ mm}^2$

High T: U-processes

Low T: boundary scattering

Data from R. Bermann, Cryogenics 5, 297 (1965)

Chemical composition: Alloy scattering



Thermal conductivity at 3000 K for $\text{GaAs}_x\text{P}_{1-x}$

After P. D. Maycock. Solid State Electronics **10**, 161 (1967)

Disorder

Thermal conductivity of SiO_2
(quartz) perpendicular
to the c-axis

- single-crystal
- same crystal with defects
induced by n-bombardment
- quartz glass

