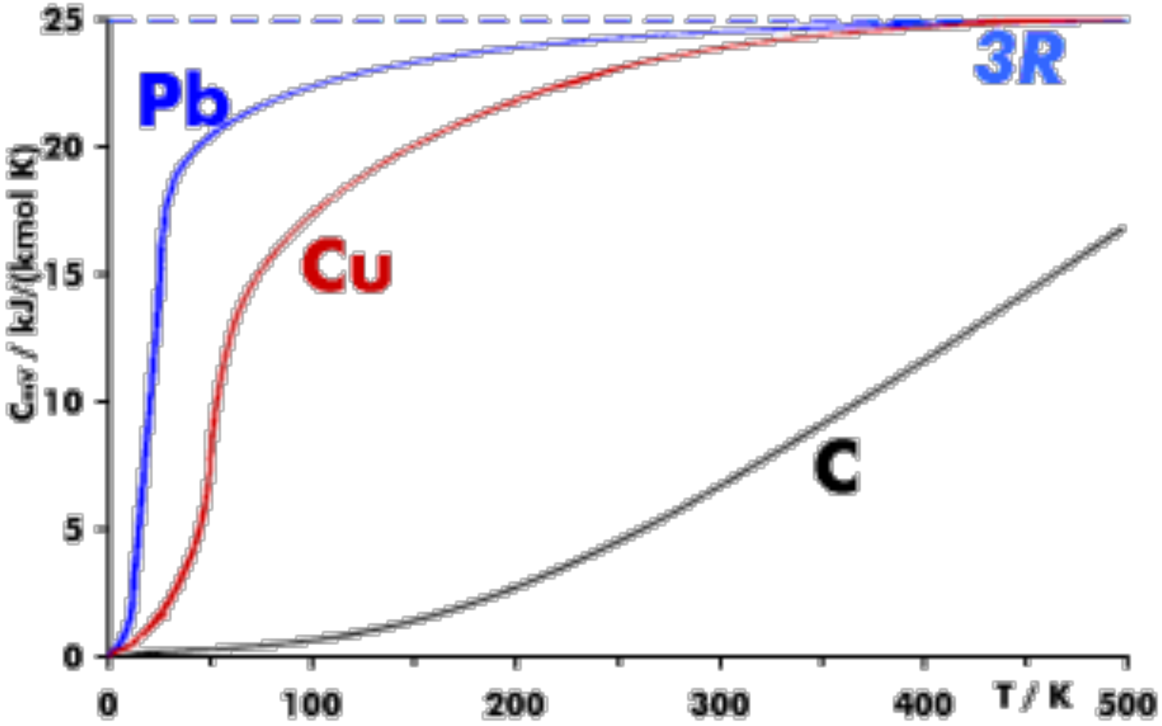
#	Dates	Title	Exercise	(1=easy, 10=hard)	Tasks
1	22.2	Introduction	VESTA	**2-3**	**Read Chap. 1**
2	01.3	Crystal structures	Daniel - info	**4**	**Read Chap. 2, Ex. 1**
3	08.03	Reciprocal space	Discuss Ex. 1	**6**	**Read Chap. 2, Ex. 2**
4	15.03	Scattering Theory	Discuss Ex. 2	**8-9**	**Read Chap. 3, Ex. 3**
5	22.03	Crystal bindings	Discuss Ex. 3	**5**	**Read Chap. 4, Ex. 4**
6	29.03	Phonons	Discuss Ex. 4	**5-6**	**Read Chap. 5, Ex. 5**
7	05.04	Thermal properties	Discuss Ex. 5	**5-6**	**Read Chap. 6, Ex. 6**
8	12.04	Electron gasses, C_{el}	Discuss Ex. 6	**5-6**	
--	19.04	EASTER HOLIDAY	-------------------	**0**	**RECAP**
9	26.04	Electronic band struc.	Discuss Ex. 7	**5-6**	
10	03.05	Semi-conductors	Discuss Ex. 8	**6**	
11	10.05	Fermi surfaces & Metals - I	Discuss Ex. 9	**8**	
12	17.05	Fermi surfaces & Metals - II	Discuss Ex. 10	**8**	
13	24.05	Guest lecture	Discuss Ex. 11	**--**	
14	31.05	Repetition		**4**	

Today’s Lecture: Heat Capacity

1. Introduction: Why do we care?
2. Debye’s Model for heat capacity (specific heat).
3. Einstein’s Model for heat capacity.
4. How to measure heat capacity.
5. Thermal conductivity.

Heat Capacity: Petit Dulong's Law / Gesetz

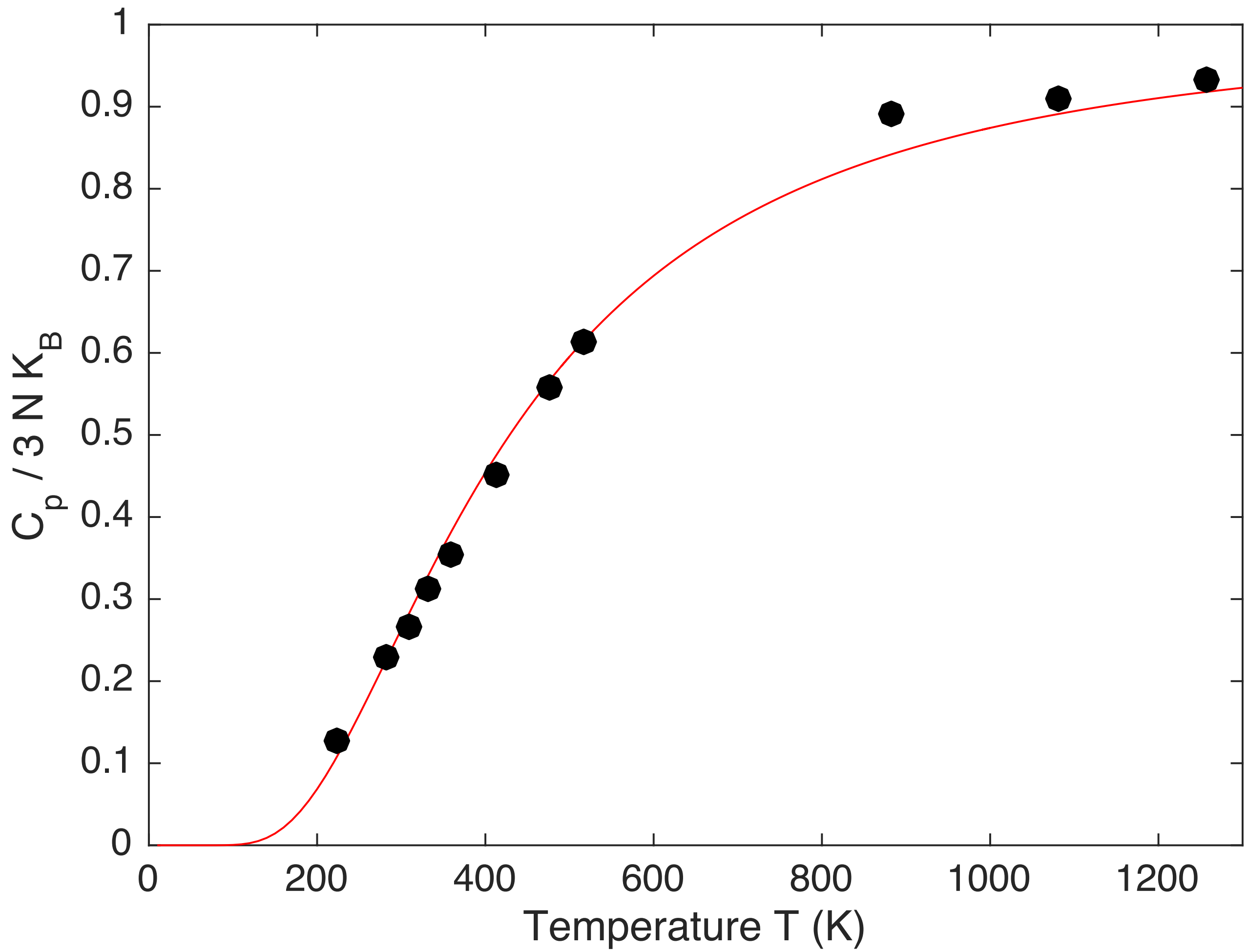


$N = n\ N_a$ (# moles x Avogadros Number)

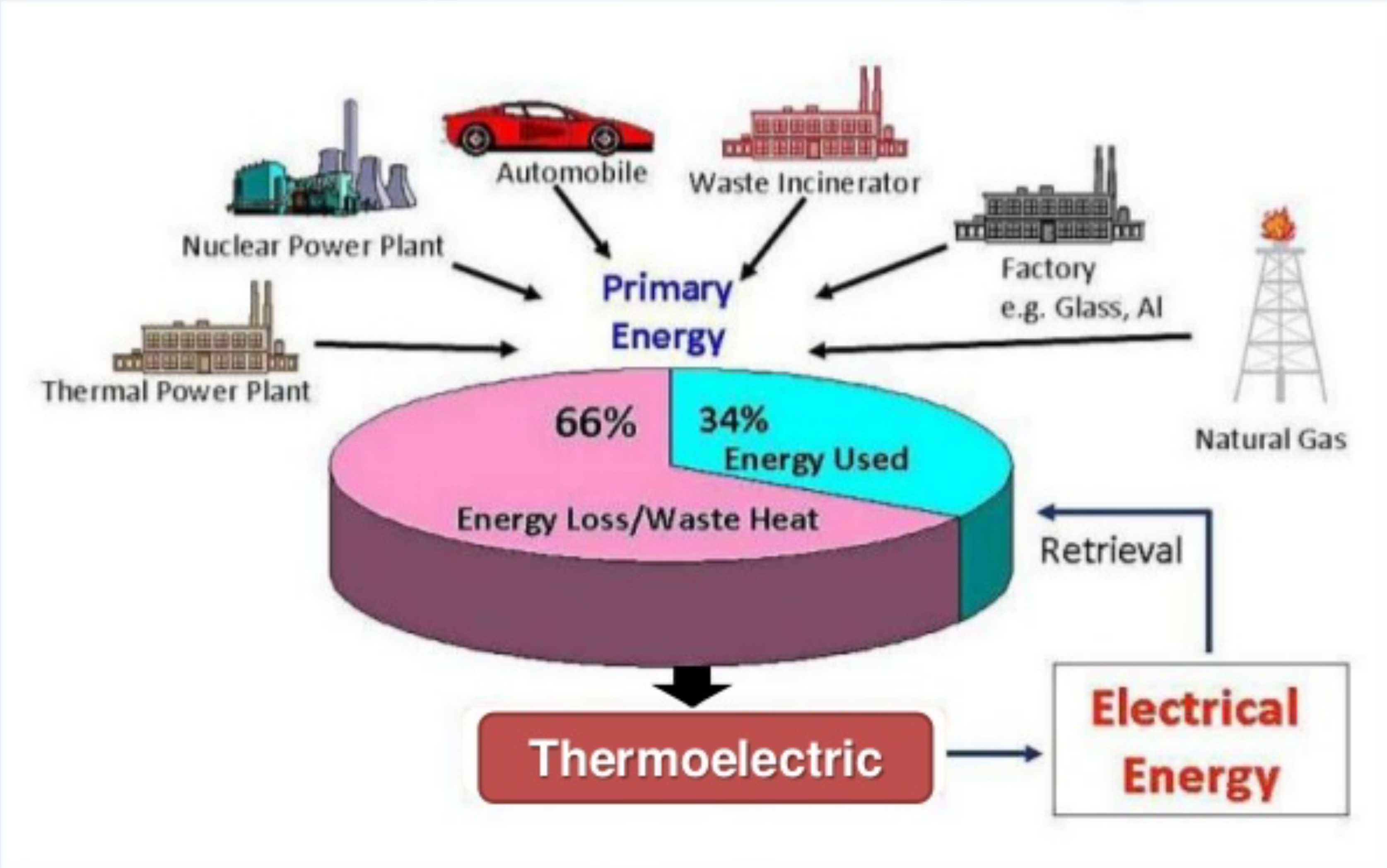
$R = N_a\ k_B$

$C/n = 3R\ /n = 3\ N_a k_B/n = 3Nk_B$

Heat Capacity: Diamond (as of 1906)



Waste Heat to Electricity



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Heat Capacity: Argon

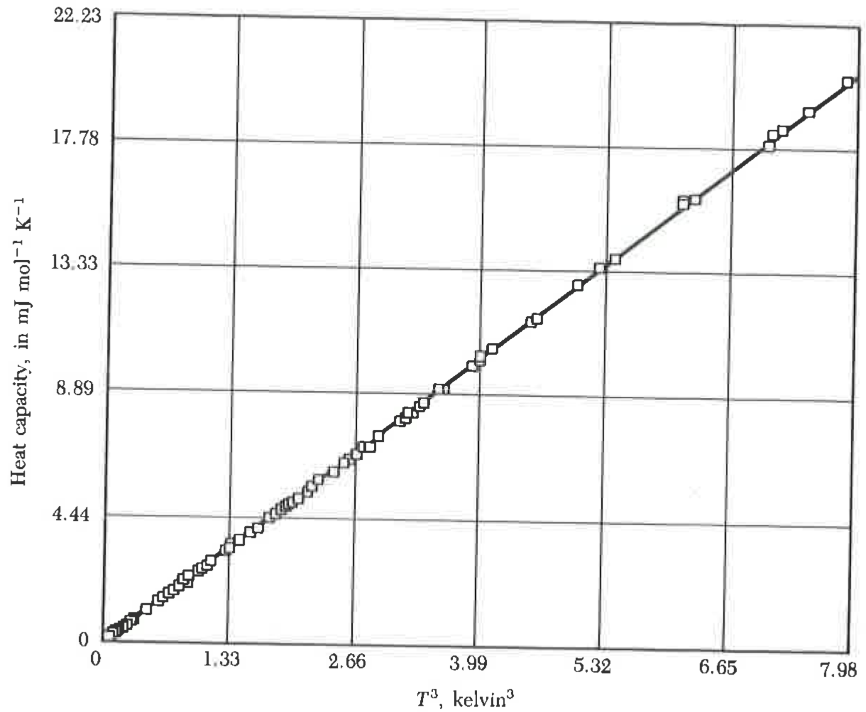

Figure 9 Low temperature heat capacity of solid argon, plotted against T^3. In this temperature region the experimental results are in excellent agreement with the Debye T^3 law with $\theta = 92.0$ K. (Courtesy of L. Finegold and N. E. Phillips.)

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Low-Temperature Heat Capacities of Solid Argon and Krypton*

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(Received 3 August 1968)

Debye Temperatures

TABLE 1 Debye Temperature and Thermal Conductivity[a]

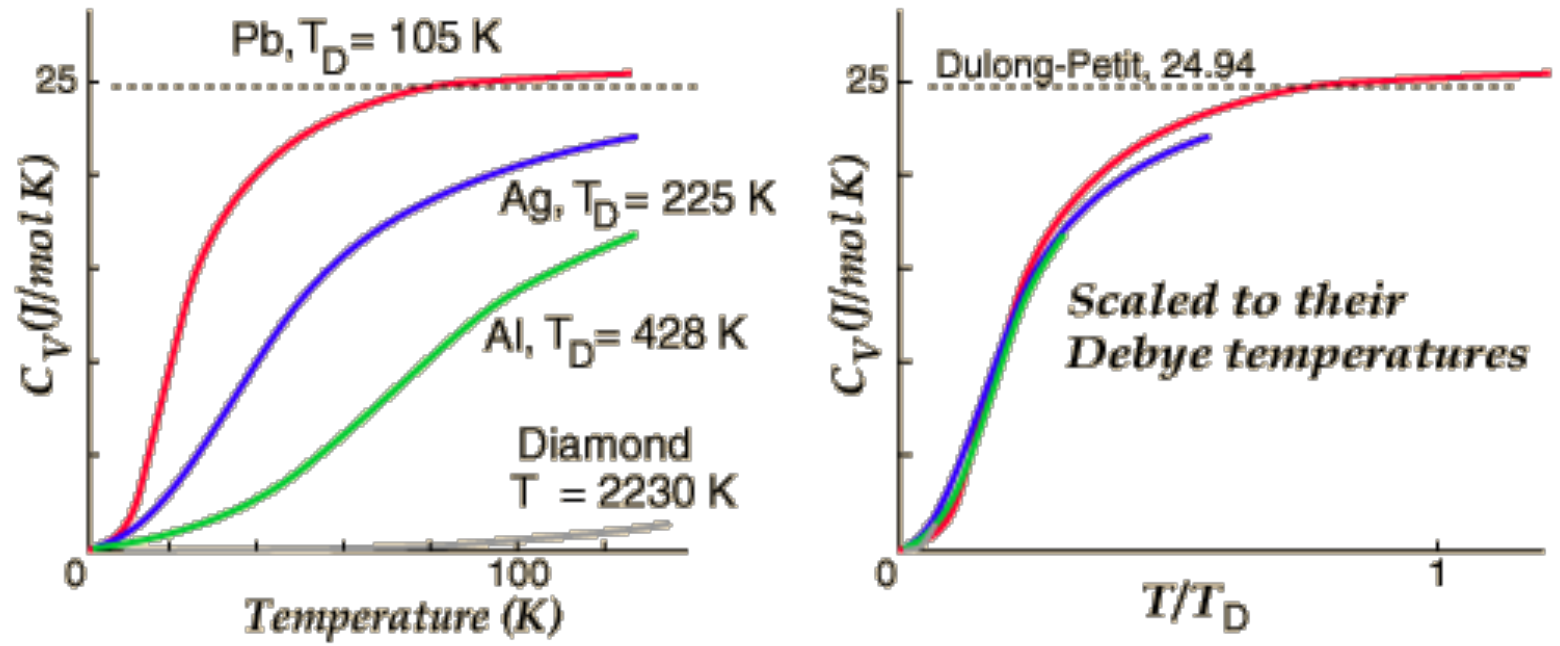
Low temperature limit of θ, in Kelvin
Thermal conductivity at 300 K, in W cm^{-1}K^{-1}

Li 344 0.85	Be 1440 2.00											B 0.27	C 2230 1.29	N	O	F	Ne 75
Na 158 1.41	Mg 400 1.56											Al 428 2.37	Si 645 1.48	P	S	Cl	Ar 92
K 91 1.02	Ca 230	Sc 360. 0.16	Ti 420 0.22	V 380 0.31	Cr 630 0.94	Mn 410 0.08	Fe 470 0.80	Co 445 1.00	Ni 450 0.91	Cu 343 4.01	Zn 327 1.16	Ga 320 0.41	Ge 374 0.60	As 282 0.50	Se 90 0.02	Br	Kr 72
Rb 56 0.58	Sr 147	Y 280 0.17	Zr 291 0.23	Nb 275 0.54	Mo 450 1.38	Tc 0.51	Ru 600 1.17	Rh 480 1.50	Pd 274 0.72	Ag 225 4.29	Cd 209 0.97	In 108 0.82	Sn ▪ 200 0.67	Sb 211 0.24	Te 153 0.02	I	Xe 64
Cs 38 0.36	Ba 110	La β 142 0.14	Hf 252 0.23	Ta 240 0.58	W 400 1.74	Re 430 0.48	Os 500 0.88	Ir 420 1.47	Pt 240 0.72	Au 165 3.17	Hg 71.9	Tl 78.5 0.46	Pb 105 0.35	Bi 119 0.08	Po	At	Rn
Fr	Ra	Ac															

Ce 0.11	Pr 0.12	Nd 0.16	Pm	Sm 0.13	Eu	Gd 200 0.11	Tb 0.11	Dy 210 0.11	Ho 0.16	Er 0.14	Tm 0.17	Yb 120 0.35	Lu 210 0.16
Th 163 0.54	Pa	U 207 0.28	Np 0.06	Pu 0.07	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

[a] Most of the θ values were supplied by N. Pearlman; references are given the *A.I.P. Handbook*, 3rd ed. the thermal conductivity values are from R. W. Powell and Y. S. Touloukian, Science **181**, 999 (1973).

Heat Capacity for different elements



Exercise

Exercise 3 *Singularity in density of states*

a) From the dispersion relation derived in the lecture for a monoatomic linear lattice of N atoms with nearest neighbour interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_{\mathrm{m}}^2 - \omega^2}}, \tag{4}$$

where ω_{m} is the maximum frequency.

b) Make a plot of equation (4).

c) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = \left(\frac{L}{2\pi}\right)^3 \left(\frac{2\pi}{A^{3/2}}\right) (\omega_0 - \omega)^{\frac{1}{2}}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

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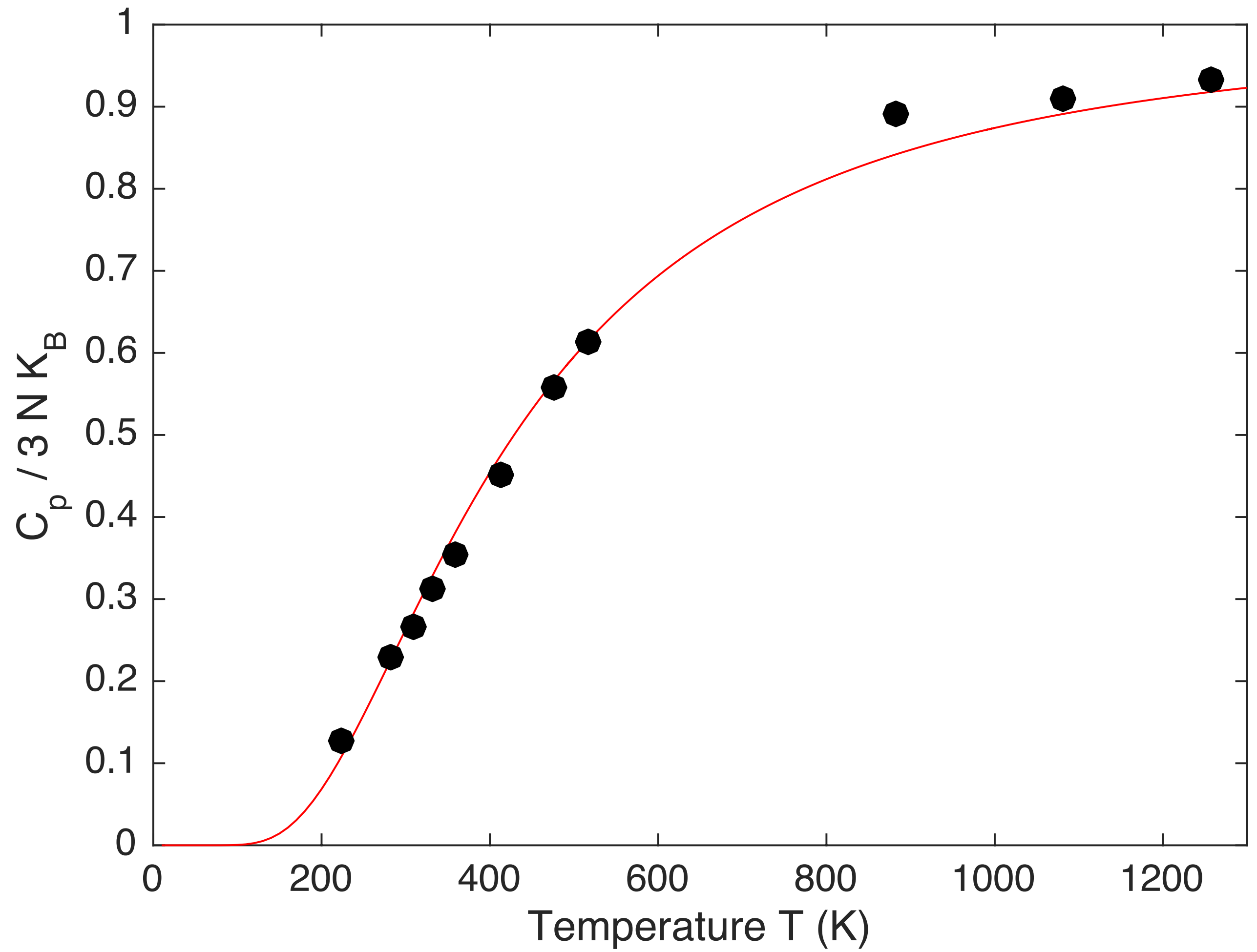
Heat Capacity: Diamond (as of 1906)



Exercise

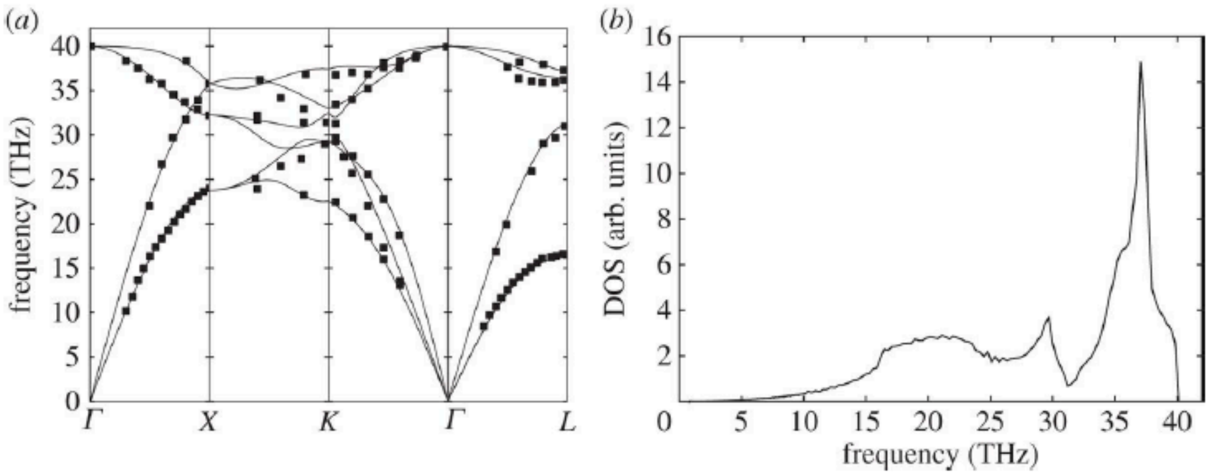
Exercise 3 *Heat capacity - Einstein model*

Einstein derived the expression

$$C = 3Nk_{\rm B}\left(\frac{\hbar\omega_0}{k_{\rm B}T}\right)^2 \frac{\exp\left(\frac{\hbar\omega_0}{k_{\rm B}T}\right)}{\left[\exp\left(\frac{\hbar\omega_0}{k_{\rm B}T}\right)-1\right]^2}. \tag{1}$$

a) In figure 1, the heat capacity of diamond is plotted as $\frac{C_p}{3Nk_{\rm B}}$ versus temperature. Einstein's model has just one free parameter: ω_0. Based on these data (given below), determine the energy scale $\hbar\omega_0$ that would give the best description of the experiment.

b) How does this energy scale compare with the energy scale of optical phonons in diamond (see figure 2)?



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Heat Capacity: Experimental setup

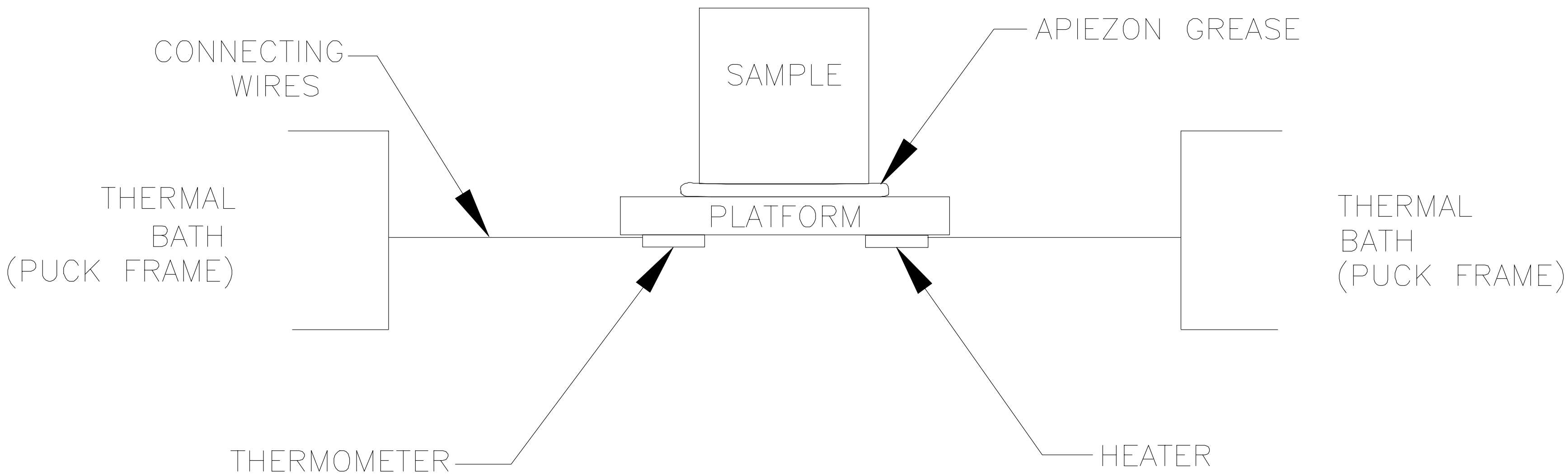

Figure 1-1. Thermal Connections to Sample and Sample Platform in PPMS Heat Capacity Option

Prof. Andreas Schilling's Laboratory.
Possibility for bachelor projects!

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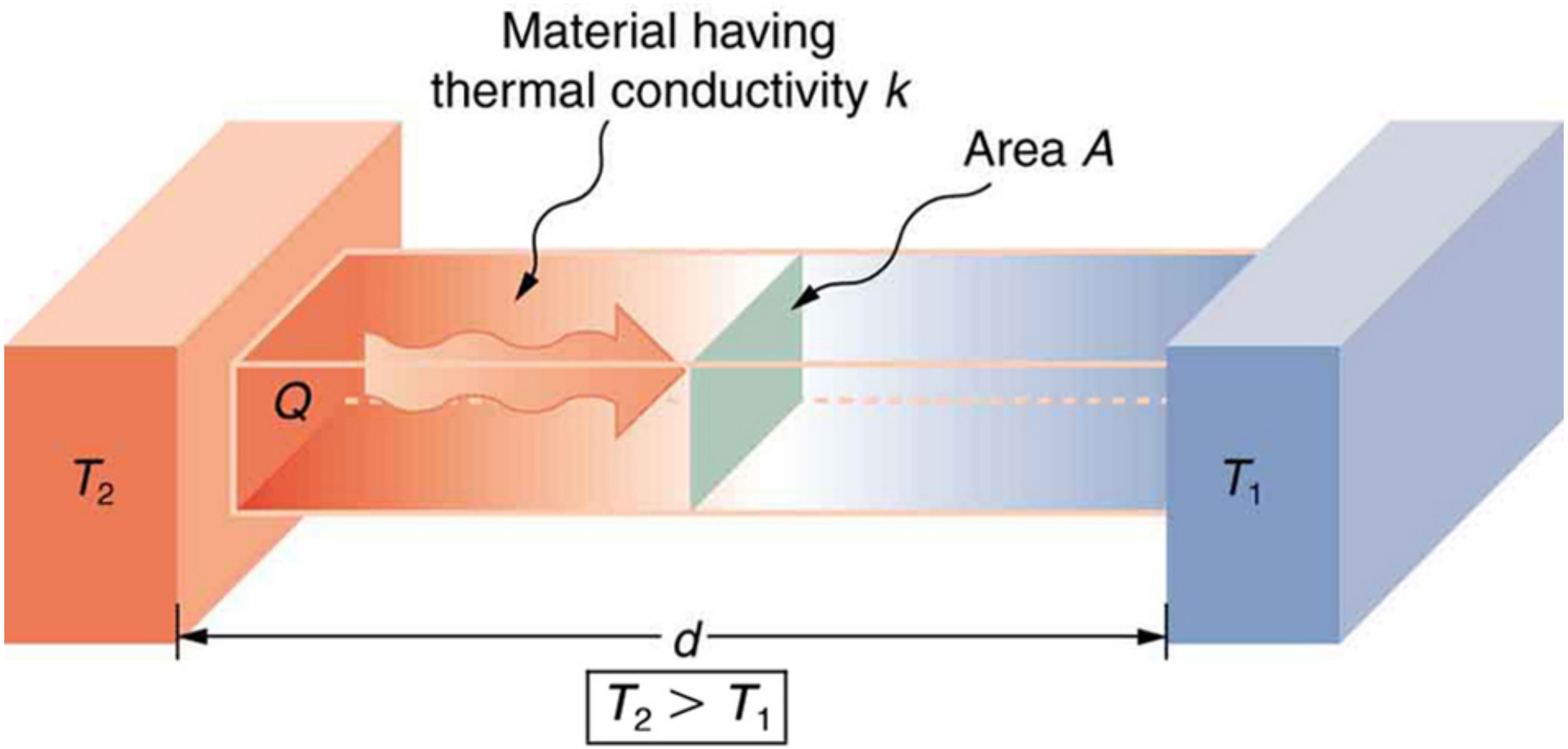
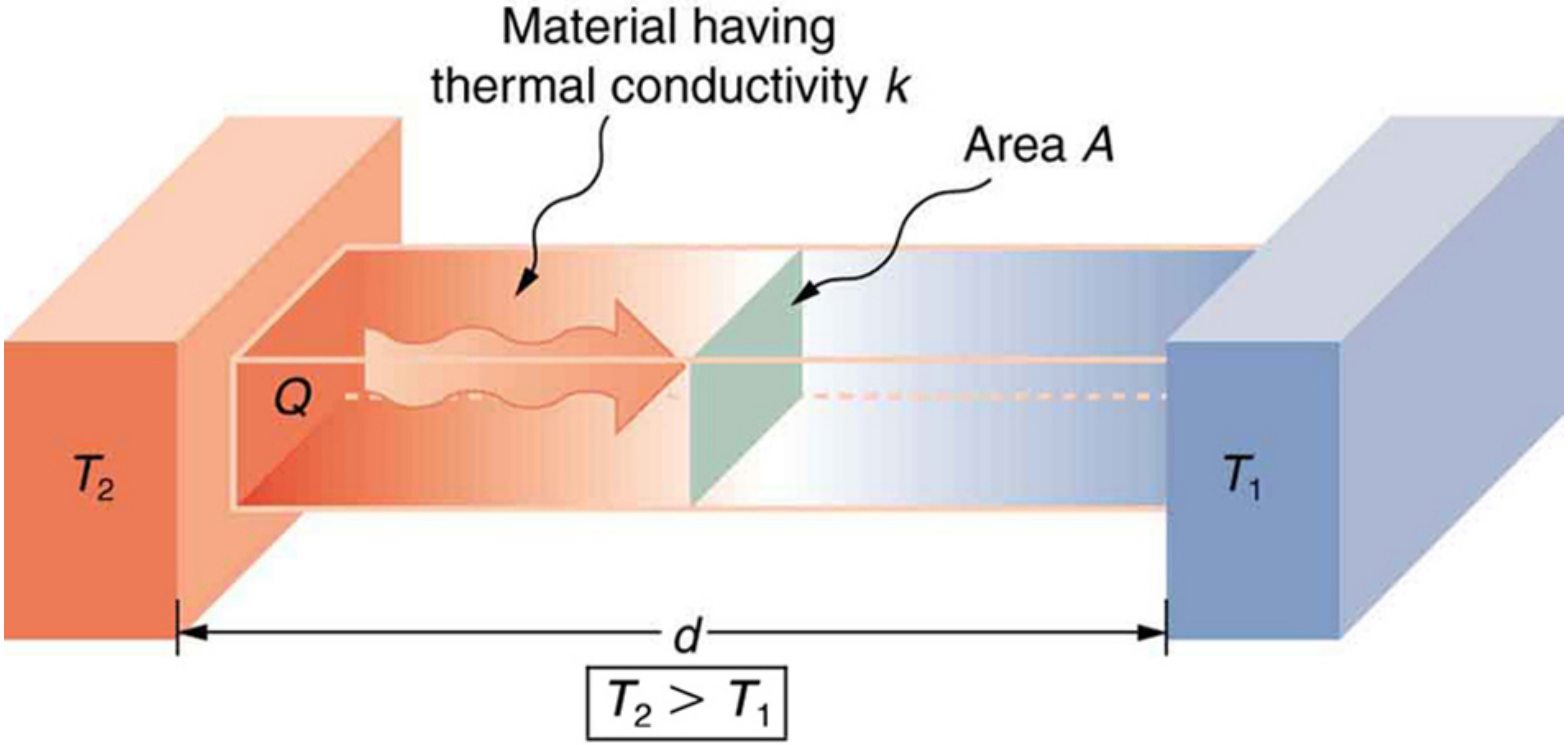
Thermal conductivity κ



$$\kappa = \frac{d}{A}\frac{P}{\Delta T} \quad \text{or} \quad \kappa\,\Delta T = \frac{d}{A}\,P$$

Where the power P=Q/t with t being time and Q = U the heat energy.

κ and Cv



$$\kappa = \frac{d}{A}\frac{P}{\Delta T} \quad \text{or} \quad \kappa\,\Delta T = \frac{d}{A}\,P$$

$$\text{C}\,\Delta T = \Delta\text{U}$$

$$\longrightarrow \kappa \propto C_V$$

Thermal Conductivity: NaF

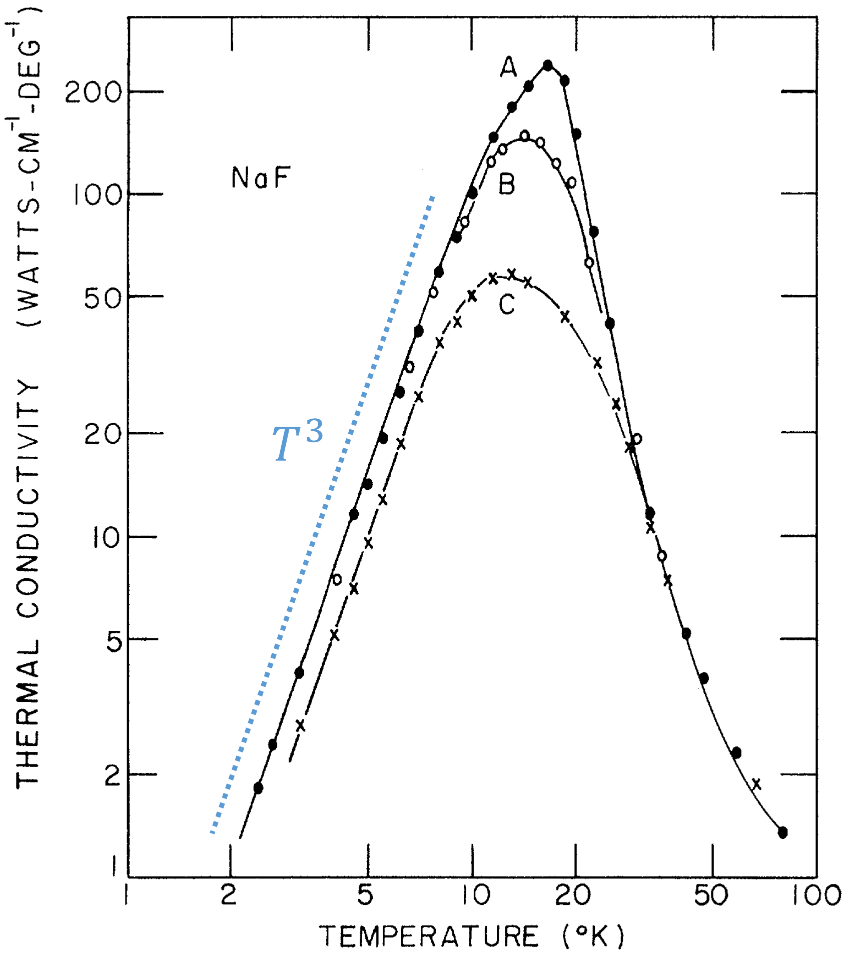
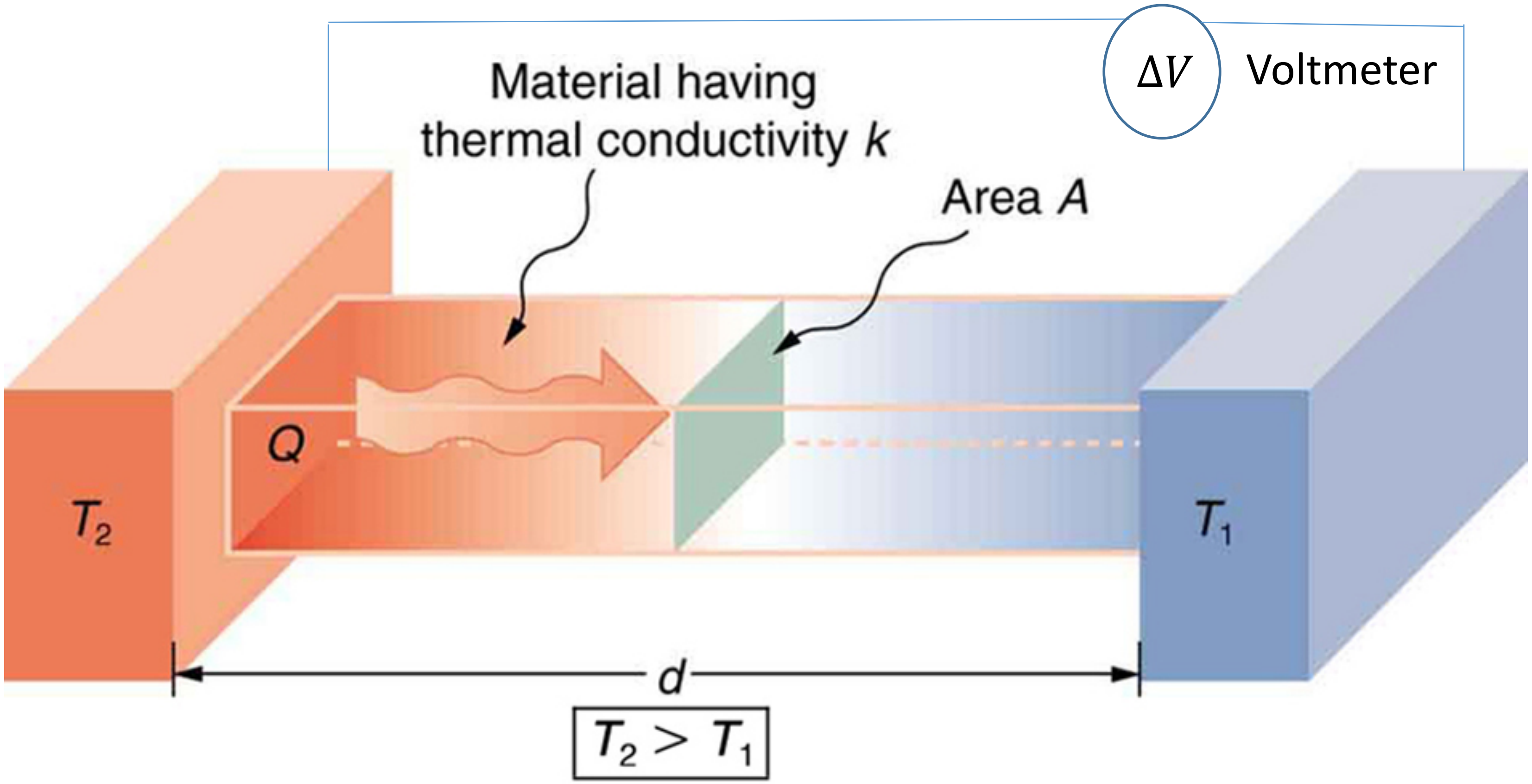


FIG. 1. Thermal conductivity versus temperature for pure NaF crystals. Curve *A*, NaF sample, this paper; curve *B*, NaF sample, Ref. 1; curve *C*, typical singly grown NaF (smaller cross section).

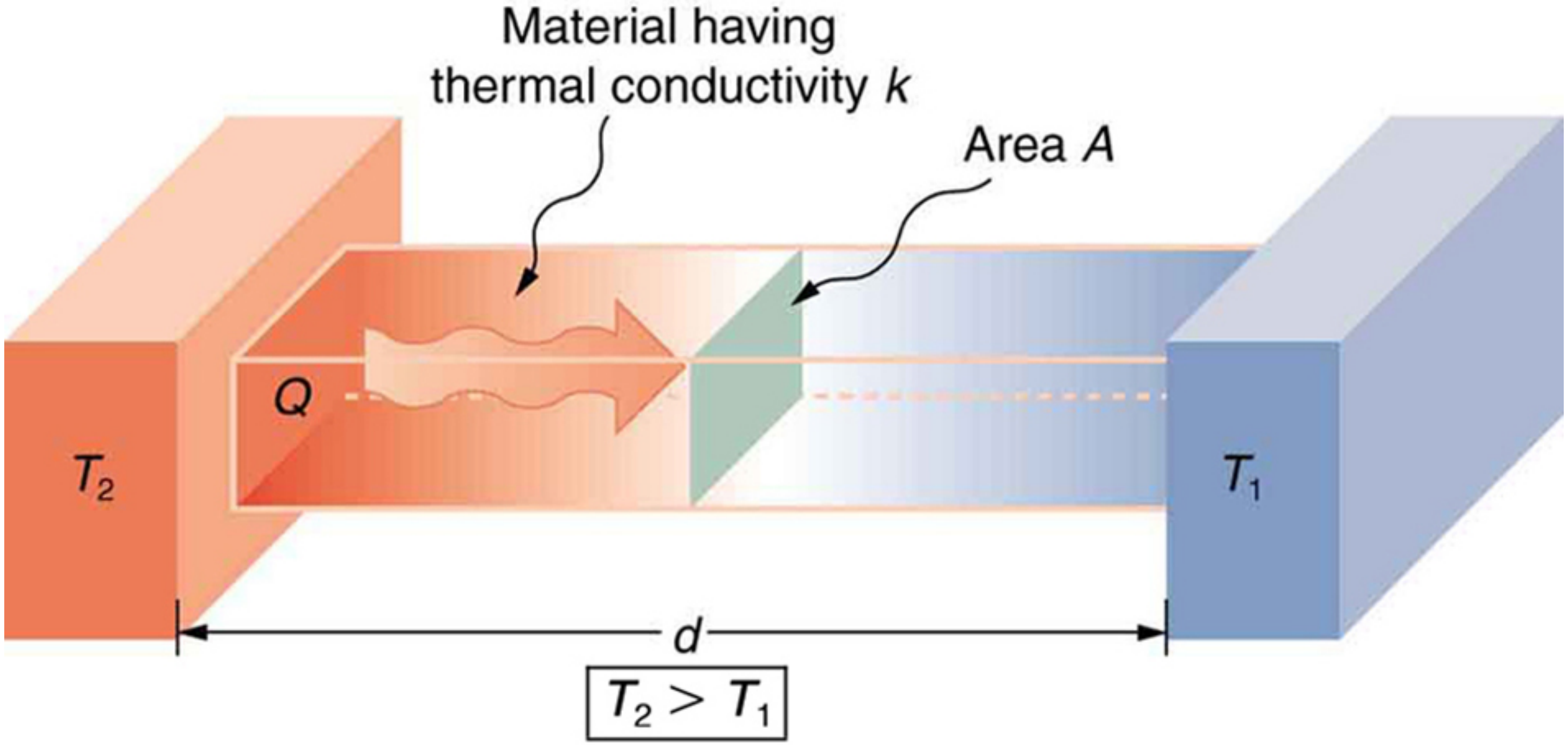
Thermal conductivity κ



$$S = \frac{\Delta V}{\Delta T} \quad \text{or} \quad S\,\Delta T = \Delta V$$

Where the ΔV is the thermoelectric voltage

S $versus$ κ



$$\kappa = \frac{d}{A}\frac{P}{\Delta T} \quad \text{or} \quad \kappa\,\Delta T = \frac{d}{A}\,P$$

$$S = \frac{\Delta V}{\Delta T} \quad \text{or} \quad S\,\Delta T = \Delta V$$