Achievements

Lecture 1: VESTA plotting of crystal structures

Lecture 2: How to describe a crystal structure

-- Crystal lattice
-- Basis

Lecture 3 +4: How to resolve crystal structures

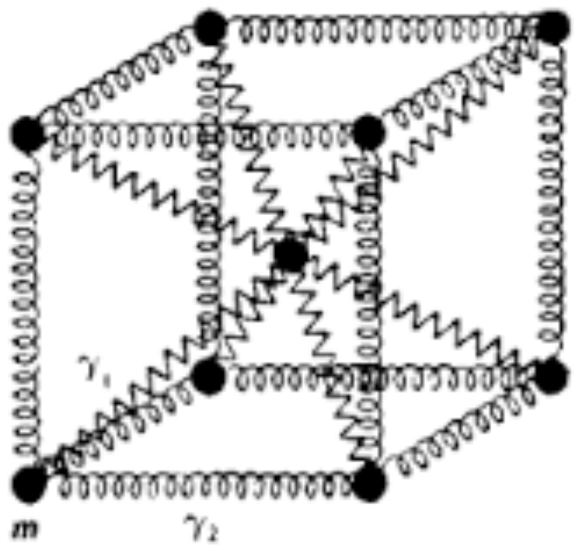
-- Reciprocal space
-- Scattering theory (Form and Structure Factor)
-- Resolving the crystal structure of a superconductor

Lecture 5: 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)

-- Anharmonic crystal interactions (2 pages)

-- Thermal conductivity (5 pages)

(2) Who is summarizing next week?

(3) Solve exercise sheet 5

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.

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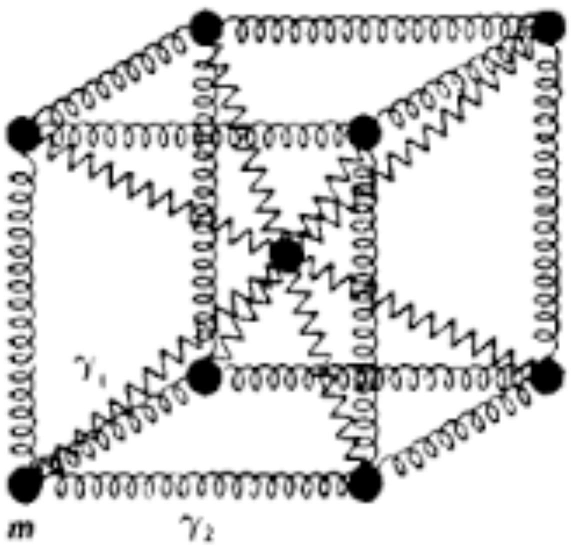
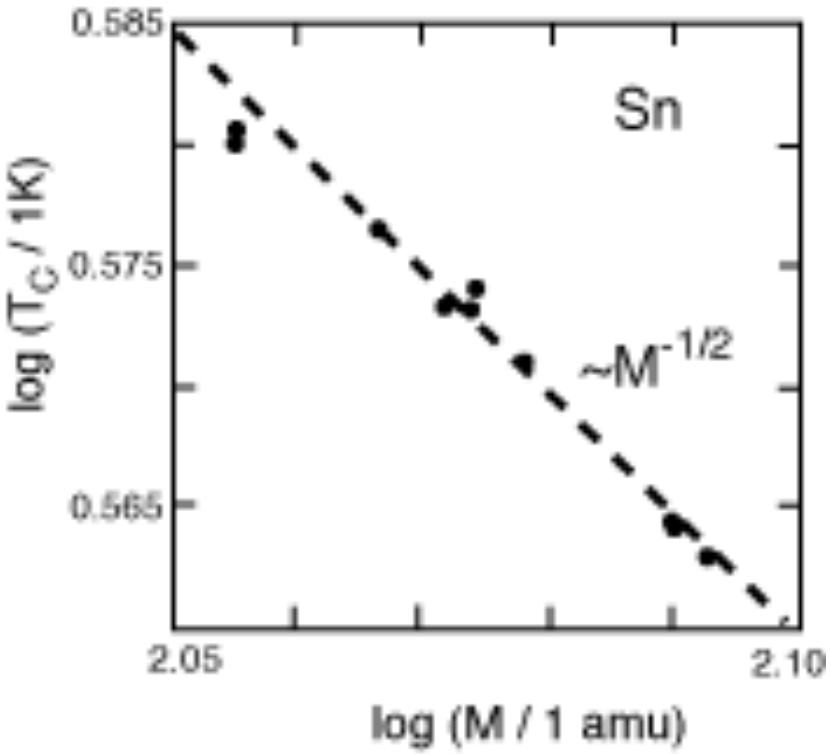
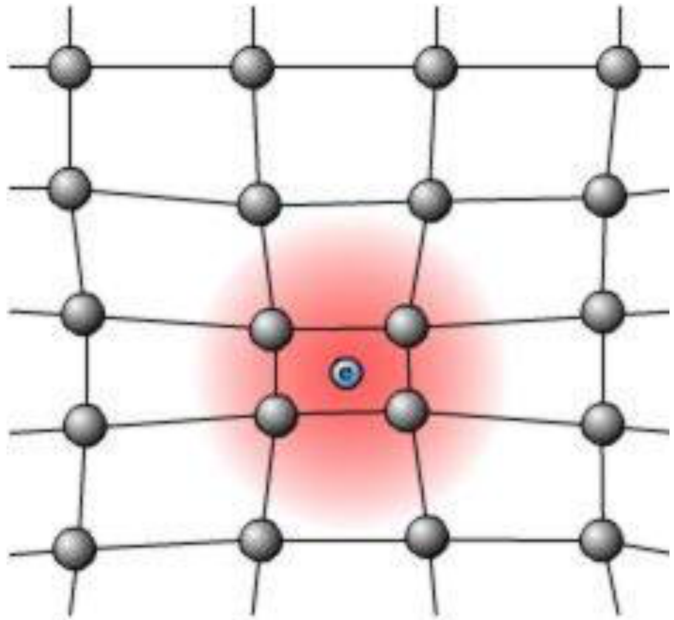


Phonons can make superconductivity

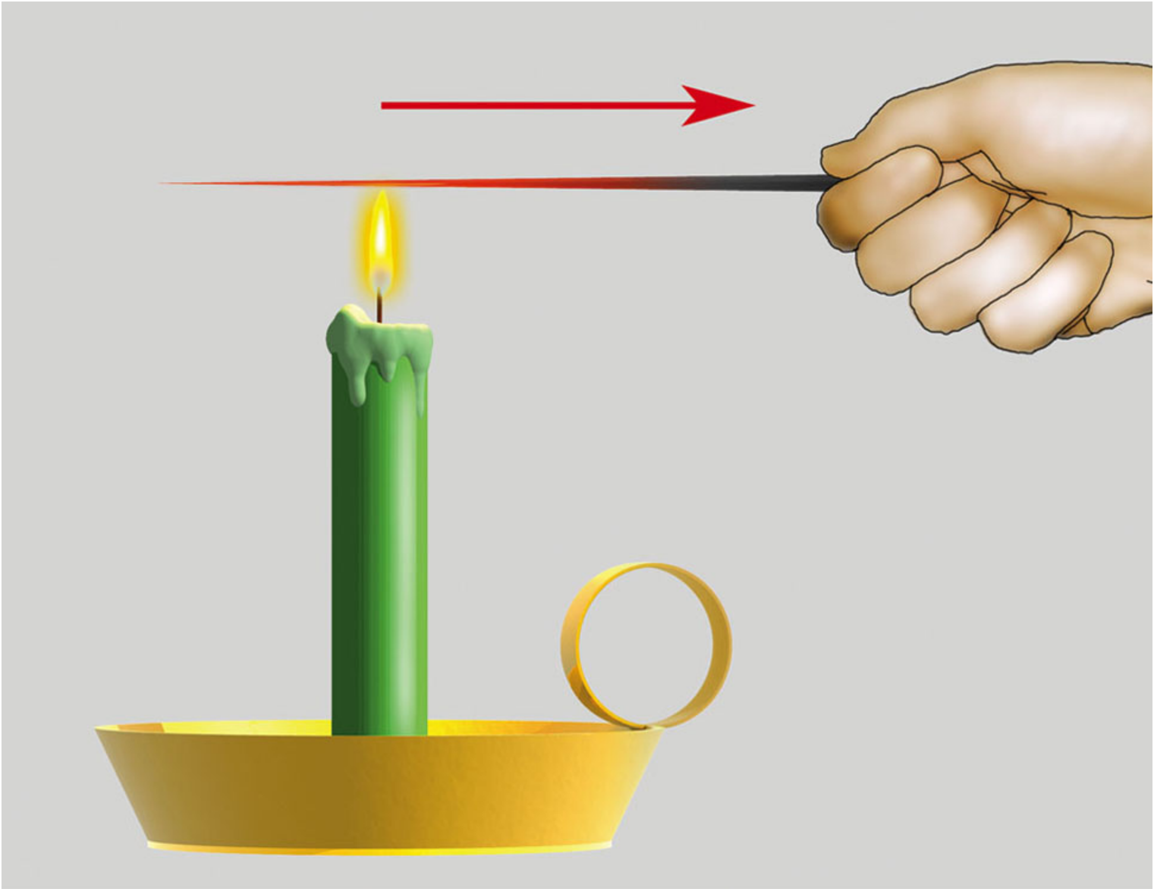


E. Maxwell, Phys. Rev. **86**, 235 (1952) and
B. Serin et al., Phys. Rev. B **86** 162 (1952))



http://www.chm.bris.ac.uk/
webprojects2000/igrant/theory.html

Phonons can conduct heat



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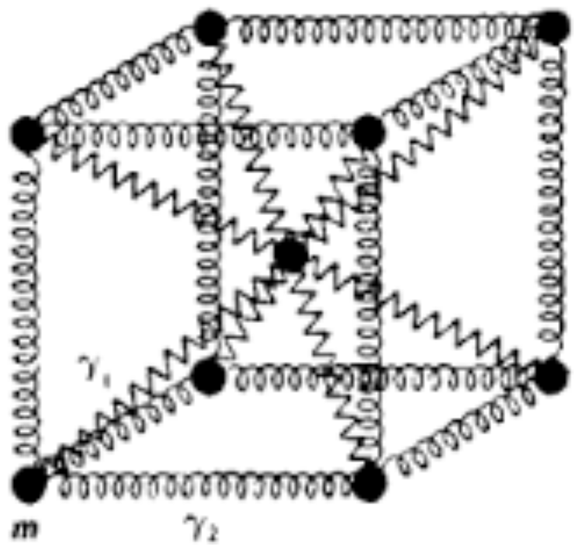
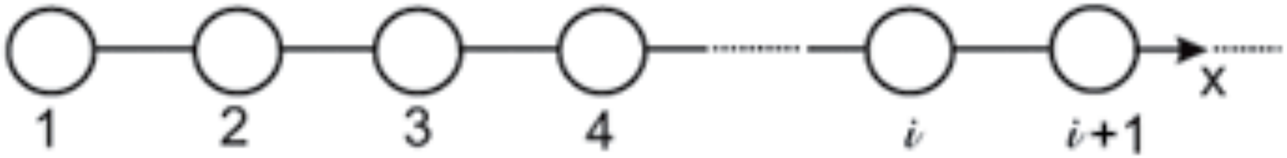
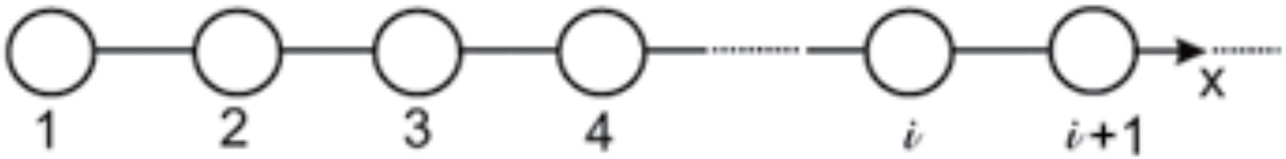


Linear chain -Models

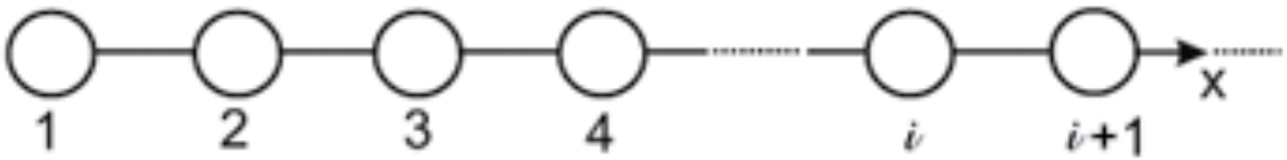


Structure factor: S = $\sum_i e^{-iqr_i}$



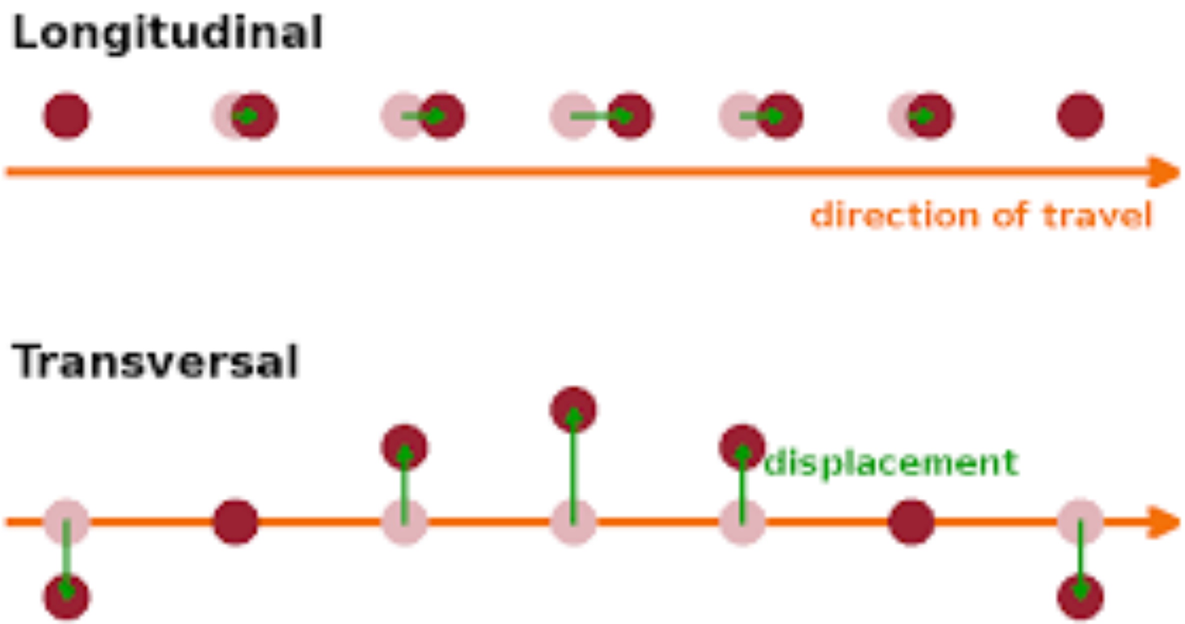
Madelungs constant: $\alpha = 2\ ln(2)$

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



Phonon dispersion: $\omega =$

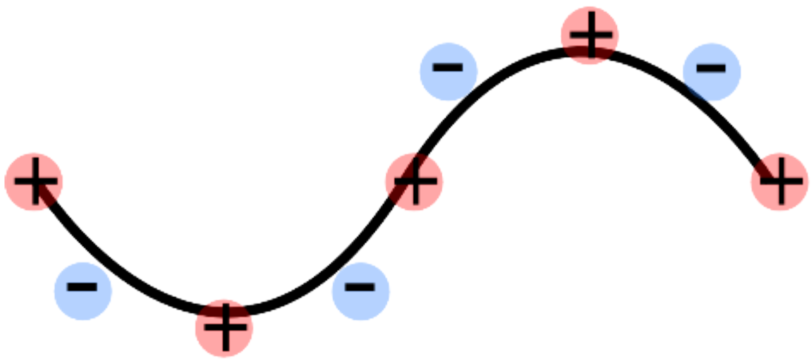
Longitudinal and Transverse Phonons



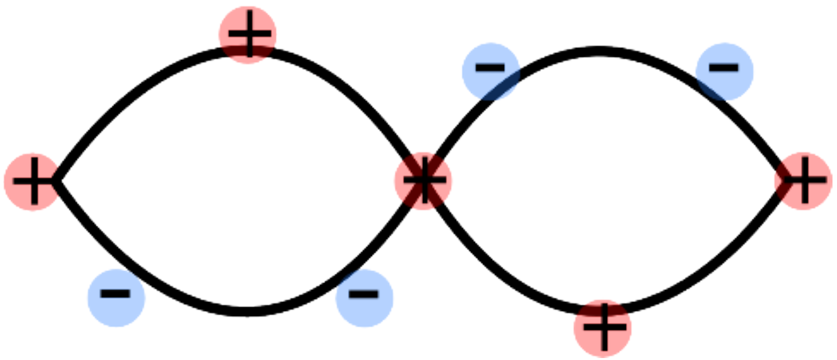
LA = Longitudinal Acoustic
LO = Longitudinal Optical
TA = Transversal Acoustic
TO = Transversal Optical

Acoustic and optical modes

Acoustical Mode



Optical Mode



LA = Longitudinal Acoustic
LO = Longitudinal Optical
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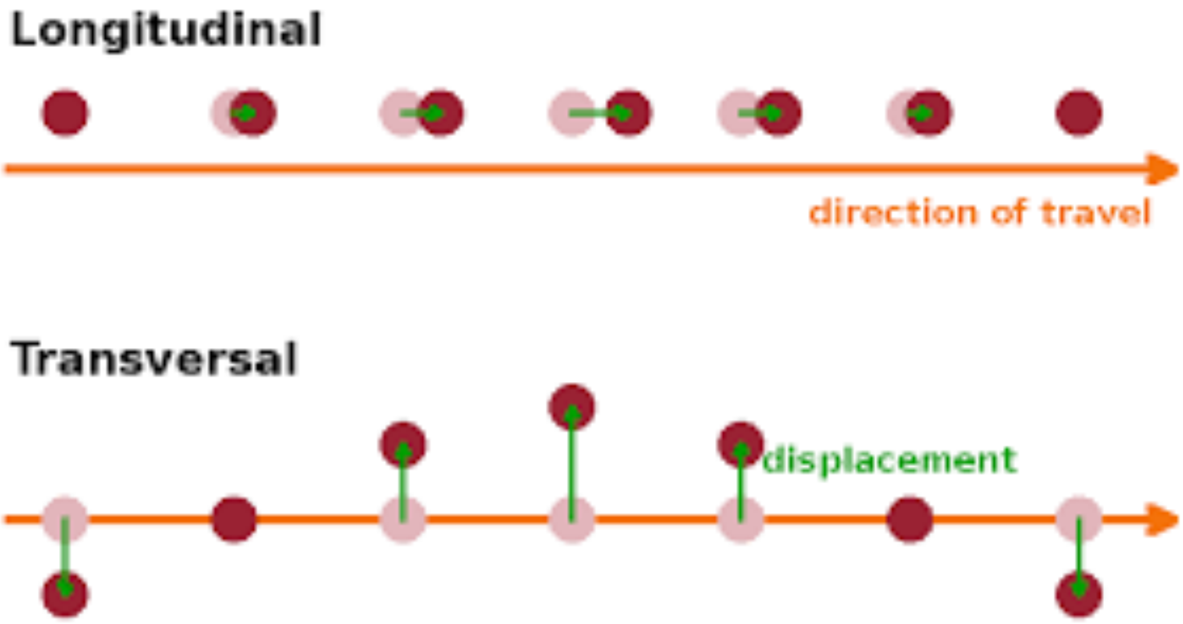
https://www2.warwick.ac.uk/fac/sci/physics/current/postgraduate/regs/mpags/ex5/phonons/

Number of phonon branches

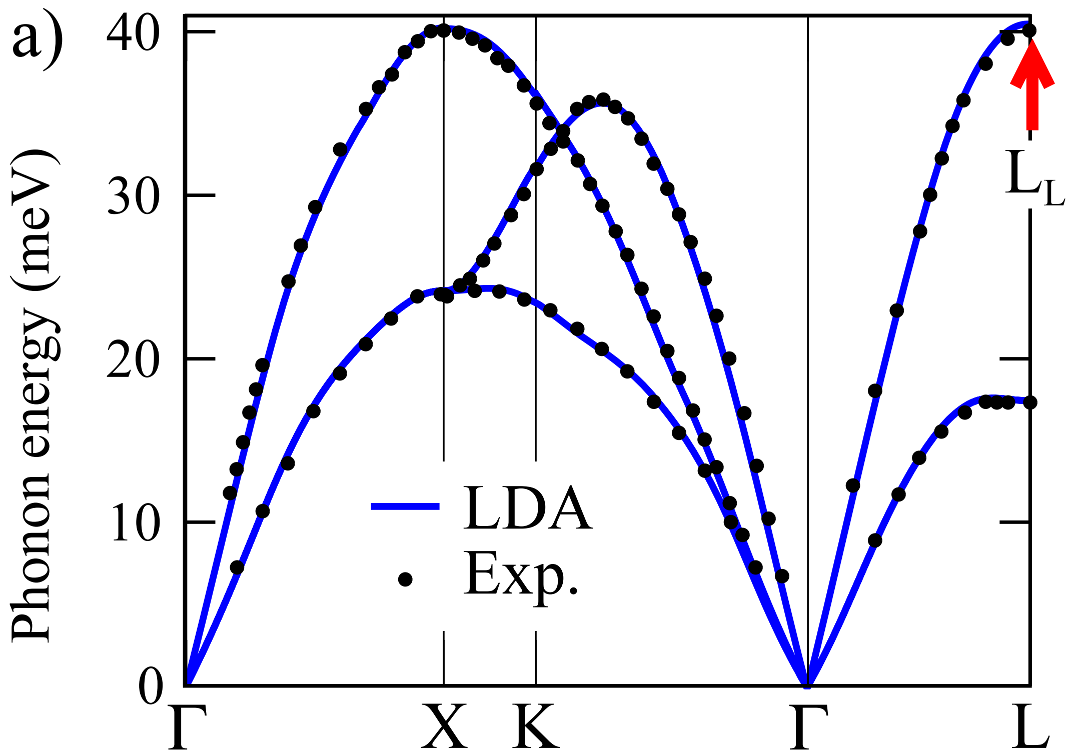


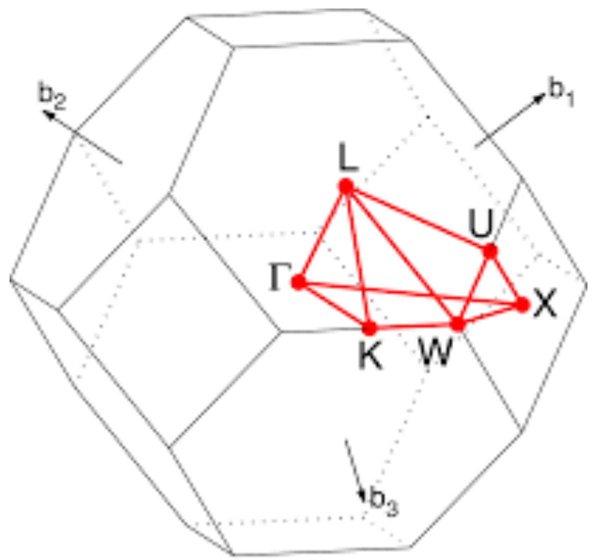
LA = Longitudinal Acoustic
LO = Longitudinal Optical
TA = Transversal Acoustic
TO = Transversal Optical

p = number of atoms in the primitive cell

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

Phonons in aluminium



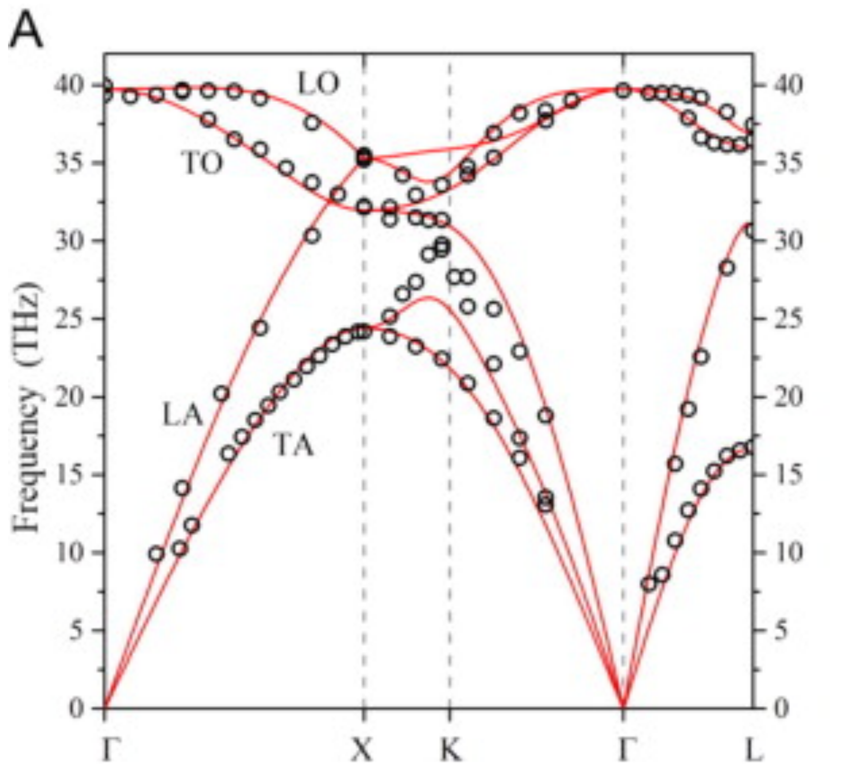


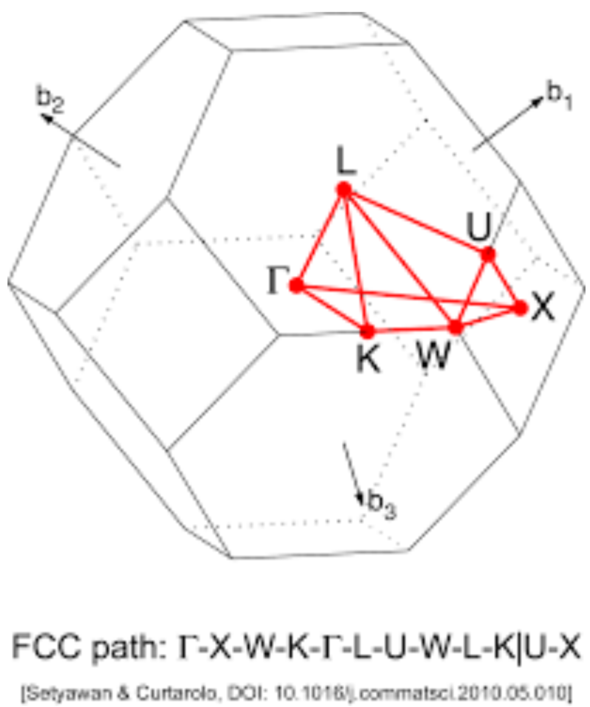
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[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





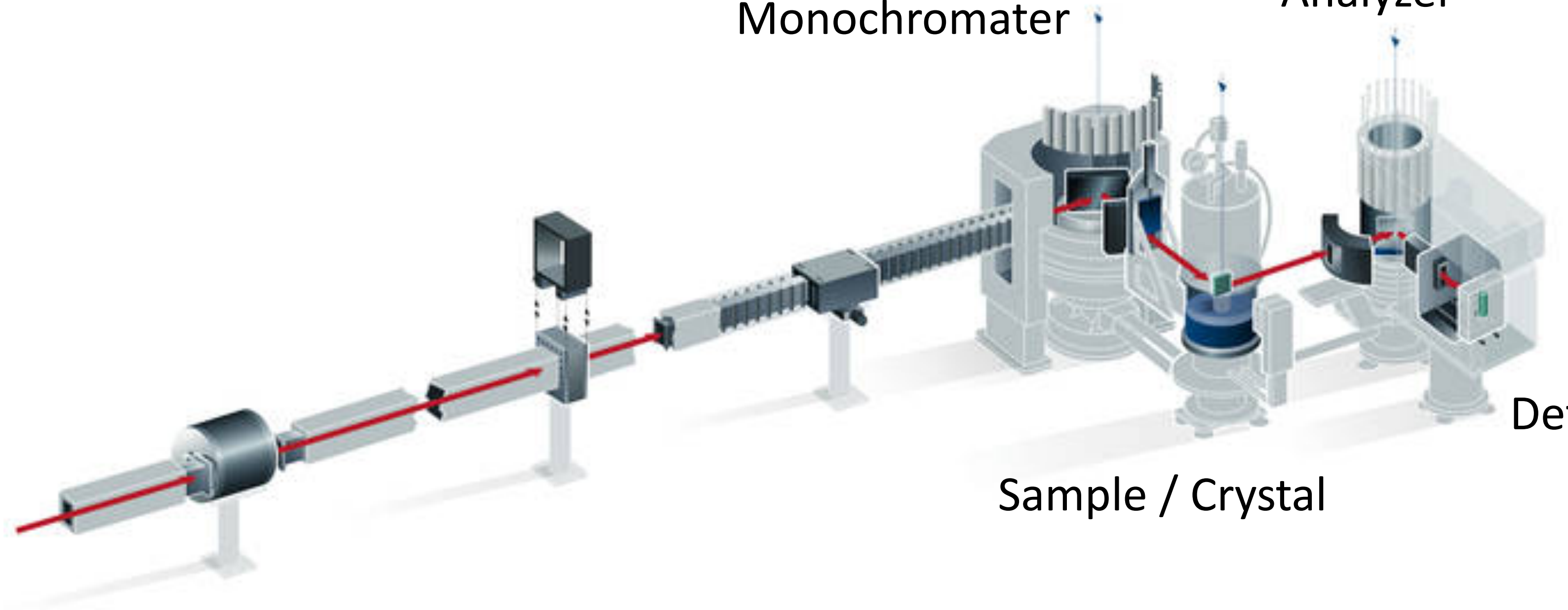
1 THz = 4.14… meV

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

3x*p* phonon branches

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

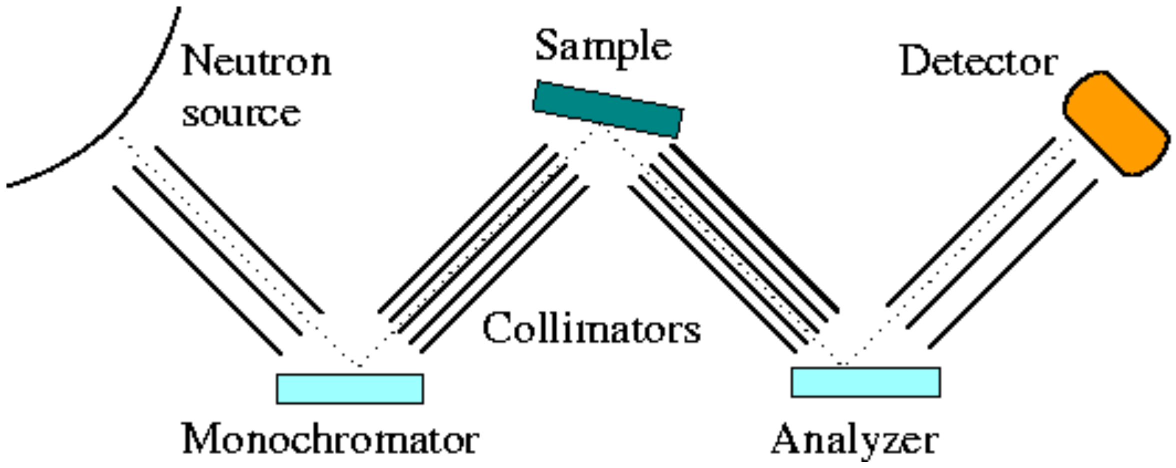
Triple axis spectrometer



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



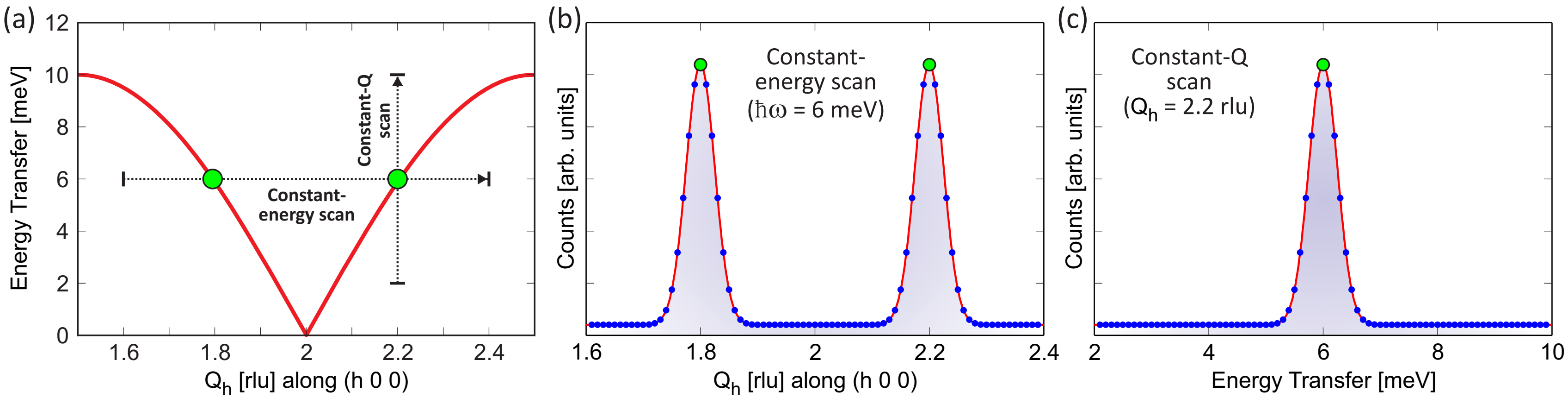


Figure 5: (a) Schematic view of how two points of the phonon dispersion curve can be measured using either (b) constant-energy scan or (c) constant-**Q** scan. By performing multiple scans it is possible to map out the complete dispersion (see below).

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

Triple axis spectrometer with x-rays

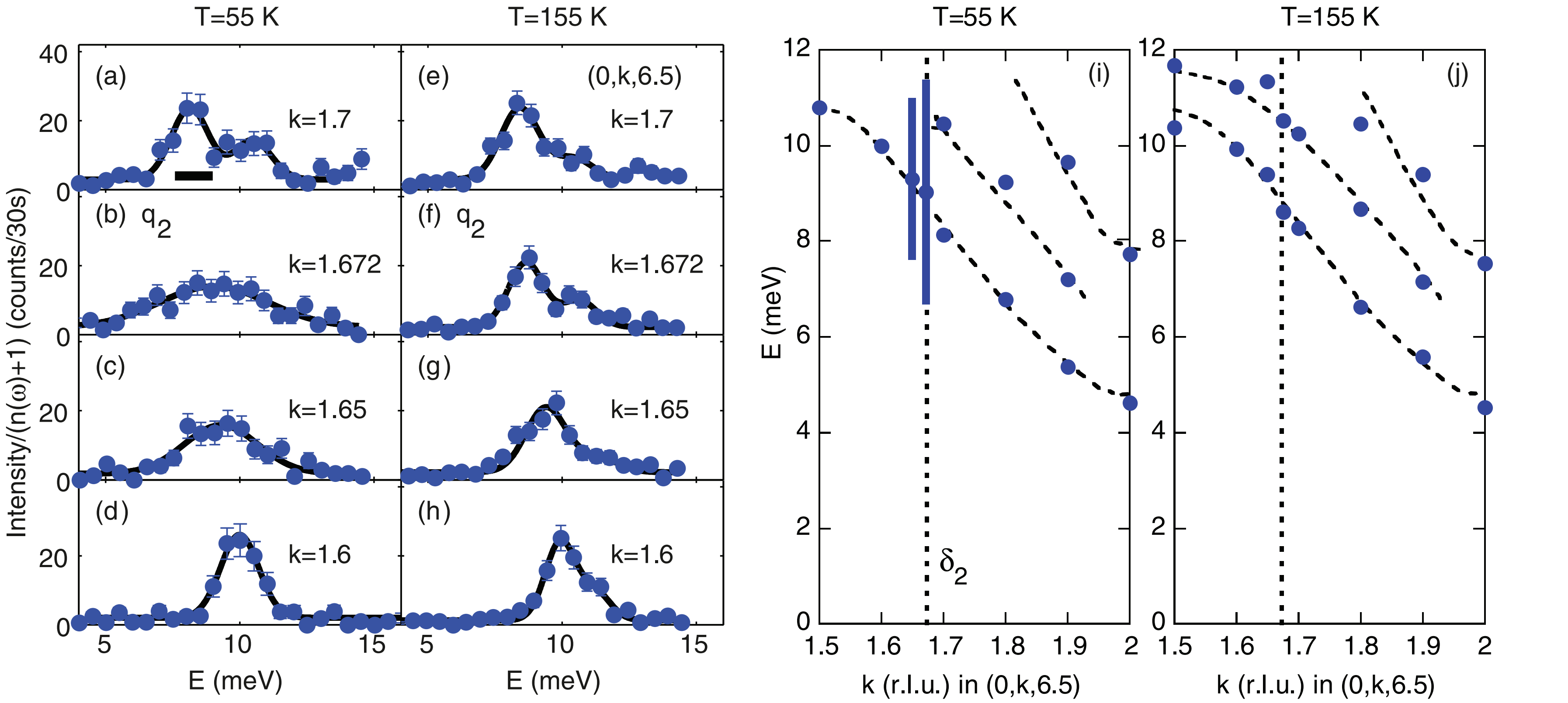
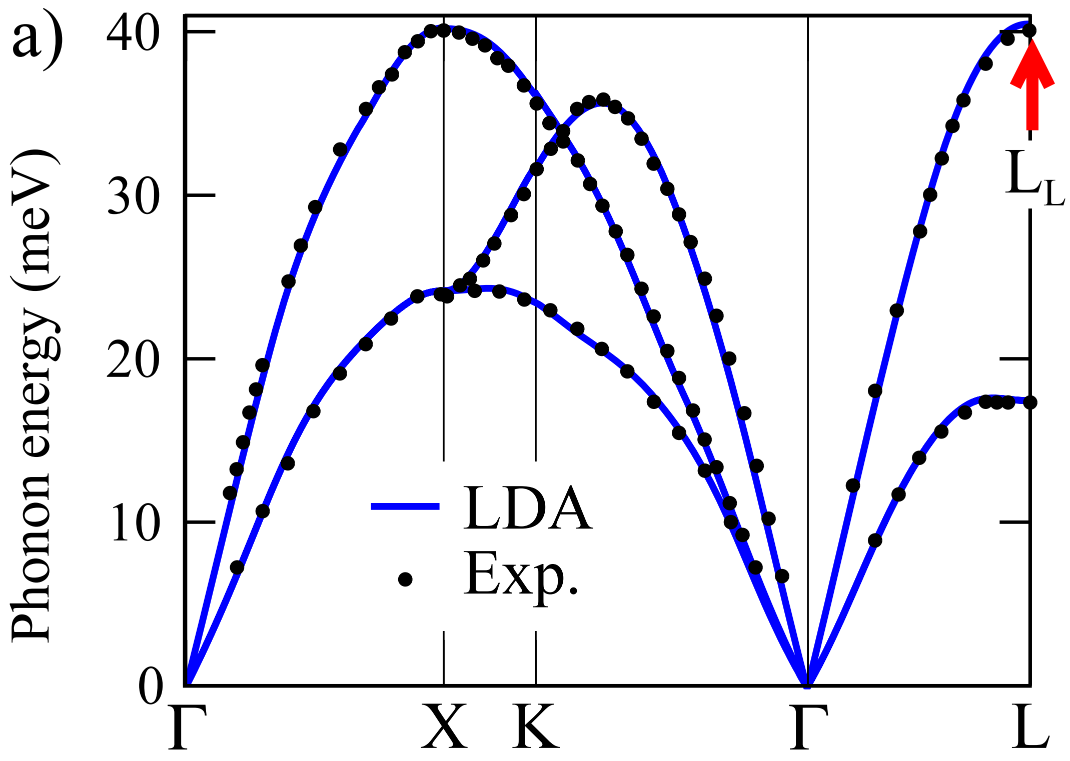
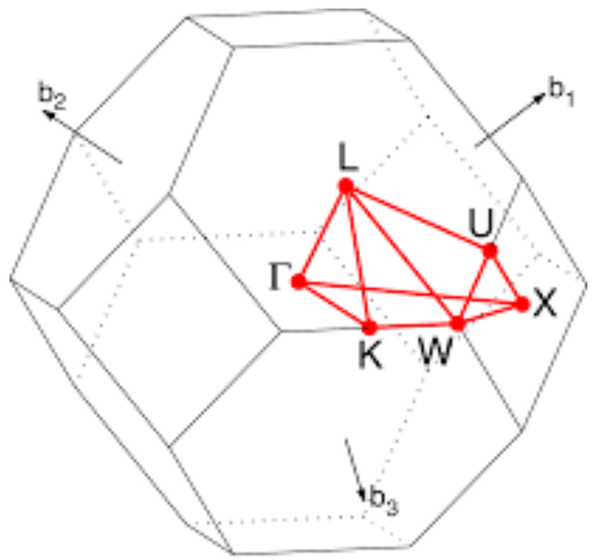


FIG. 5. (Color online) [(a)–(h)] IXS E scans of the low-energy phonons for wave vectors along the $(0,k,6.5)$ line. Solid lines are fits to a sum of Gaussian functions. Data have been multiplied by $1 - \exp[-E/(k_B T)]$ to correct for the Bose factor. The horizontal bar in panel (a) is the instrumental 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

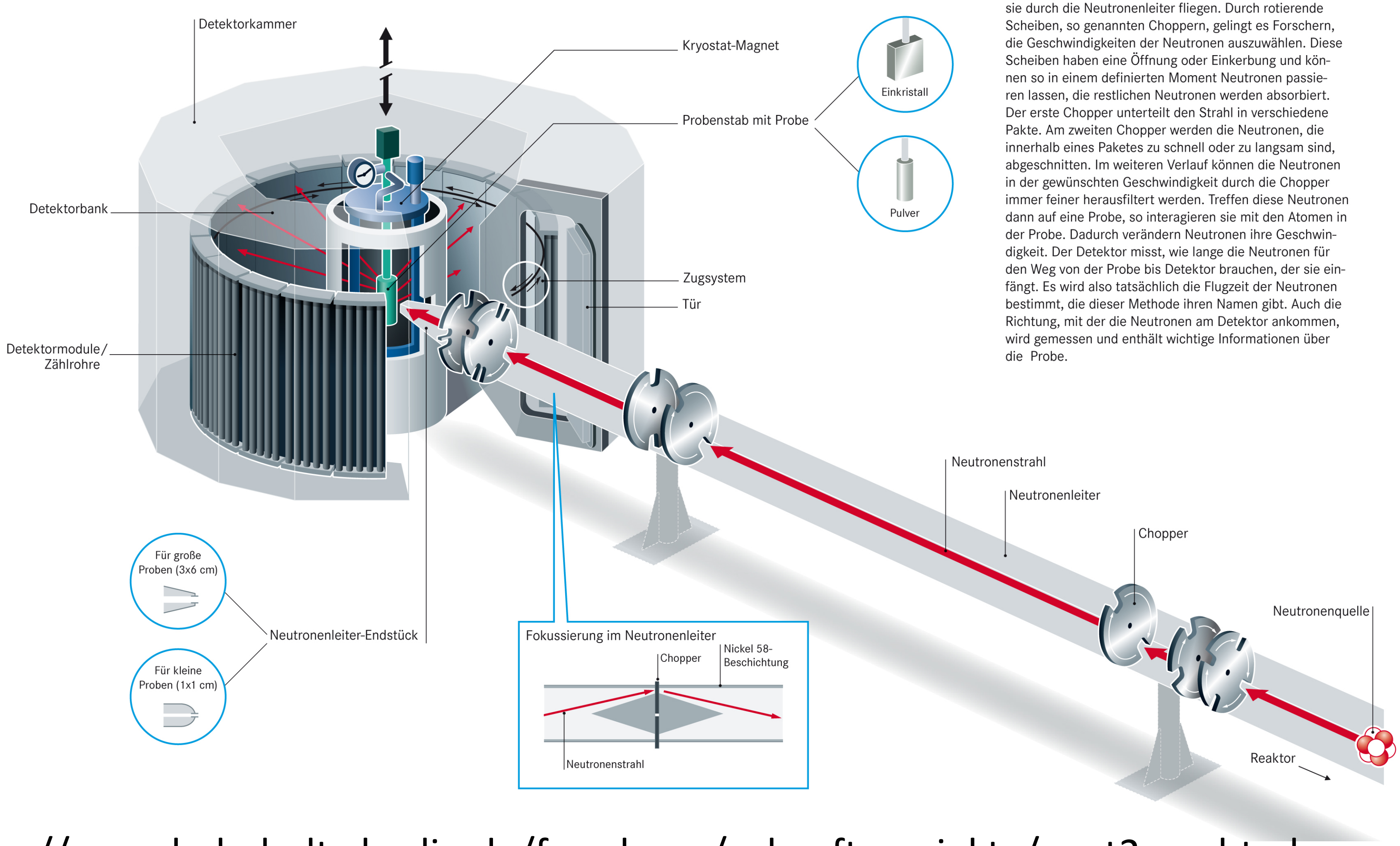
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

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

Time-of-flight spectrometry

Flugzeitspektrometer NEAT II

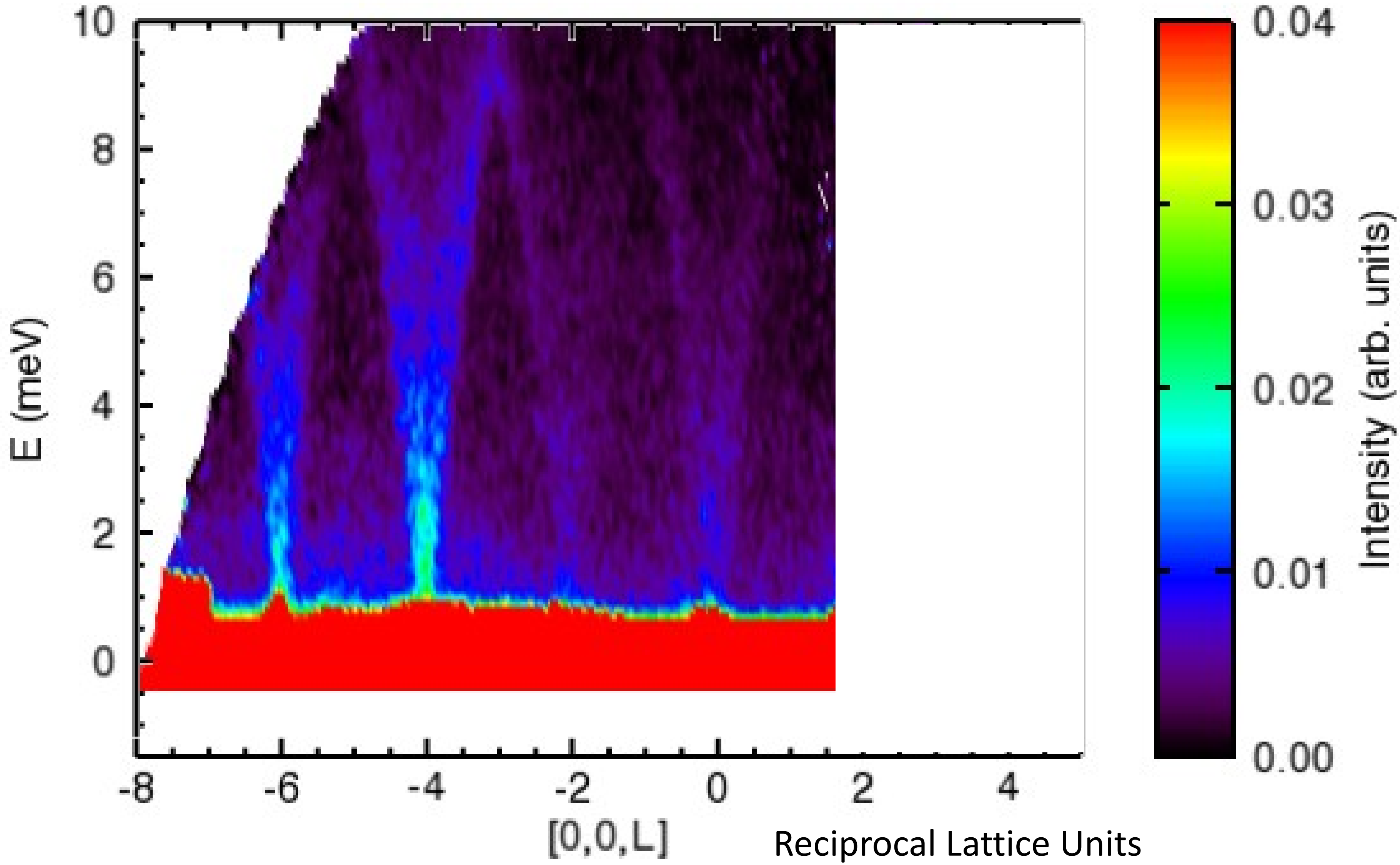
Infografik: E. Strickert



Die Neutronen gelangen von der Neutronenquelle BER II über Neutronenleiter zur Probe. Die Neutronen haben unterschiedliche Geschwindigkeiten (Wellenlängen), wenn sie durch die Neutronenleiter fliegen. Durch rotierende Scheiben, so genannten Choppern, gelingt es Forschern, die Geschwindigkeiten der Neutronen auszuwählen. Diese Scheiben haben eine Öffnung oder Einkerbung und können so in einem definierten Moment Neutronen passieren lassen, die restlichen Neutronen werden absorbiert. Der erste Chopper unterteilt den Strahl in verschiedene Pakte. Am zweiten Chopper werden die Neutronen, die innerhalb eines Paketes zu schnell oder zu langsam sind, abgeschnitten. Im weiteren Verlauf können die Neutronen in der gewünschten Geschwindigkeit durch die Chopper immer feiner herausfiltert werden. Treffen diese Neutronen dann auf eine Probe, so interagieren sie mit den Atomen in der Probe. Dadurch verändern Neutronen ihre Geschwindigkeit. Der Detektor misst, wie lange die Neutronen für den Weg von der Probe bis Detektor brauchen, der sie einfängt. Es wird also tatsächlich die Flugzeit der Neutronen bestimmt, die dieser Methode ihren Namen gibt. Auch die Richtung, mit der die Neutronen am Detektor ankommen, wird gemessen und enthält wichtige Informationen über die Probe.

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

Acoustic Phonon in Sr_2RuO_4



Reciprocal Lattice Units