Achievements

How to describe a crystal structure

-- Crystal lattice
-- Basis

How to resolve crystal structures

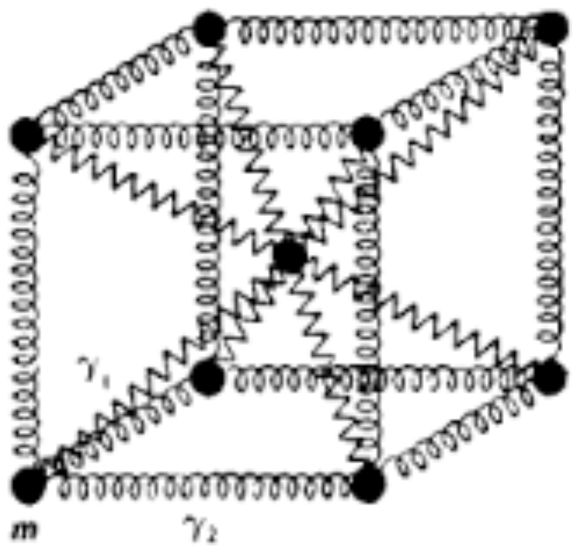
-- Reciprocal space
-- Scattering theory (Form and Structure Factor)
-- Resolving the crystal structure of a superconductor

How to crystals bind together

-- van der Waals, ionic, covalent crystal bindings

Lecture 6-7: Crystal vibrations (phonons)

-- Tasks
-- Why is phonons important
-- Theory & concepts
-- How to measure phonons



Tasks

(1) Read chapter 5

-- Phonon heat capacity (12 pages) Mandatory reading!!

-- Anharmonic crystal interactions (2 pages) Elective reading!!

-- Thermal conductivity (5 pages) Mandatory reading!!

(2) Solve exercise sheets

(3) Who is summarizing next week? Student presentation?
Einstein Model.

Exam dates: 7 & 8th June?

Exercises

Exercise 1 *Elastic waves in lattices and continuous media*
In continuous media the 1D wave equation reads

$$\frac{\partial^2 \xi(x,t)}{\partial t^2} = v^2 \frac{\partial^2 \xi(x,t)}{\partial x^2}, \tag{1}$$

with the speed of sound $v = \sqrt{E/\rho}$, elastic modulus E, and density ρ. For a linear chain of atoms with distance a, mass m, and spring constant C we get

$$m \frac{\partial^2 \xi_n}{\partial t^2} = C\left(\xi_{n+1} + \xi_{n-1} - 2\xi_n\right). \tag{2}$$

Show that in the limit of continuous media ($\lambda \gg a$) equation (2) transitions into equation (1). Calculate E as a function of C, m, and a.

Exercise 2 *Linear chain of atoms with different spring constants*
Calculate the dispersion relation $\omega(k)$ for a linear chain of identical atoms of mass m, distance between atoms $d = a/2$, and alternating spring constants C_1 and C_2. (The unit cell with two identical atoms has thus a lattice constant of a.) Draw $\omega(k)$ for $C_1/C_2 = 1.0$, 0.6, 0.3, and 0.1.

Exercise 3 *Acoustic and optic waves in 2D*
Sketch the longitudinal and transverse waves for optic and acoustic modes in a 2D NaCl structure with lattice constant a. The wavevector with $\lambda = 4a$ is in the [1 0] direction.

Exercises

Exercise 4 *Neutron and photon dispersion relations*

Particles have dispersion relations. For example, the energy E of electrons and neutrons is given by:

$$E = \frac{\hbar^2 k^2}{2m} \tag{3}$$

where m is the particle mass and $p = \hbar k$ is the momentum. Photons (light) by contrast have the following dispersion:

$$E = \hbar c k \tag{4}$$

where c is the speed of light and $\hbar = h/(2\pi)$ with h being Planck's constant.

a) For a neutron moving with $2\,\text{km/s}$, what is its kinetic energy E (in meV)? (Hint: look up the mass of a neutron.) What is its wavelength $\lambda = 2\pi/k$? Derive the following relation for neutrons:

$$\lambda[\text{Å}] = \frac{9.045}{\sqrt{E[\text{meV}]}}. \tag{5}$$

b) With the wavelength calculated in (a), calculate the energy of a photon.

c) To experimentally study excitations such as phonons, meV energy resolution is needed. Let the instrumental resolving power be defined by $\Delta E/E$ where ΔE is the energy resolution. If $\Delta E = 1\,\text{meV}$, what is the resolving power of neutrons and photons with a wavelength of $4\,\text{Å}$.

Exercises

Exercise 5 *Measuring phonons*

In a previous lecture, we discussed the recent discovery of high-temperature superconductivity in H_2S. We found that under the high pressure needed to crystallize this gas, the crystal structure is bcc.

a) Is the (200) Bragg peak allowed (non-zero) or forbidden (zero) by the structure factor for a monoatomic crystal?

b) If the conventional lattice parameter is 3 Å, and we use neutrons moving with 2 km/s, what is the scattering angle of the (200) Bragg peak and what is the energy of the scattered neutrons?

c) What is the expectation for the phonon branches (dispersions) of a mono atomic bcc lattice? Can we expect optical phonons? What is the expectation for H_2S?

d) Let's assume that the phonon velocity of an acoustic branch is 4 meV per reciprocal lattice unit ($2\pi/a$) in the long wavelength limit $k \to 0$. What is the phonon energy at $\mathbf{Q} = (2.1,0,0)$ (where $\mathbf{Q}$ is in reciprocal units)?

e) If we fix the analyser at our triple axis instrument to measure neutrons with energy 7 meV, what should be the energy of the incident neutrons to measure the phonon at $\mathbf{Q} = (2.1,0,0)$?

Exercises

Exercise 6 *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

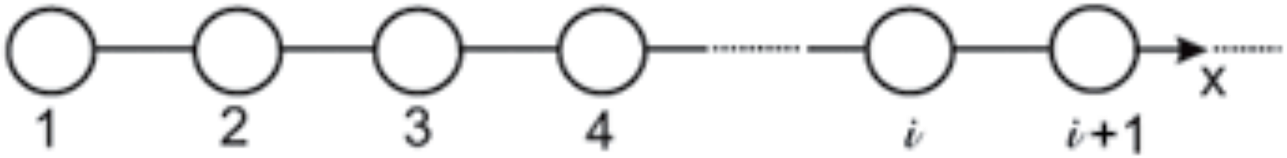
$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_{\mathrm{m}}^2 - \omega^2}}, \tag{6}$$

where ω_{m} is the maximum frequency.

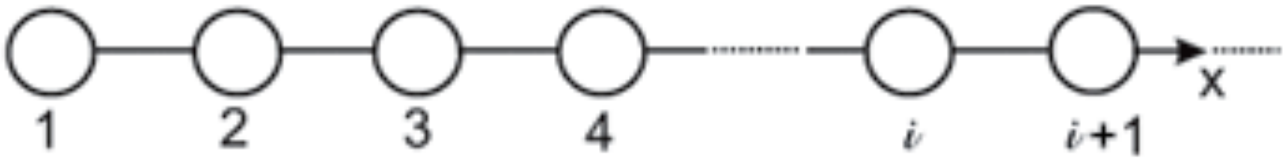
b) Make a plot of equation (6).

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.

Linear chain -Models

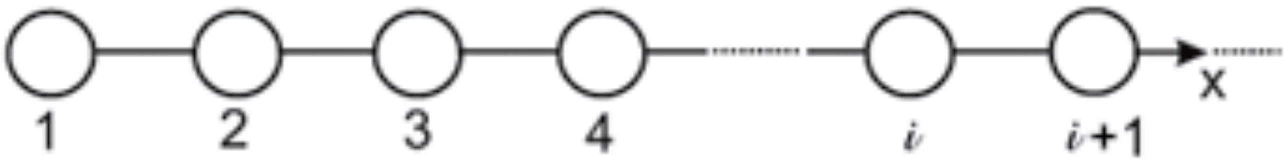


Structure factor: S = $\sum_i e^{-iqr_i}$



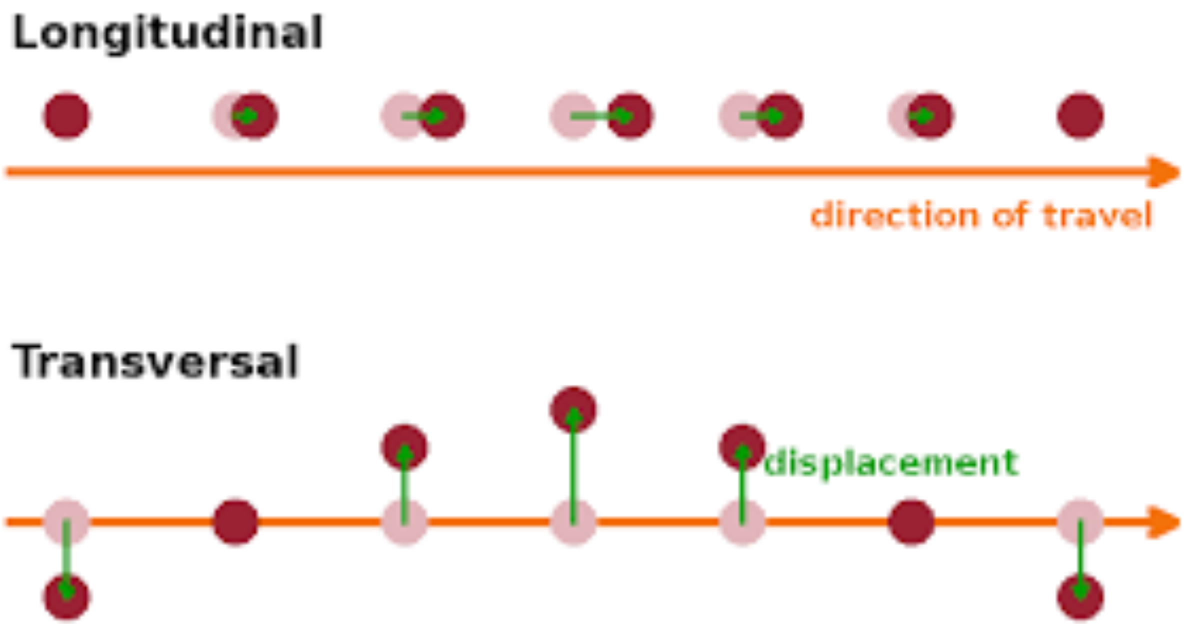
Madelungs constant: $\alpha = 2\, ln(2)$

Distortion Energy : $E = 0.5 * constant * \delta^2$



Phonon dispersion: $\omega =$

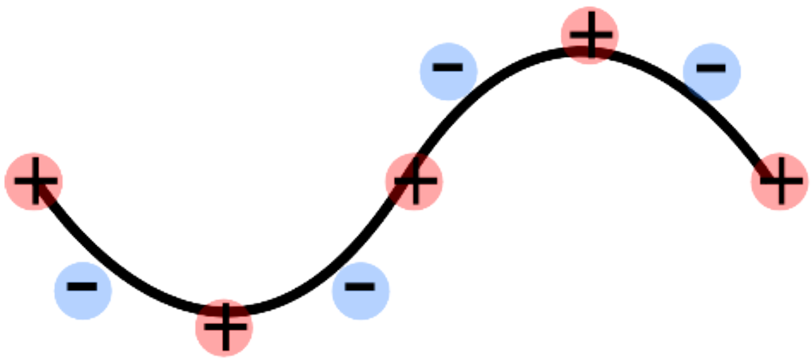
Longitudinal and Transverse Phonons



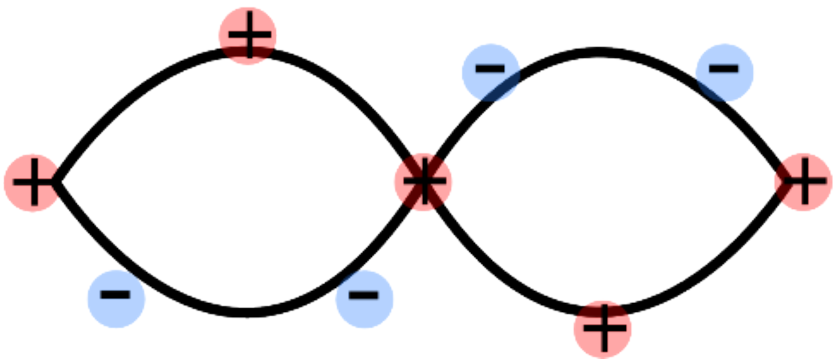
LA = Longitudinal Acoustic
LO = Longitudinal Optical
TA = Transversal Acoustic
TO = Transversal Optical

Acoustic and optical modes

Acoustical Mode



Optical Mode



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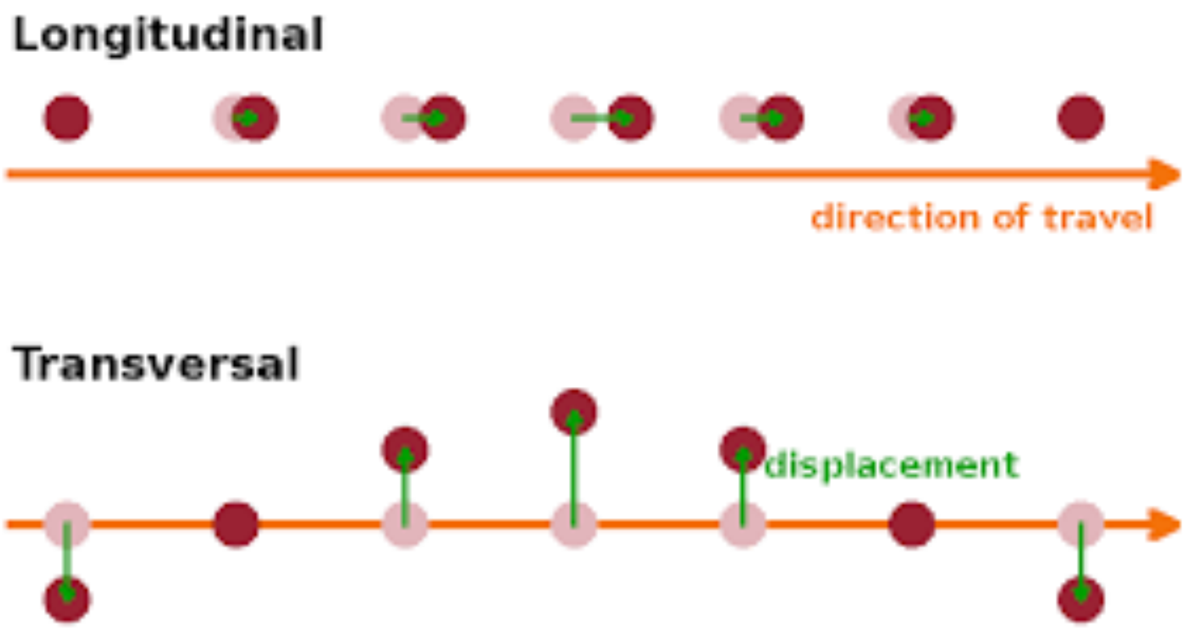
https://www2.warwick.ac.uk/fac/sci/physics/current/postgraduate/regs/mpags/ex5/phonons/

Number of phonon branches



LA = Longitudinal Acoustic
LO = Longitudinal Optical
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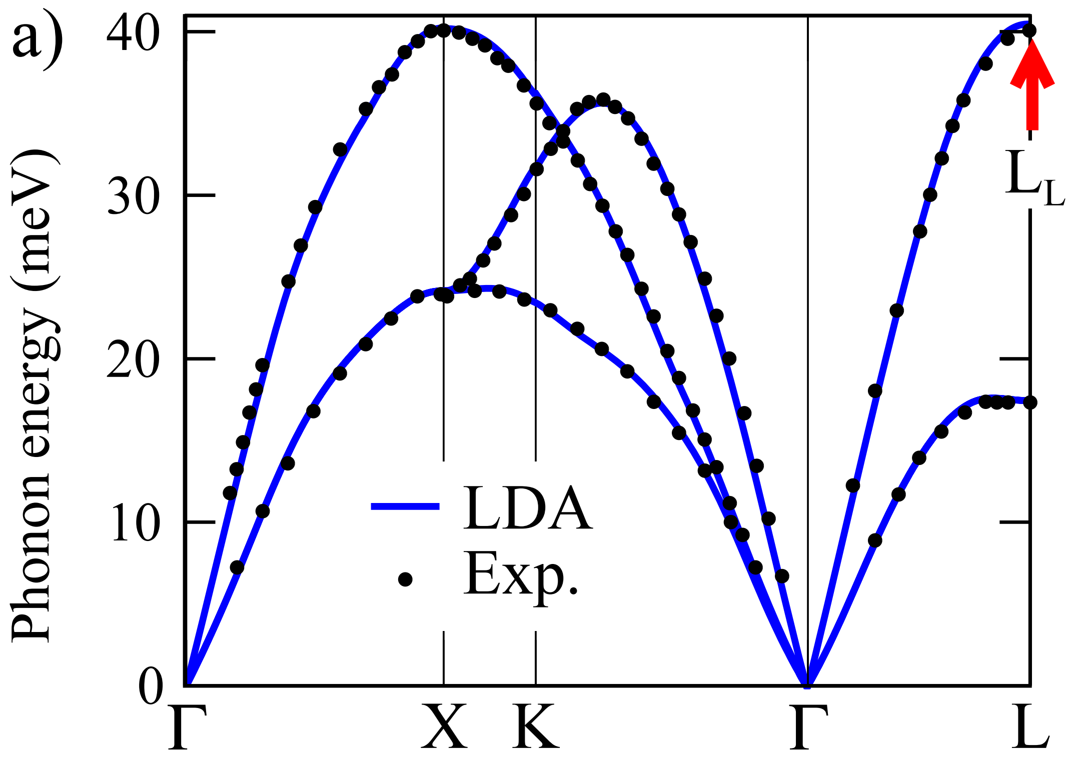
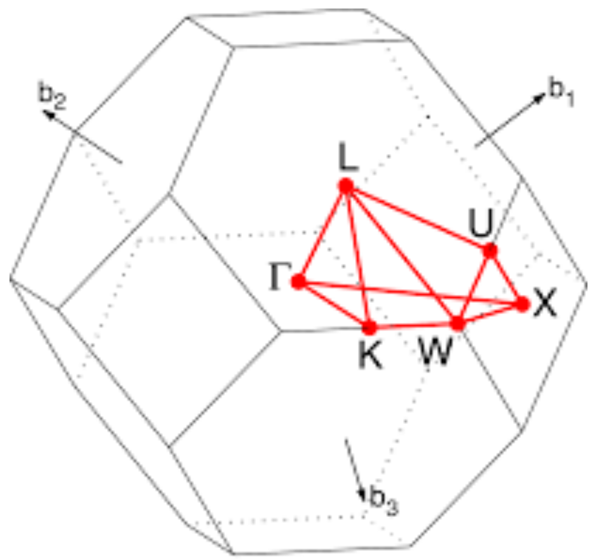
TO = Transversal Optical

p = number of atoms in the primitive cell

3 acoustic branches
3p-3 optical branches
Total 3p phonon branches

Phonons in aluminium



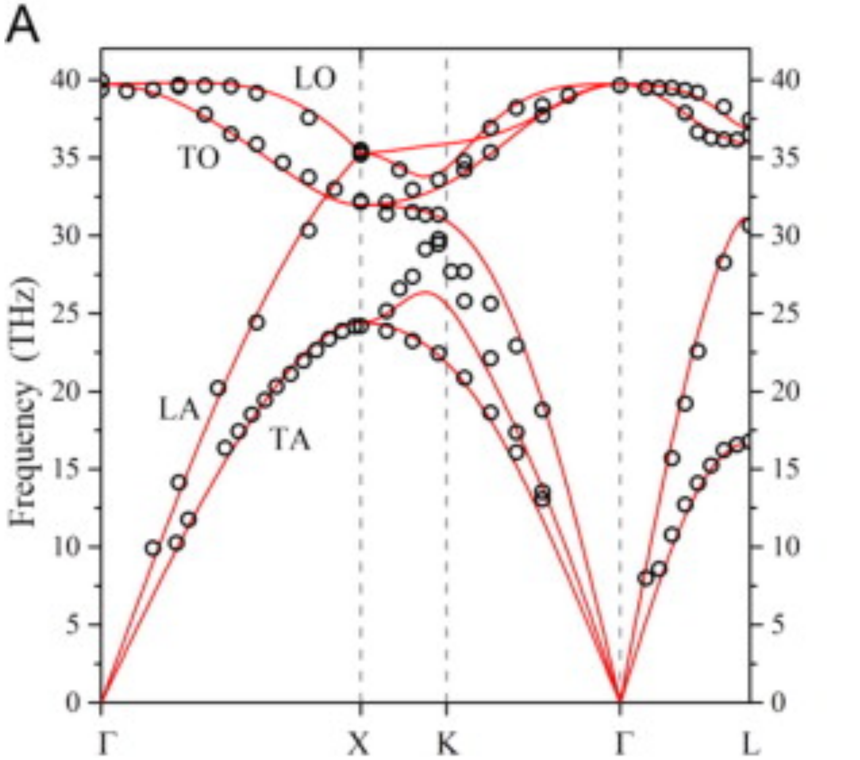


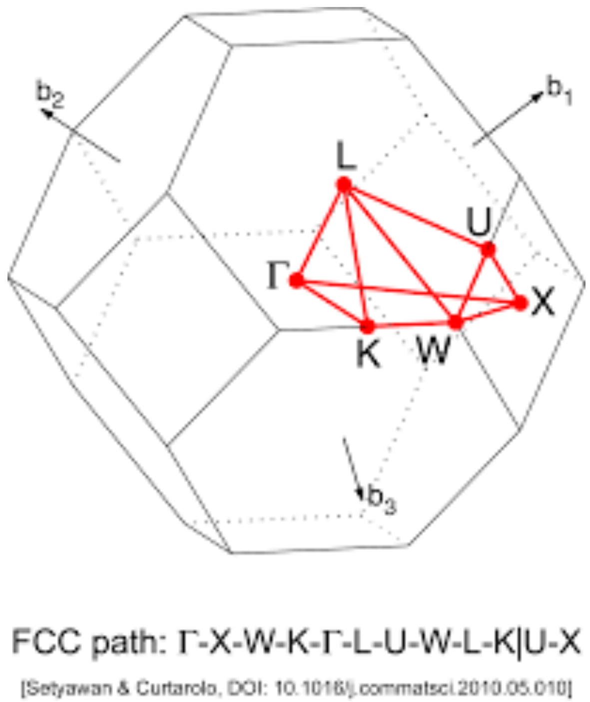
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

http://iopscience.iop.org/article/10.1088/0953-8984/24/5/053202

Phonons in diamond





1 THz = 4.14… meV

p = number of atoms in the basis of the primitive cell

3x*p* phonon branches

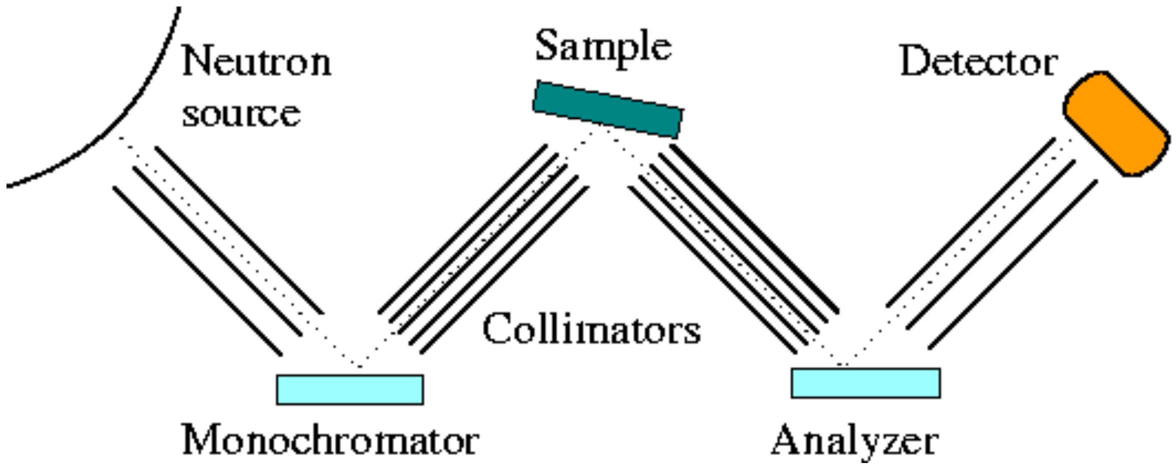
3 Acoustic branches and 3*p*-3 optical branches

Triple axis spectrometer

https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/flex/index_en.html

The Nobel Prize in Physics 1994
Bertram N. Brockhouse, Clifford G. Shull

Triple axis spectrometer



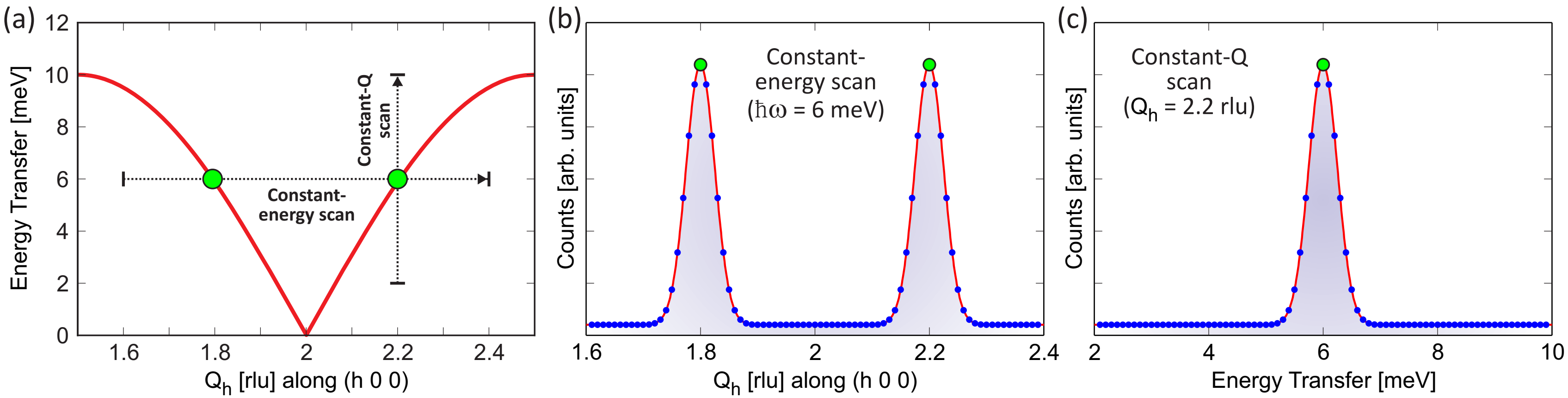


Figure 5: (a) Schematic view of how two points of the phonon dispersion curve can be measured using either (b) constant-energy scan or (c) constant-**Q** scan. By performing multiple scans it is possible to map out the complete dispersion (see below).

https://www.psi.ch/lns/TrainingEN/INS_Student_Practicum_PSI.pdf

Triple axis spectrometer with x-rays

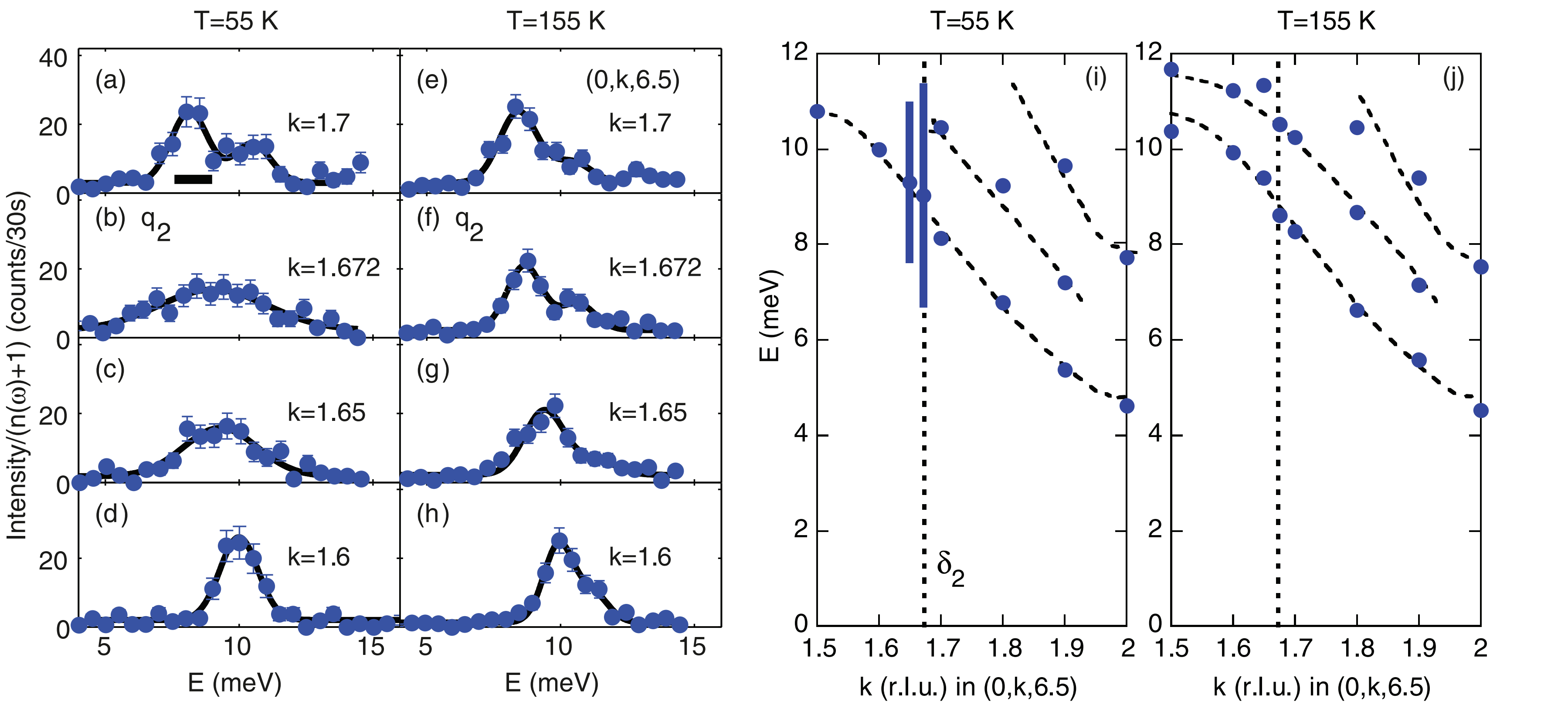
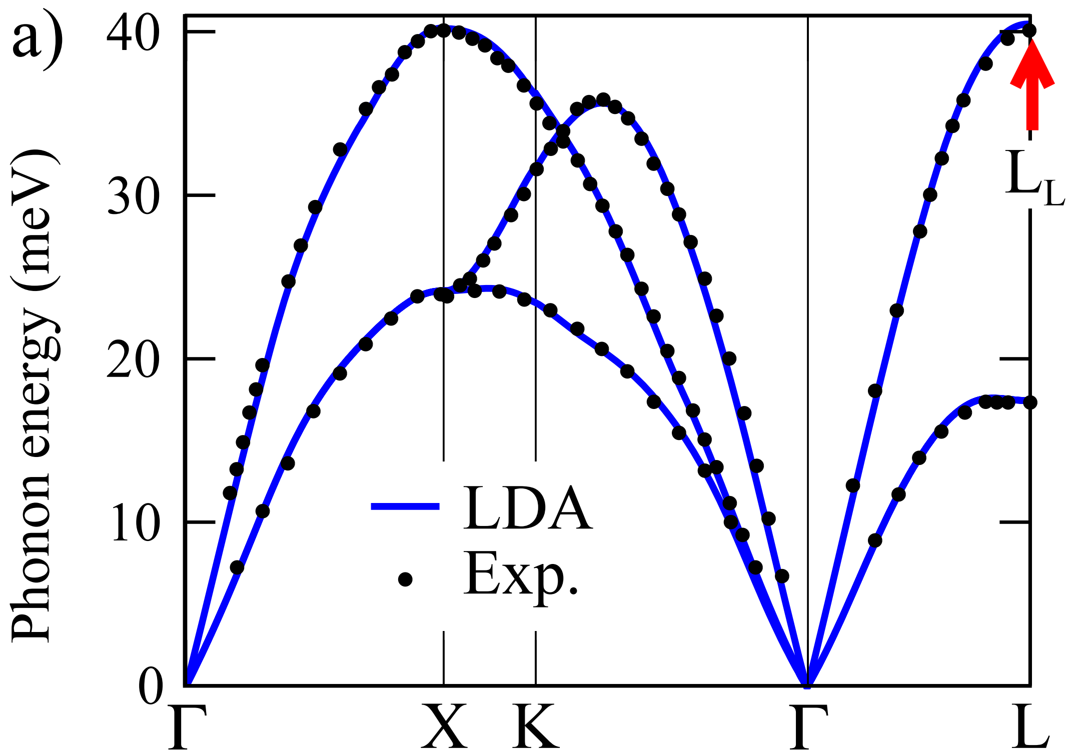
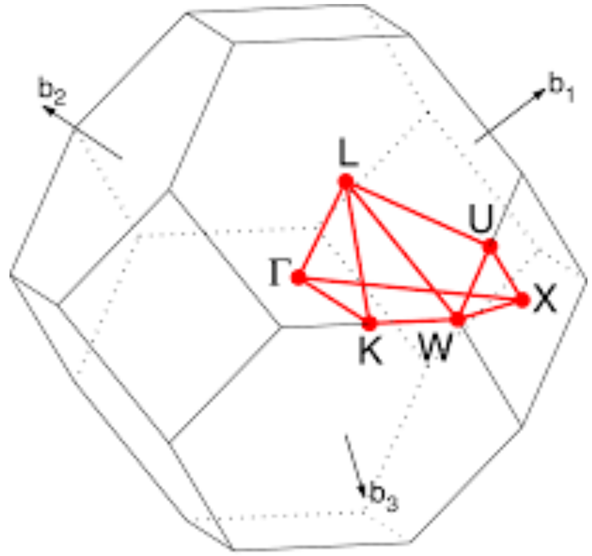


FIG. 5. (Color online) [(a)–(h)] IXS E scans of the low-energy phonons for wave vectors along the $(0,k,6.5)$ line. Solid lines are fits to a sum of Gaussian functions. Data have been multiplied by $1 - \exp[-E/(k_B T)]$ to correct for the Bose factor. The horizontal bar in panel (a) is the instrumental resolution. [(i) and (j)] Phonon dispersion curves along the $(0,k,6.5)$ line for $T = 55$ and 155 K. The solid circles represent the phonon peak positions determined from fitting data such as that in (a)–(h); the dashed lines are guides to the eye for the different branches. The resolution-deconvolved phonons widths are represented by vertical bars. The vertical dotted line is the CDW ordering wave vector.

Phonons in aluminium



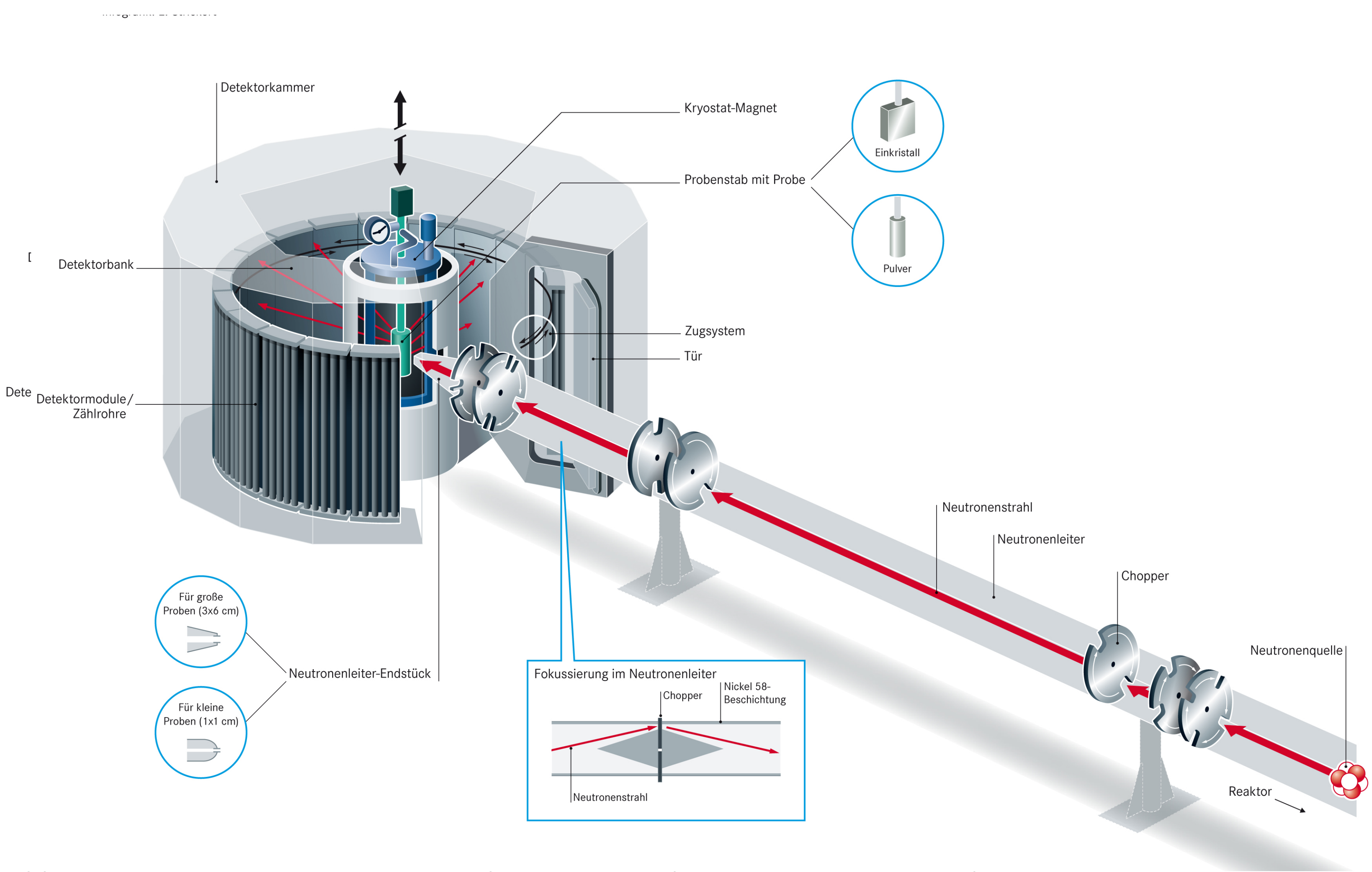


FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

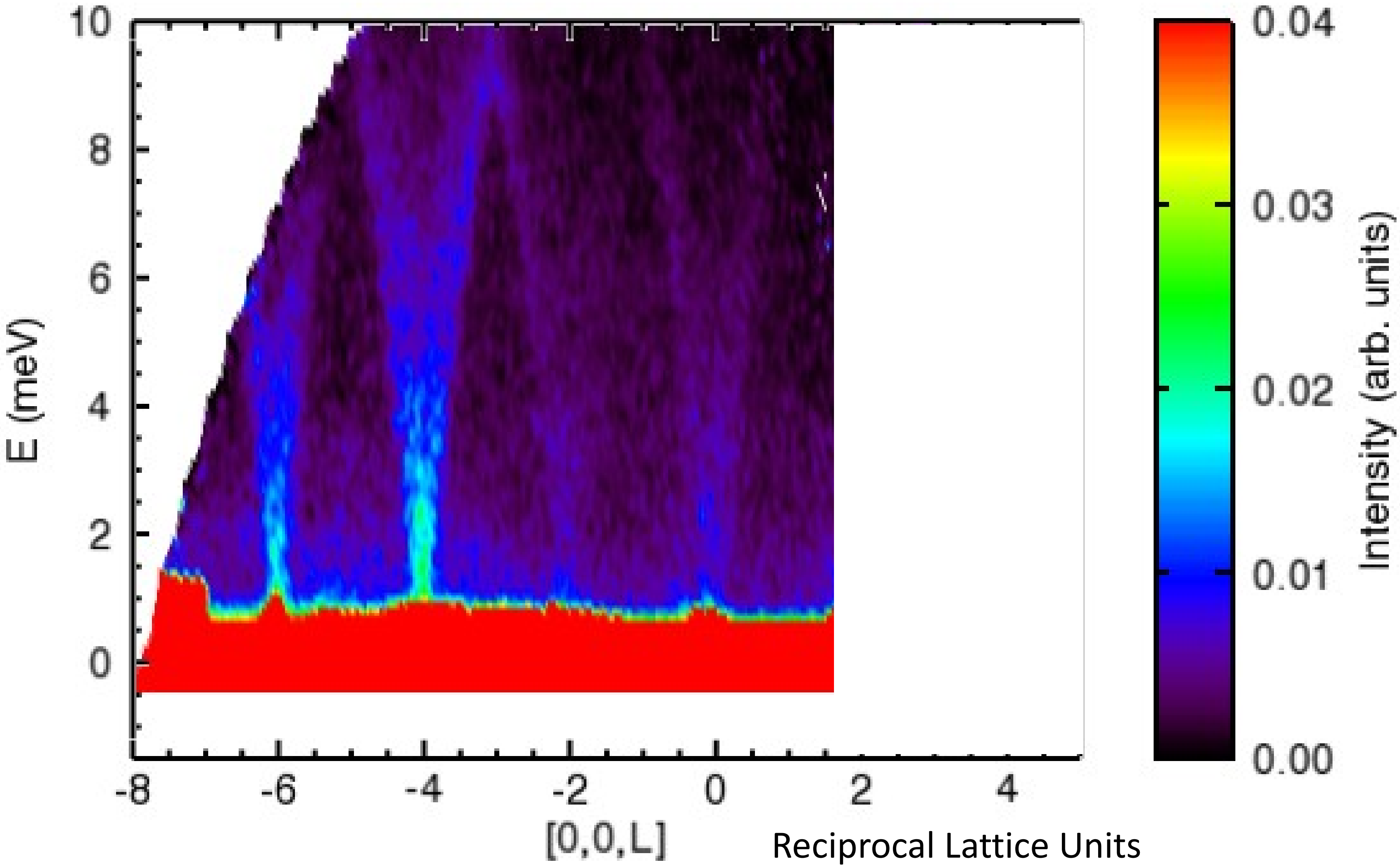
http://iopscience.iop.org/article/10.1088/0953-8984/24/5/053202

Time-of-flight spectrometry



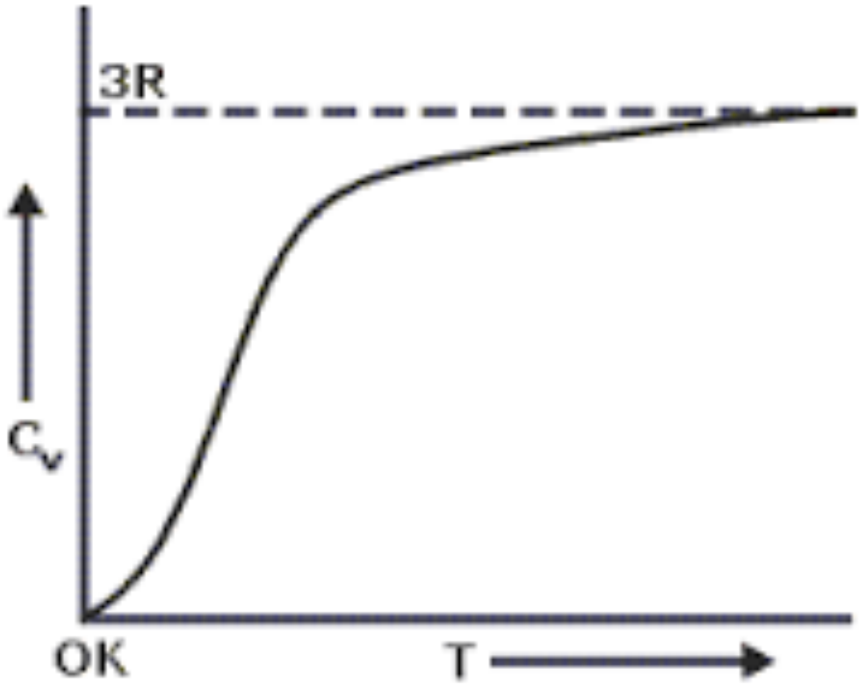
https://www.helmholtz-berlin.de/forschung/zukunftsprojekte/neat2_en.html

Acoustic Phonon in Sr_2RuO_4



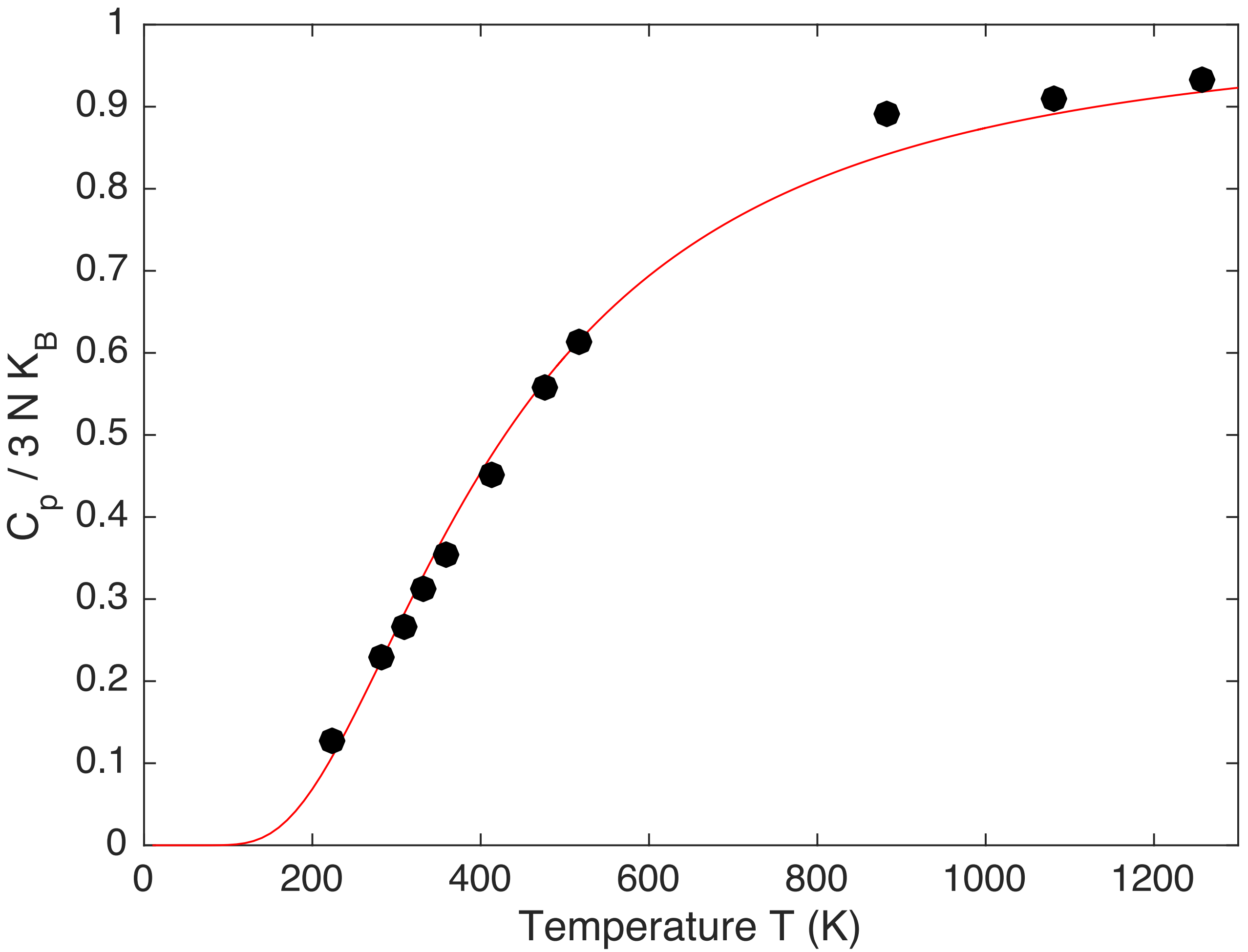
Reciprocal Lattice Units

Heat Capacity: Petit Dulong's Law / Gesetz



Variation of C_V with T

Heat Capacity: Diamond (as of 1906)



Waste Heat to Electricity