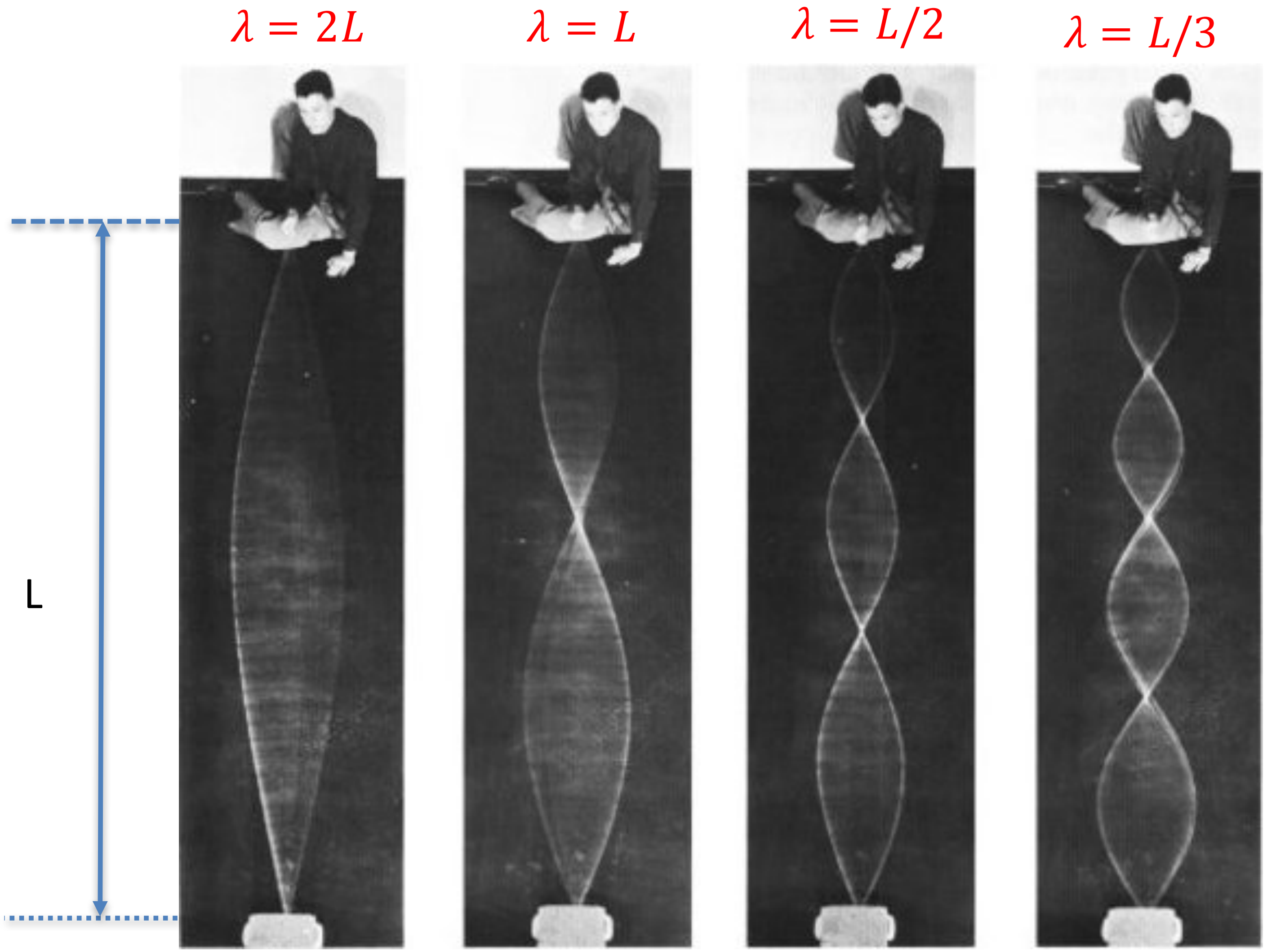
Today's Lecture: Phonons II

- Topic 1
  - Revisit of linear mono-atomic chain
  - Periodic boundary conditions
  - Number phonon modes
  - Density of states

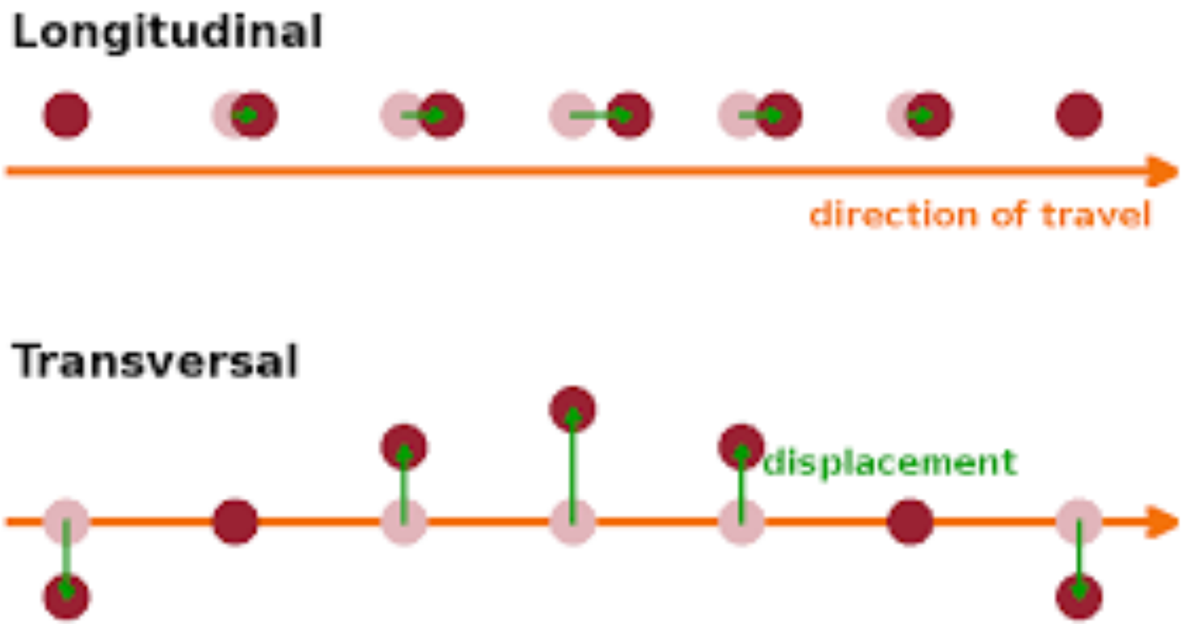
- Topic 2
  - Revisit of linear bi-atomic chain
  - Acoustic and optical phonons

- Topic 3
  - How to measure phonons
  - Inelastic neutron and x-ray scattering



$\lambda = 2L$
$\lambda = L$
$\lambda = L/2$
$\lambda = L/3$
L

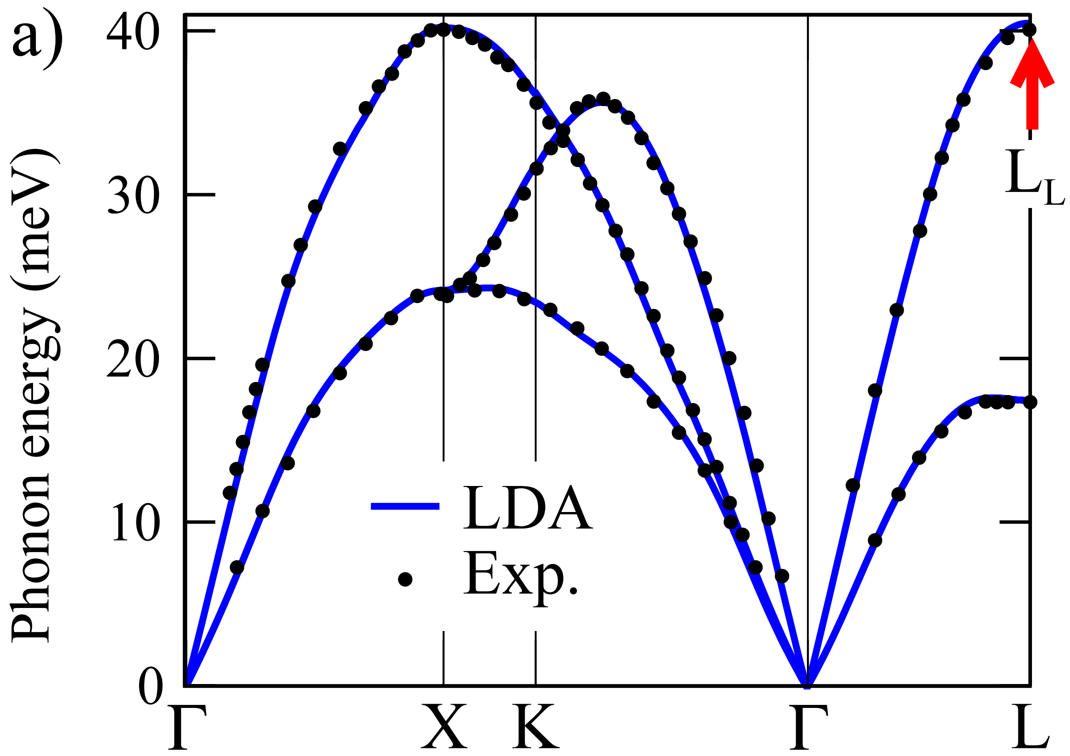
Longitudinal and Transverse Phonons

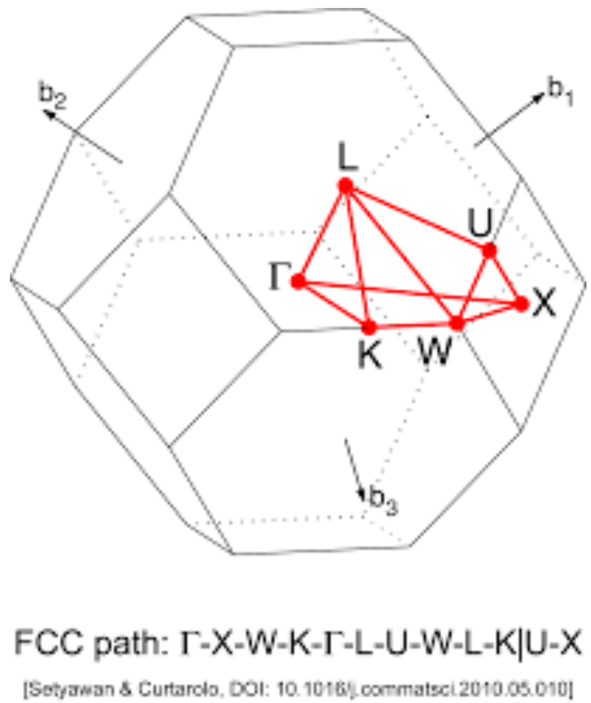


LA = Longitudinal Acoustic
TA = Transversal Acoustic

1 LA modes
2 TA modes

Phonons in aluminium





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

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Phonon dispersion
Linear Chain with two atoms

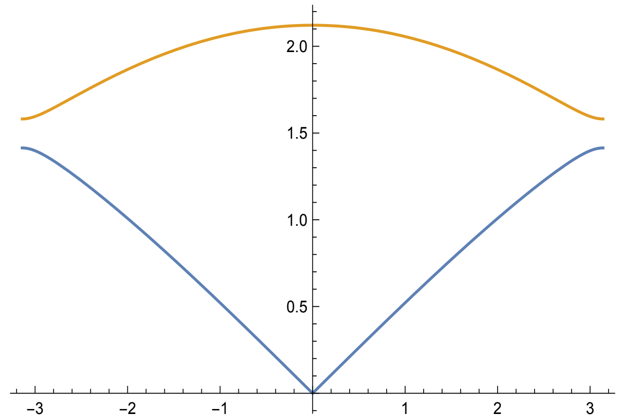
$$aa = \omega^2 * M_1 - 2 * C;$$
$$bb = C * \left(1 + e^{i*k*a}\right);$$
$$cc = C * \left(1 + e^{-i*k*a}\right);$$
$$dd = \omega^2 * M_2 - 2 * C;$$

In[5]:= $\text{Solve}\left[\text{Det}\left[\begin{pmatrix} aa & bb \\ cc & dd \end{pmatrix}\right] == 0, \omega\right]$

Out[5]=
$$\left\{\left\{\omega \to -\sqrt{\frac{C}{M_1} + \frac{C}{M_2} - \frac{\sqrt{C^2 M_1^2 + C^2 e^{-i a k} M_1 M_2 + C^2 e^{i a k} M_1 M_2 + C^2 M_2^2}}{M_1 M_2}}\right\},\right.$$
$$\left\{\omega \to \sqrt{\frac{C}{M_1} + \frac{C}{M_2} - \frac{\sqrt{C^2 M_1^2 + C^2 e^{-i a k} M_1 M_2 + C^2 e^{i a k} M_1 M_2 + C^2 M_2^2}}{M_1 M_2}}\right\},$$
$$\left\{\omega \to -\sqrt{\frac{C}{M_1} + \frac{C}{M_2} + \frac{\sqrt{C^2 M_1^2 + C^2 e^{-i a k} M_1 M_2 + C^2 e^{i a k} M_1 M_2 + C^2 M_2^2}}{M_1 M_2}}\right\},$$
$$\left.\left\{\omega \to \sqrt{\frac{C}{M_1} + \frac{C}{M_2} + \frac{\sqrt{C^2 M_1^2 + C^2 e^{-i a k} M_1 M_2 + C^2 e^{i a k} M_1 M_2 + C^2 M_2^2}}{M_1 M_2}}\right\}\right\}$$

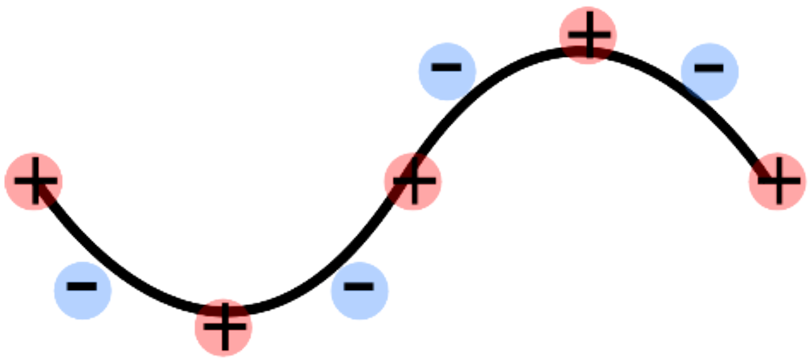
In[3]:= $\text{Plot}\left[\left\{\sqrt{\frac{1}{1} + \frac{1}{0.8} - \frac{\sqrt{1 + 0.8 * e^{-i\,k} + 0.8 * e^{i\,k} + 0.8 * 0.8}}{0.8}},\right.\right.$
$\left.\left.\sqrt{\frac{1}{1} + \frac{1}{0.8} + \frac{\sqrt{1 + 0.8 * e^{-i\,k} + 0.8 * e^{i\,k} + 0.8 * 0.8}}{0.8}}\right\}, \{k, -3.14, 3.14\}\right]$

Out[3]=

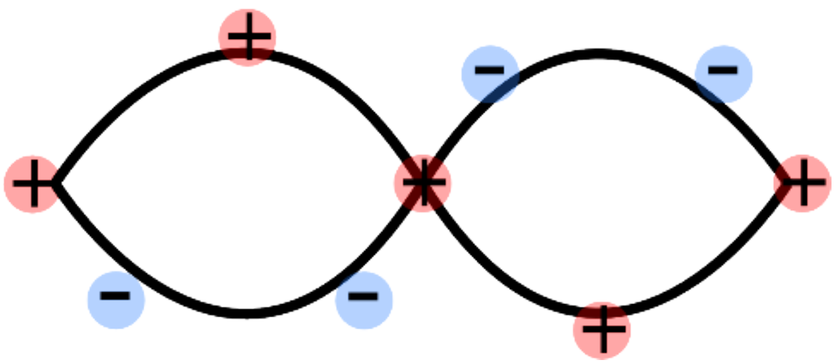


Acoustic and optical modes

Acoustical Mode



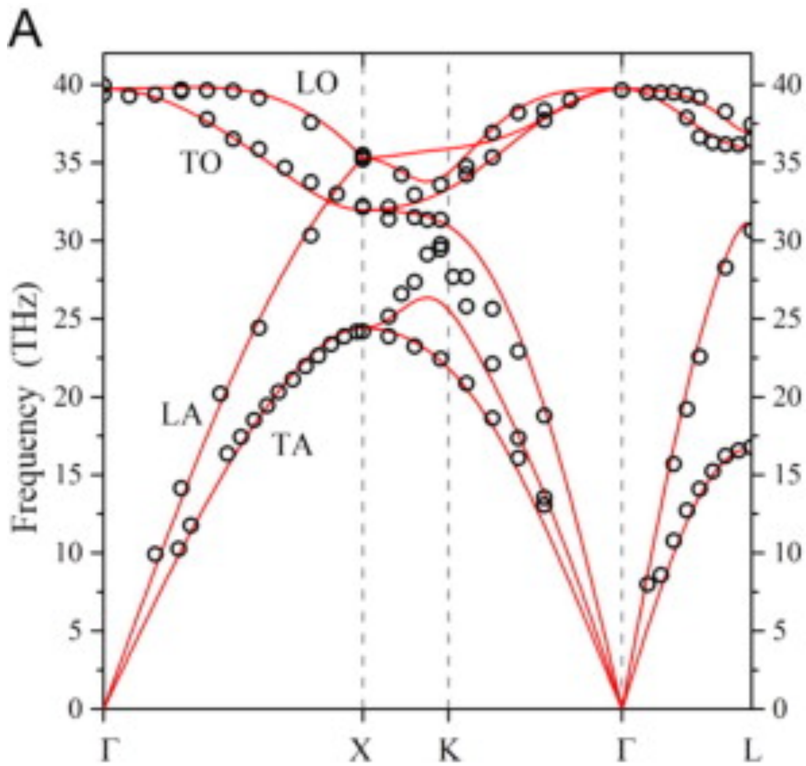
Optical Mode

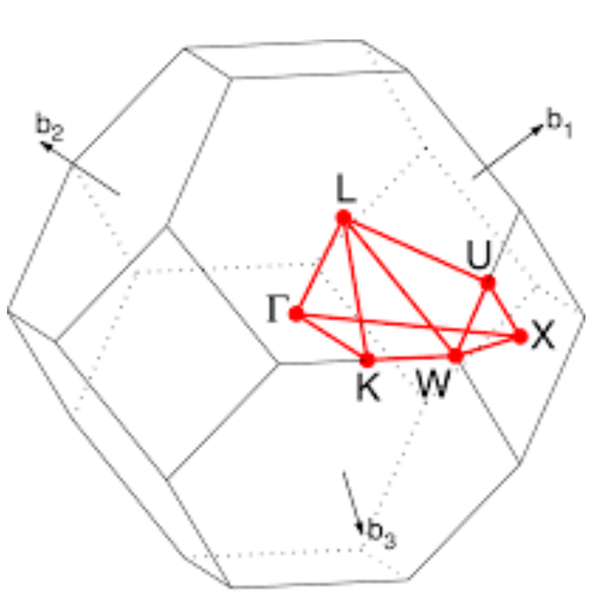


LA = Longitudinal Acoustic
LO = Longitudinal Optical
TA = Transversal Acoustic
TO = Transversal Optical

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

Phonons in diamond





FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

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

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

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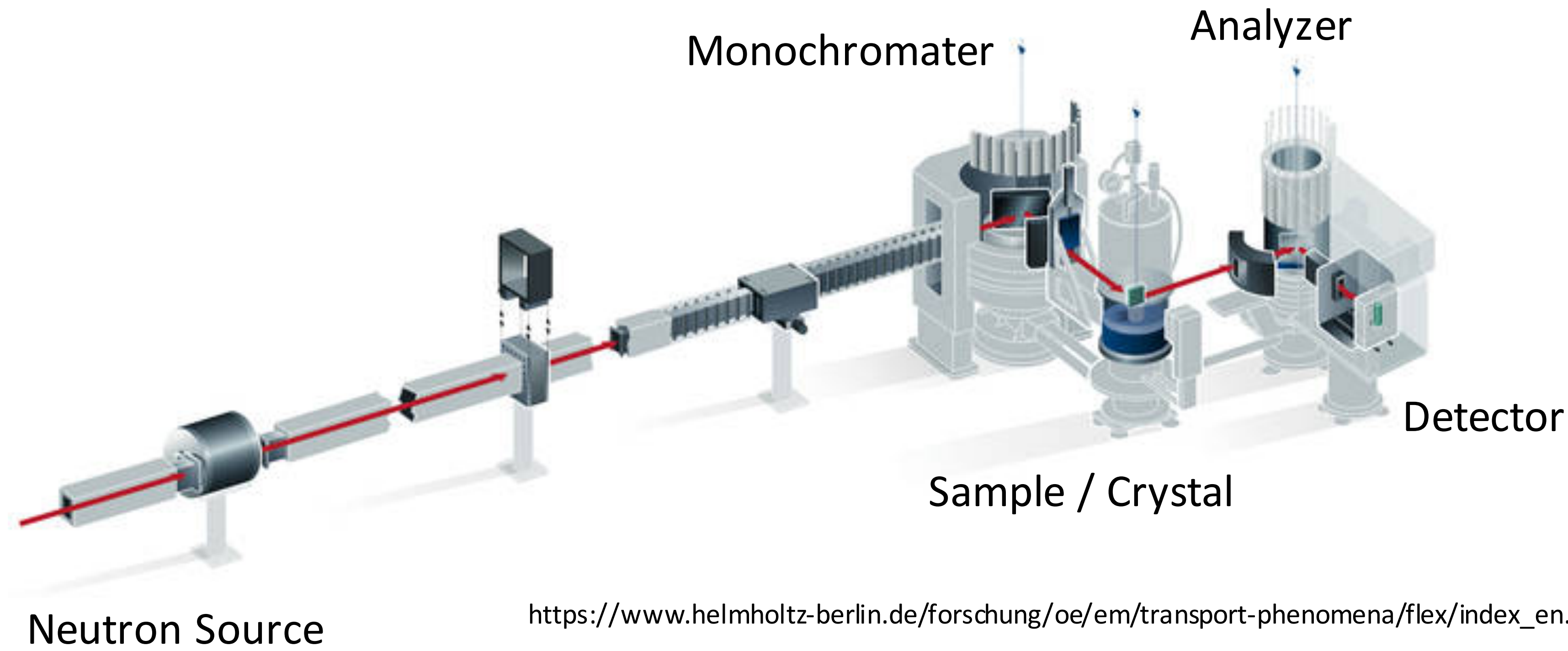
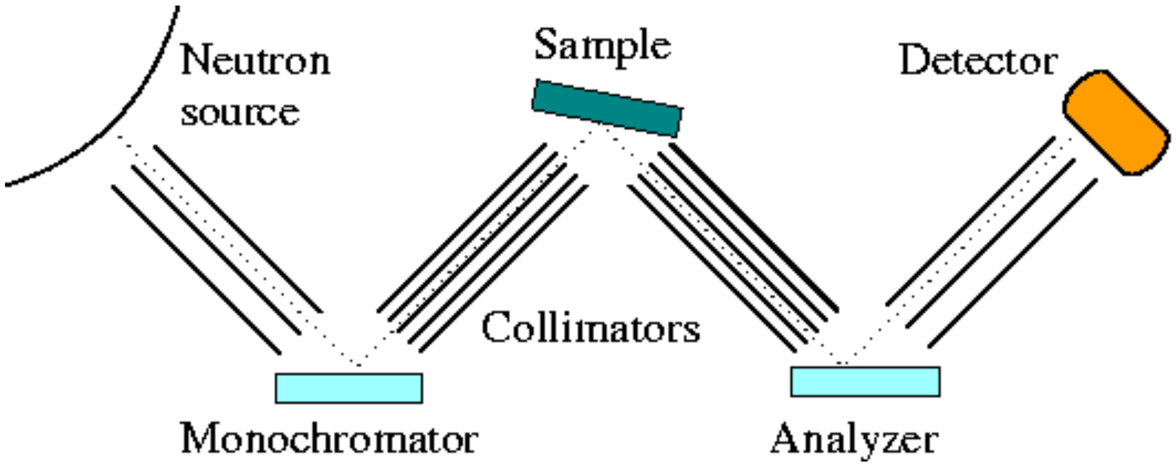
Triple axis spectrometer



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



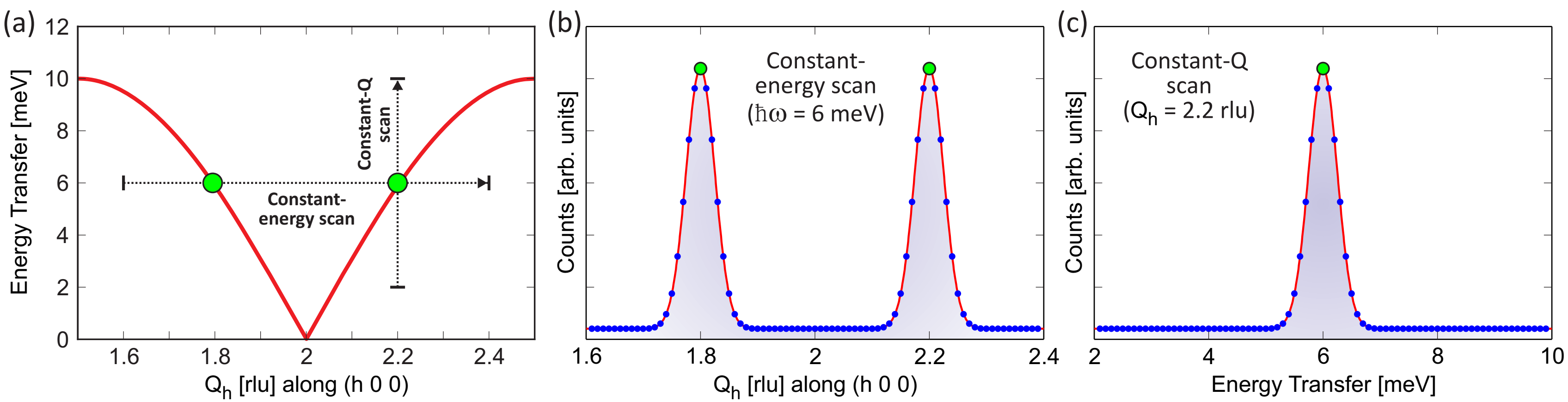


Figure 5: (a) Schematic view of how two points of the phonon dispersion curve can be measured using either (b) constant-energy scan or (c) constant-**Q** scan. By performing multiple scans it is possible to map out the complete dispersion (see below).

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

Triple axis spectrometer with x-rays

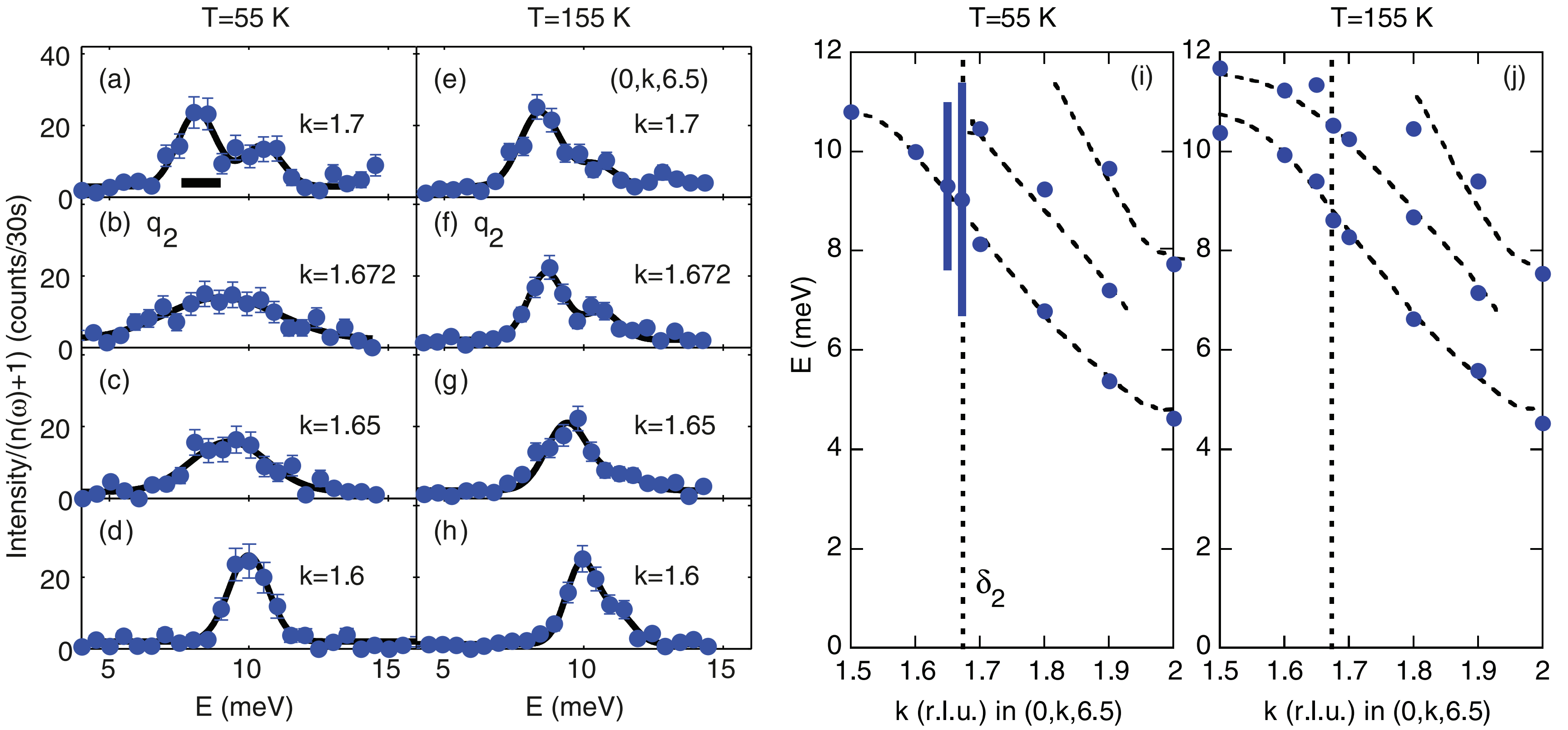
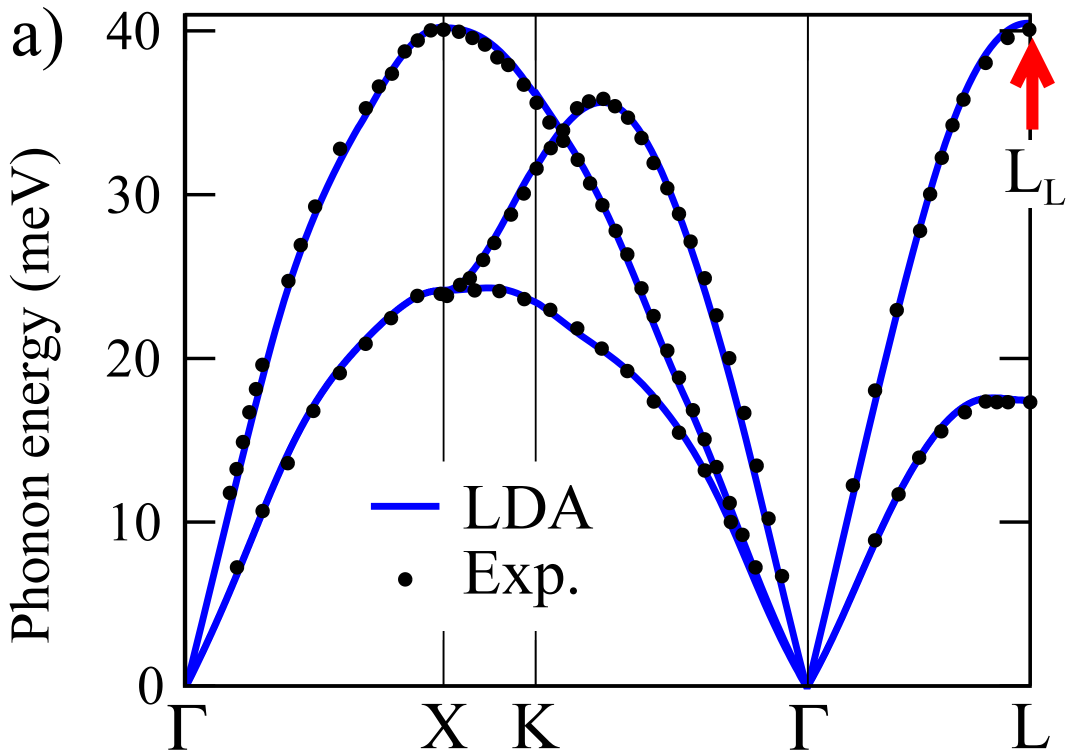
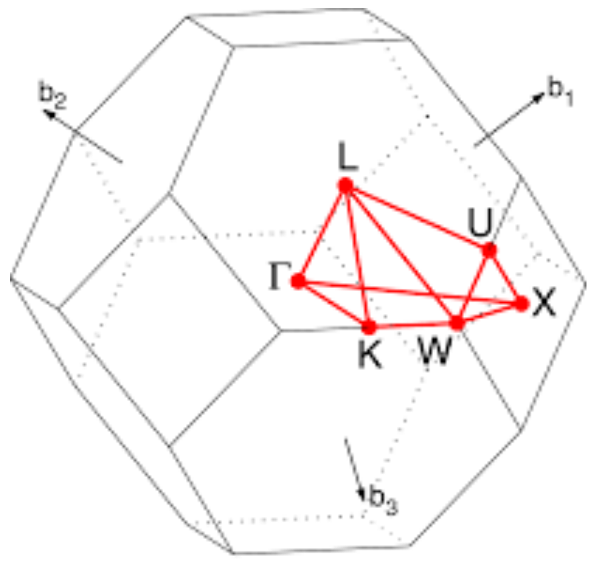


FIG. 5. (Color online) [(a)–(h)] IXS E scans of the low-energy phonons for wave vectors along the $(0,k,6.5)$ line. Solid lines are fits to a sum of Gaussian functions. Data have been multiplied by $1 - \exp[-E/(k_B T)]$ to correct for the Bose factor. The horizontal bar in panel (a) is the instrumental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

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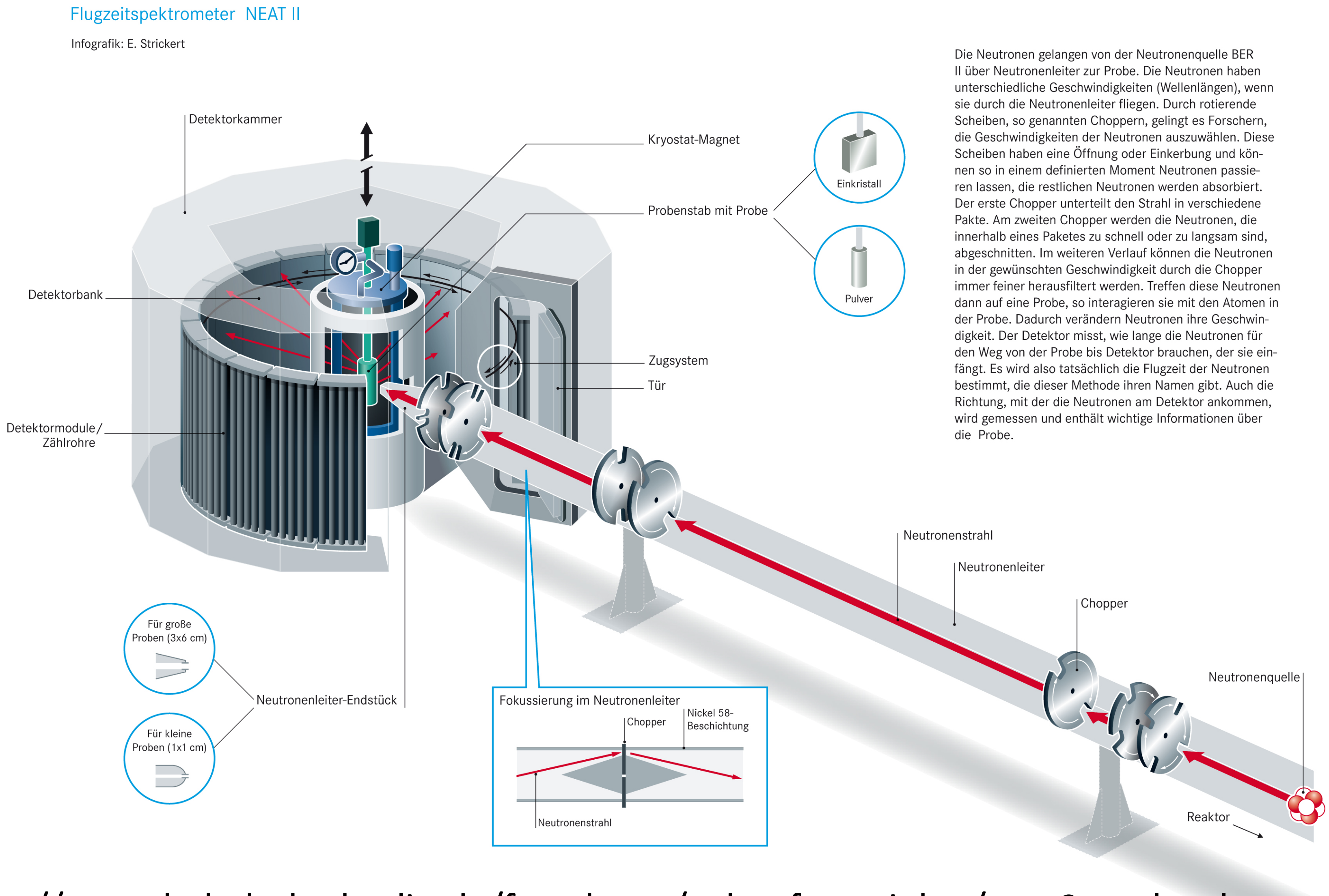
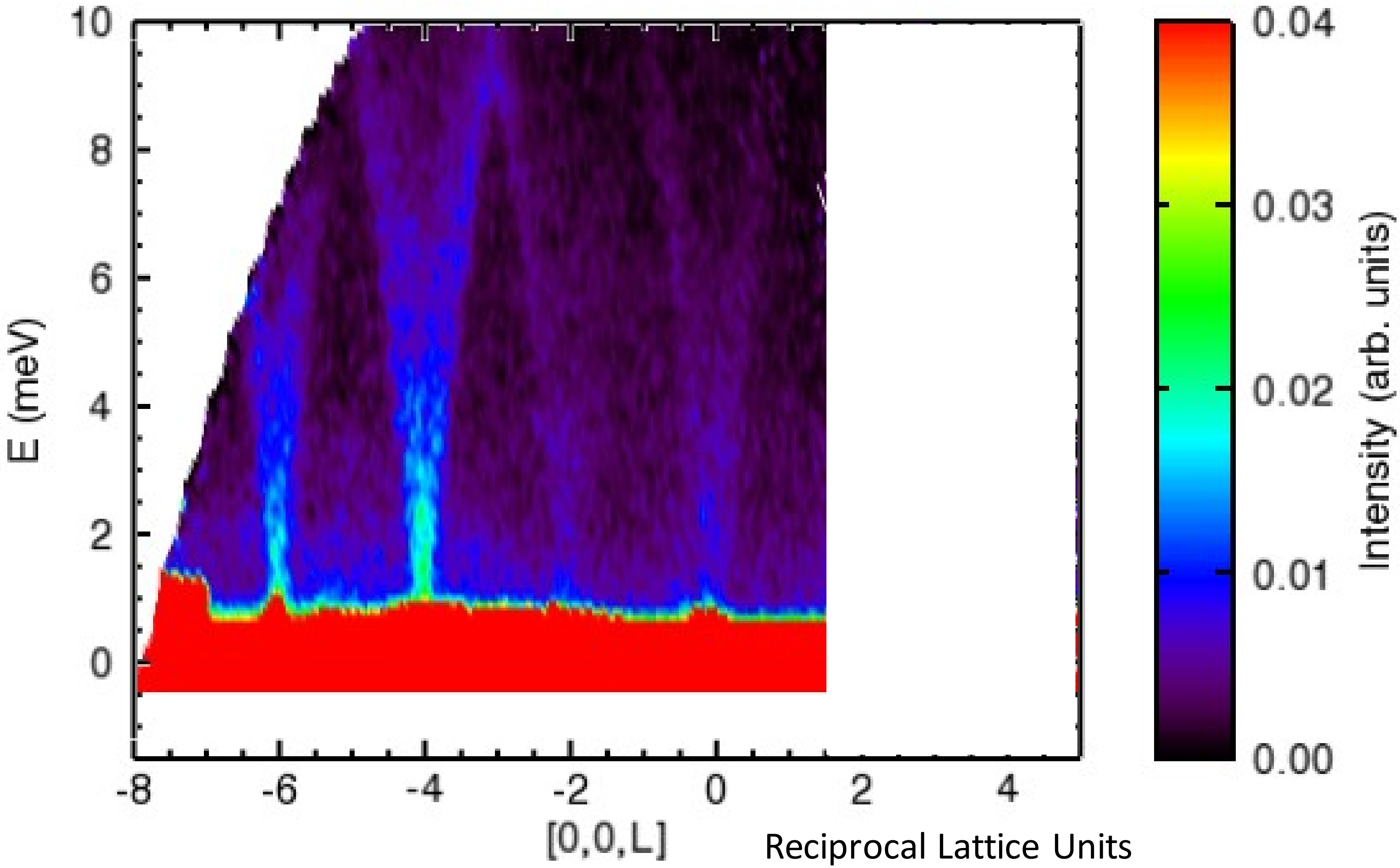
Time-of-flight spectrometry



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

Acoustic Phonon in Sr_2RuO_4



Reciprocal Lattice Units