6. Phonons

6.1 Specific heat — Debye model:

assumptions:

- solids are elastic, isotropic homogenous continua
- excitations: sound waves with linear dispersion
- Bose-Einstein distribution

internal energy:

cut-off frequency → Debye frequency

$$U(T) = \int_0^{\hbar\omega_\mathrm{D}} \hbar\omega\, \mathcal{D}(\omega)\, f(\omega, T)\, \mathrm{d}\omega$$

$\mathcal{D}(\omega) \propto \omega^2$

specific heat:

$$C_V = \frac{\partial U}{\partial T} = 9Nk_\mathrm{B} \left(\frac{T}{\Theta}\right)^3 \int_0^{x_\mathrm{D}} \frac{x^4 \mathrm{e}^x}{\left(\mathrm{e}^x - 1\right)^2}\, \mathrm{d}x$$

$x_\mathrm{D} = \hbar\omega_\mathrm{D}/k_\mathrm{B}T$

$x = \hbar\omega/k_\mathrm{B}T$

$\Theta = \hbar\omega_\mathrm{D}/k_\mathrm{B}$

6.1 Specific Heat

Limiting cases:

(i) $T \to \infty \longrightarrow x \to 0$

$$\lim_{x\to 0} \int_0^{x_\mathrm{D}} \frac{x^4\,\mathrm{e}^x}{(\mathrm{e}^x-1)^2}\mathrm{d}x \approx \int_0^{x_\mathrm{D}} \frac{x^4\cdot 1}{x^2}\mathrm{d}x = \frac{x_\mathrm{D}^3}{3} = \frac{1}{3}\left(\frac{\Theta}{T}\right)^3$$

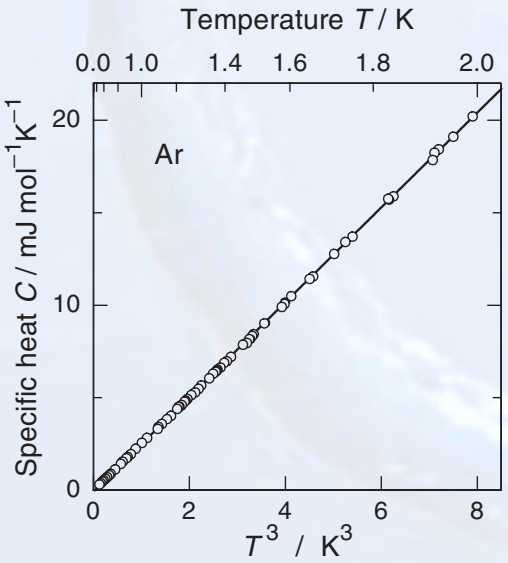
$(\mathrm{e}^x-1)^2 \approx (1+x-1)^2$

$$\longrightarrow \boxed{C_V = 3Nk_\mathrm{B}}$$ Dulong-Petit law

(ii) $T \to 0 \longrightarrow x_\mathrm{D} \to \infty$

$$C_V = 9Nk_\mathrm{B}\left(\frac{T}{\Theta}\right)^3 \underbrace{\int_0^{\infty} \frac{x^4\mathrm{e}^x}{(\mathrm{e}^x-1)^2}\mathrm{d}x}_{4\pi^4/15} = \frac{12\pi^4}{5}Nk_\mathrm{B}\left(\frac{T}{\Theta}\right)^3$$

$$\longrightarrow \boxed{C_V = \frac{12\pi^4}{5}Nk_\mathrm{B}\left(\frac{T}{\Theta}\right)^3}$$



- perfect agreement with theory
- only small temperature range
- Debye temperature $\Theta = 92\,\mathrm{K}$

6.1 Specific Heat

Element	Θ (K)	Element	Θ (K)	Element	Θ (K)	Element	Θ (K)
Ar	92	Cu	347	Mn	409	Sc	346
Ac*	100	Er	118	Mo	423	Se	152
Ag	227	Fe	477	N*	70	Si	645
Al	433	Ga	325	Na	156	Sm	169
Am	121	Gd	182	Nb	276	Sn	199
As	282	Ge	373	Nd	163	Sr	147
Au	162	H (para)	122	Ne	75	Ta	245
B	1480	H (orth)	114	Ni	477	Tb	176
Ba	111	^{3}He	19–33	Np	259	Te	152
Be	1481	Hf	252	O*	90	Th	160
Bi	120	Hg	72	Os	467	Ti	420
C (Dia.)	2250	Ho	190	Pa	185	Tl	78
C (Gra.)	413	I	109	Pb	105	Tm	200
Ca	229	In	112	Pd	271	U	248
Cd	210	Ir	420	Pr	152	V	399
Ce	179	K	91	Pt	237	W	383
Cl*	115	Kr	72	Rb	56	Xe	64
Cm	123	La	145	Re	416	Y	248
Co	460	Li	344	Rh	512	Yb	118
Cr	606	Lu	183	Ru	555	Zn	329
Cs	40	Mg	403	Sb	220	Zr	290

6.1 Specific Heat

Compound	Θ (K)	Compound	Θ (K)	Compound	Θ (K)
AgBr*	140	$Cr_2Cl_3^*$	360	MgO*	800
AgCl*	180	FeS_2^*	630	MoS_2^*	290
$As_2O_3^*$	140	KBr	173	RbBr	131
$As_2O_5^*$	240	KCl	235	RbCl	165
$AuCu_3$	285	KI	131	RbI	103
BN*	600	InSb	206	SiO_2 (Quartz)	470
CaF_2	508	LiF	736	TiO_2^* (Rutile)	450
$CrCl_2^*$	80	LiCl	422	ZnS	315

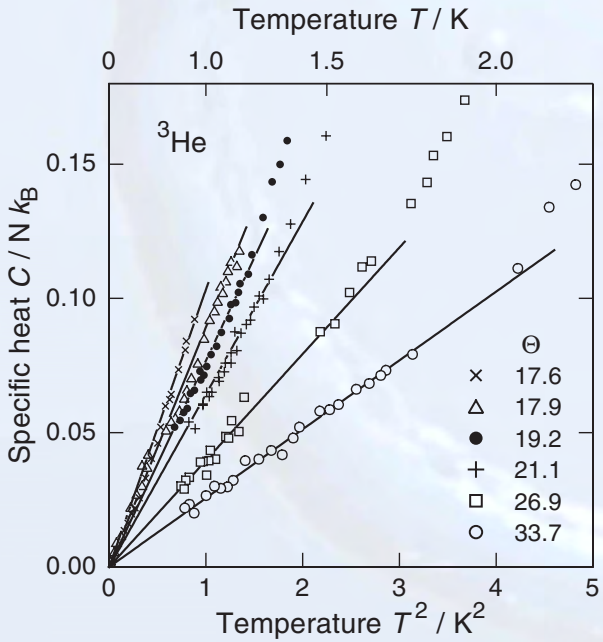
6.1 Specific Heat

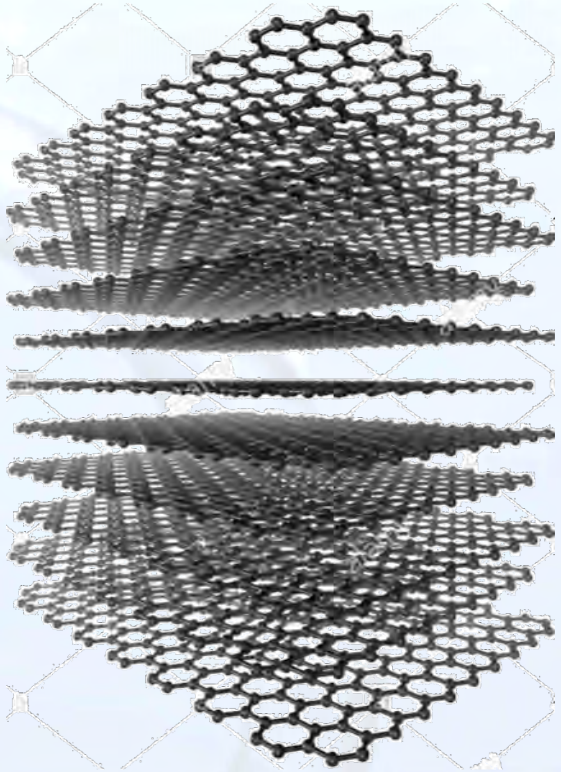
low-dimensional systems

$$D(\omega) \propto \omega^{d-1} \longrightarrow C_V \propto T^d$$

$$d = 2 \longrightarrow C_V \propto T^2$$

example: ^{3}He atoms on graphite (sub-mono layers)





- high temperatures and low densities ⟶ gas: $C_V \approx N k_B$
- for $n > 0.078\,\text{Å}^{-2}$ ⟶ two-dimensional solid crystals
- increasing density ⟶ Θ increases
- density $0.078 \ldots 0.092$ per Å^2 ⟶ $\Theta = 17.6 \ldots 37.7\,\text{K}$
- at high temperatures melting of 2d-crystals

6.2 Heat transport

Fourier equation $\boldsymbol{j} = -\Lambda \nabla T$

$$\Lambda = \frac{1}{3} C v \ell$$

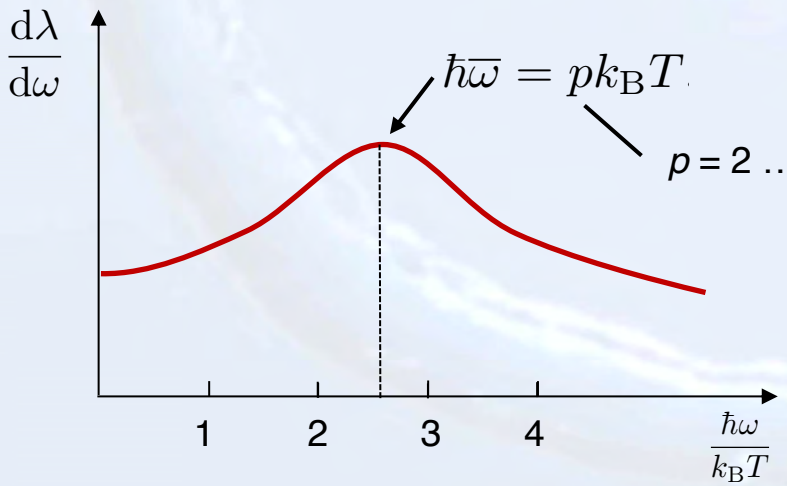
in general

$$\Lambda = \frac{1}{3} \sum_i \int c_i(\omega)\, v_i(\omega)\, \ell_i(\omega)\, \mathrm{d}\omega$$

spectral specific heat

different “particles” ⟶ phonon branches

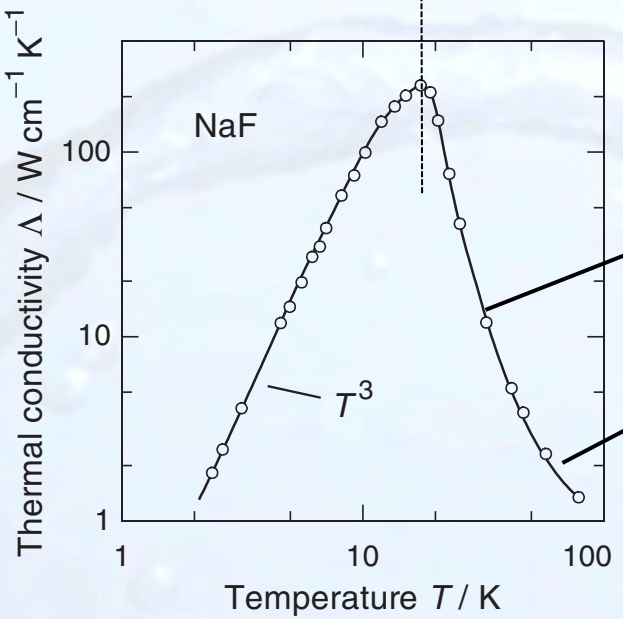
dominate phonon approximation (Debye)



- summation and integration can be avoided
- in addition: linear dispersion

6.2 Heat Transport

phonon-defect scattering ← → phonon-phonon scattering

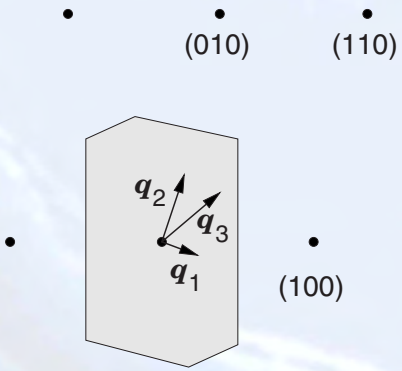


$$\Lambda \propto \ell_{\mathrm{U}} \propto \mathrm{e}^{\Theta/2T}$$

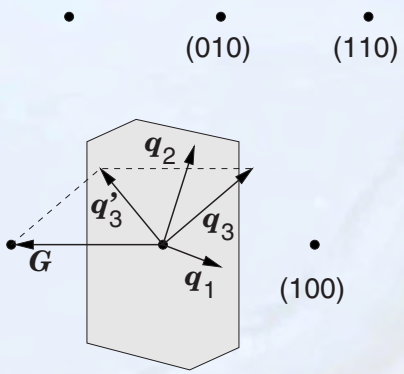
$$\Lambda \propto T^{-1}$$

number of umklapp processes increases with temperature

normal process



umklapp process



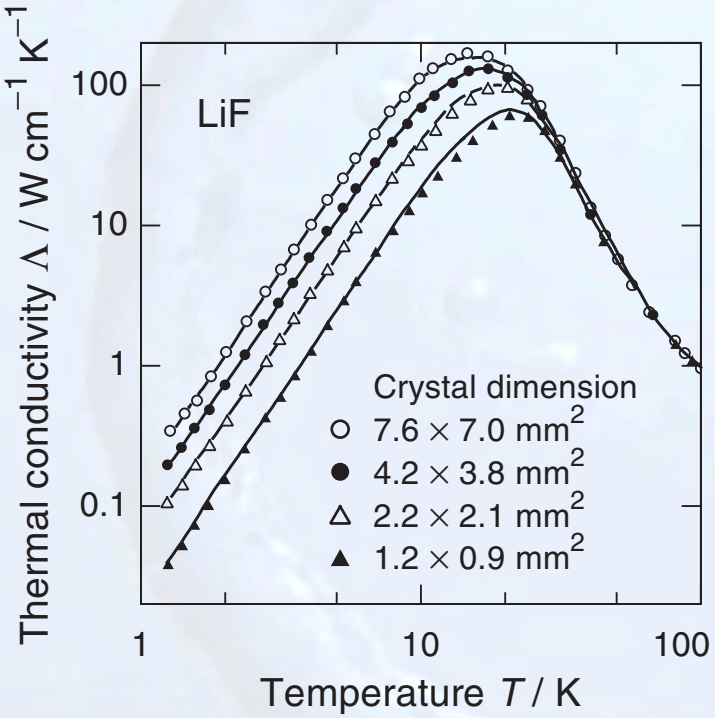
6.2 Heat Transport

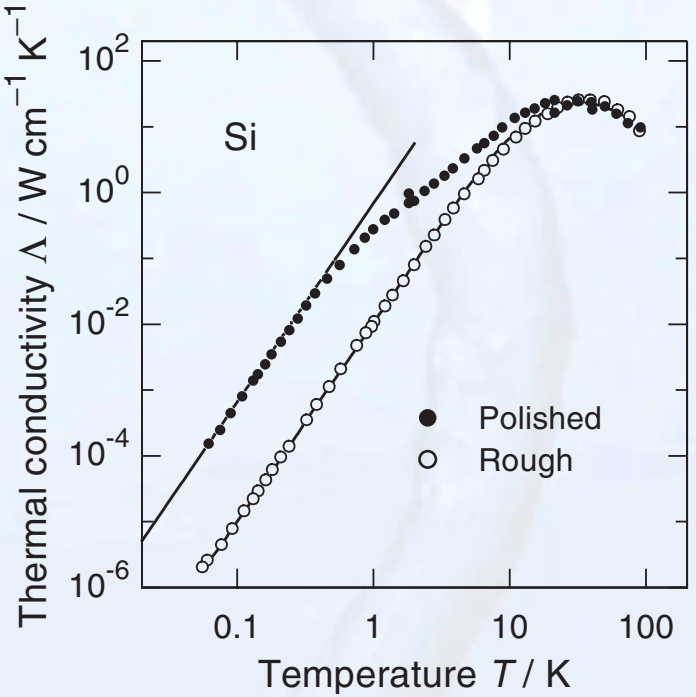
phonon-defect scattering

a) surfaces

$$\Lambda = \frac{1}{3} C v \ell \xrightarrow{\ell \approx d} \Lambda \approx \frac{1}{3} C_V v d \propto T^3$$

Casimir regime





- depends on sample cross-section
- temperature dependence as expected

- roughed: mean free path factor 50 shorter
- polished: mean free path 7 cm, sample length

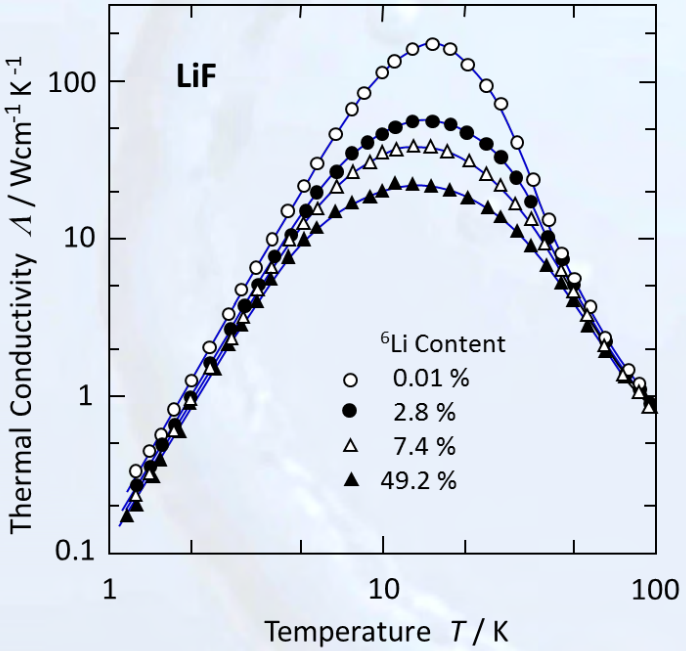
6.2 Heat Transport

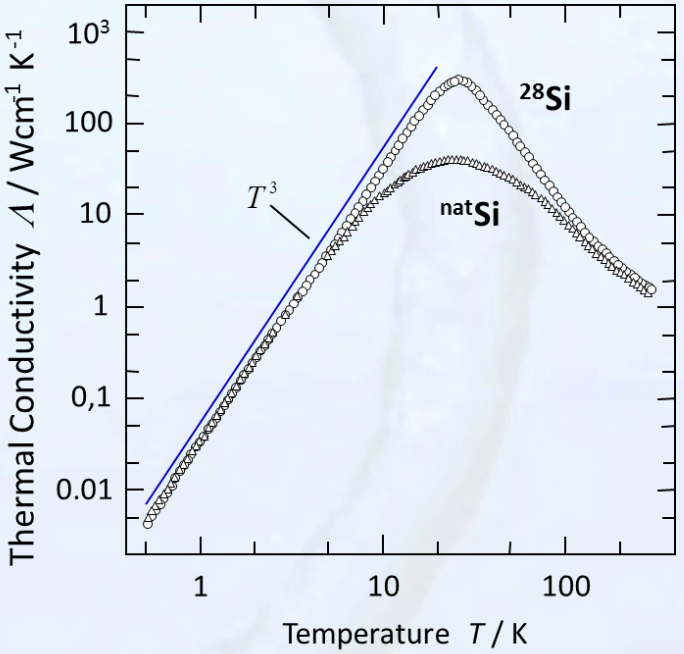
b) influence of point defects (elastic scattering)

⟶ Rayleigh scattering, since $\lambda_{\text{phonon}} \gg d_{\text{defect}}$

$$\ell^{-1} = \frac{n_{\text{p}} V_{\text{A}}^2}{4\pi} \left(\frac{\Delta M}{M}\right)^2 q^4 \propto \omega^4$$

is important at intermediate temperatures, since at low temperature q is too small and at high temperatures phonon-phonon scattering dominates



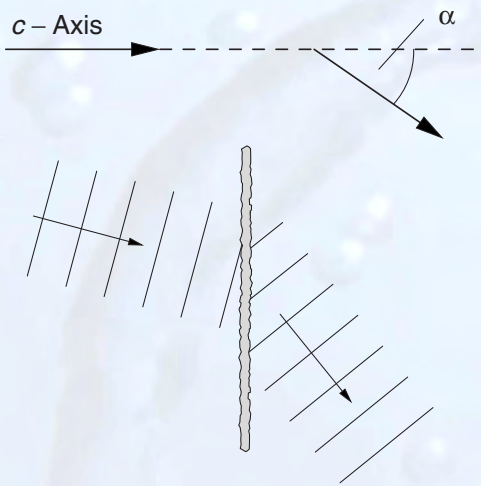


- adding ^{6}Li reduces heat transport
- maximum becomes rounded

- ^{nat}Si: 10% of all Si atoms have mass difference
- ^{28}Si: sharp peak ⟶ little scattering on point defects

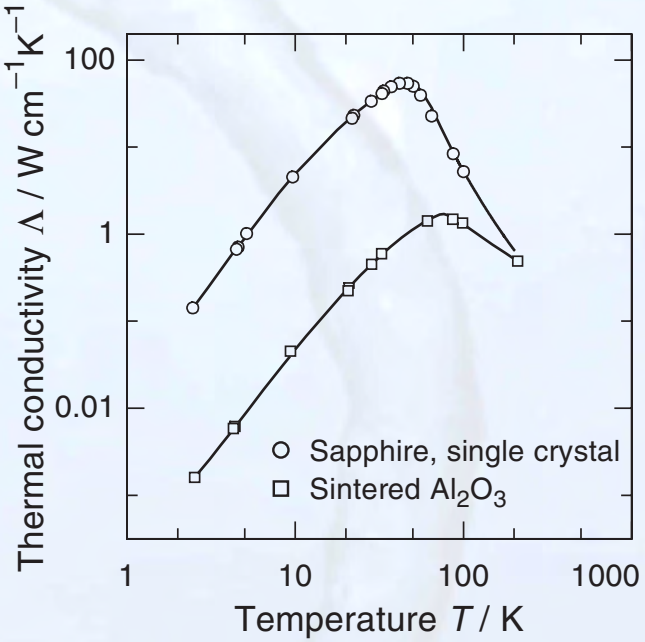
6.2 Heat Transport

c) grain boundaries



$$\ell \approx L/\langle \sin^2 \alpha \rangle$$

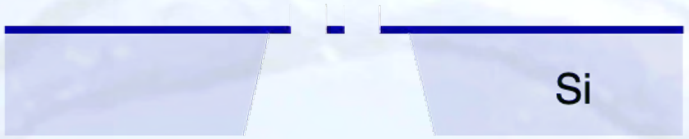
average size of crystallites



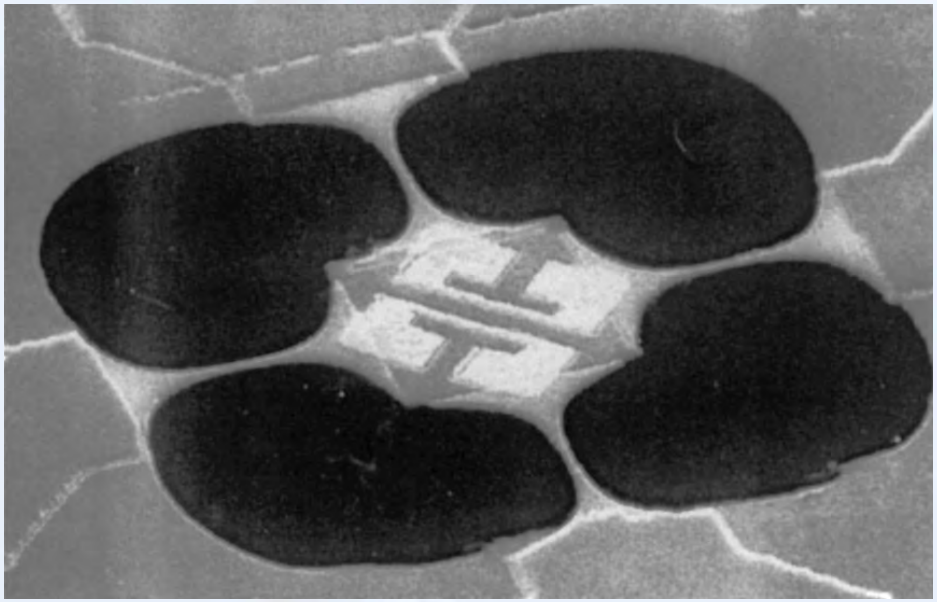
- sapphire single crystal: 1.5 mm
- sintered Al_2O_3 powder 5 … 30 µm

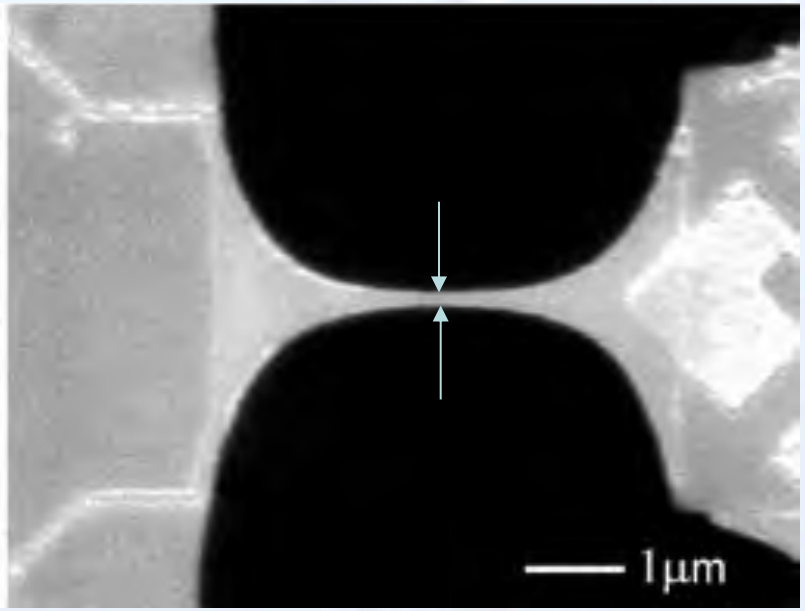
6.3 Thermal Conductivity in One-dimensional Samples

Geometry of setup:



Si_3N_4 silicon nitride





4 × 4 µm^3 island with gold resistors as heaters and thermometers

minimal width of bridge $w < 200$ nm

6.3 Thermal Conductivity in One-dimensional Samples

heat flow: $J = \frac{1}{L} \sum_{q} \hbar \omega_q v_q$

L: length of sample; q: all thermally excited phonons

summation ⟶ integration

$$J = \sum_i \frac{1}{L} \int_0^\infty \mathcal{D}_i^1(q)\, \hbar \omega_i\, v_i\, [f_\mathrm{h}(\omega, T) - f_\mathrm{c}(\omega, T)]\, \mathrm{d}q$$

i: phonons modes; v_i: group velocity

assumptions

- transmission coefficient for coupling between bath and thin bar = 1
- $\mathcal{D}_i^1(q) = L/2\pi\,, \quad q \longleftrightarrow \omega\,, \quad \frac{\partial q}{\partial \omega}$ cancels with $v = \frac{\partial \omega}{\partial q}$
- small temperature difference ΔT

  ⟶ $[f_\mathrm{h}(\omega, T) - f_\mathrm{c}(\omega, T)]$ can be expanded, keep only terms linear in ΔT

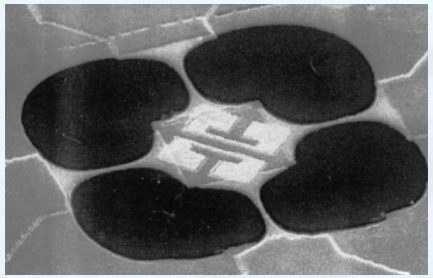
$$G = \frac{J}{\Delta T} = \frac{k_\mathrm{B}^2 T}{h} \sum_i \int_0^\infty \frac{x^2 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} \mathrm{d}x = N_i \underbrace{\frac{\pi^2}{3} \frac{k_\mathrm{B}^2 T}{h}}_{\text{quantum of thermal conductance } G_0} = N_i G_0$$

N_i: number of contributing modes

$$\boxed{G = N_i G_0}$$

Quantized of Heat Conduction: Sample Geometry

for given geometry



$N_i = 4 \times 4$ legs $= 16$

modes:
1 longitudinal (dilatation)
1 torsional
2 bending

$$G_0 = (9.456 \times 10^{-13}\,\mathrm{W\,K^{-2}})\,T$$

- transition roughly at 0.8 K

$$T_{\mathrm{crossover}} \approx \frac{h\nu}{2wk_{\mathrm{B}}} \approx 0.8\,\mathrm{K}$$

expected for: $q_{\mathrm{th}} \approx k_{\mathrm{B}}T/(\hbar v) < \Delta q = \frac{\pi}{w}$

spacing between lowest lying modes