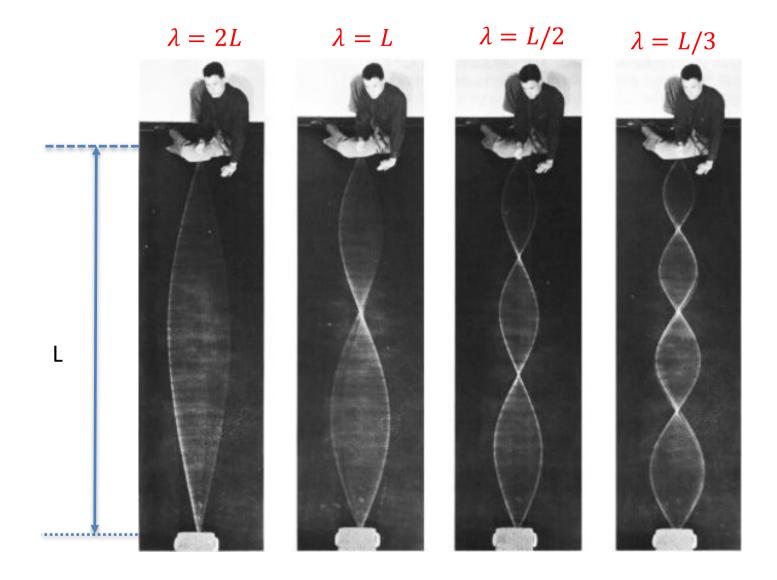
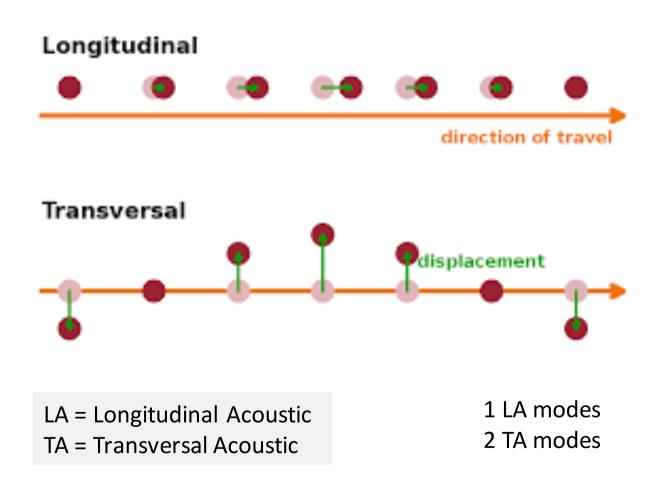
Today's Lecture: Phonons II

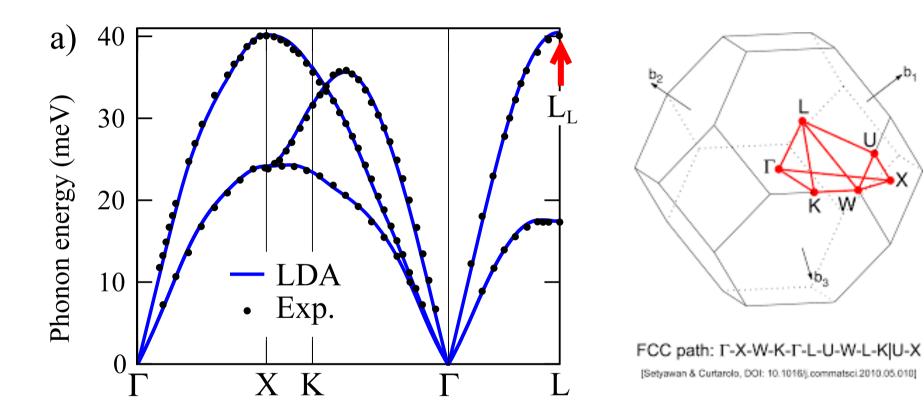
- Topic 1
 - Revisit of linear mono-atomic chain
 - Periodic boundary conditions
 - Number phonon modes
 - Density of states
- Topic 2
 - Revisit of linear bi-atomic chain
 - Acoustic and optical phonons
- Topic 3
 - How to measure phonons
 - Inelastic neutron and x-ray scattering



Longitudinal and Transverse Phonons



Phonons in aluminium

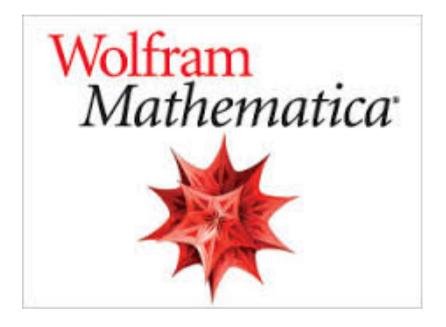


http://iopscience.iop.org/article/10.1088/0953-8984/24/5/053202

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

Phonon dispersion Linear Chain with two atoms



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

$$ln[5] = Solve[Det[(aa bb cc dd))] = 0, \omega]$$

$$\text{Out} \text{[S]= } \left\{ \left\{ \omega \rightarrow -\sqrt{\frac{C}{M_1} + \frac{C}{M_2}} - \frac{\sqrt{C^2 \; M_1^2 + C^2 \; e^{-i \; a \; k} \; M_1 \; M_2 + C^2 \; e^{i \; a \; k} \; M_1 \; M_2 + C^2 \; M_2^2}}{M_1 \; M_2} \; \right\} \text{,}$$

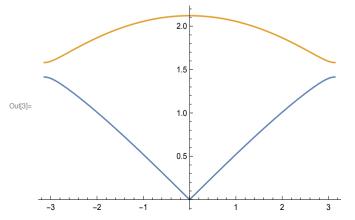
$$\left\{\omega \to \sqrt{ \, \frac{C}{M_1} + \frac{C}{M_2} \, - \, \frac{\sqrt{C^2 \, M_1^2 + C^2 \, e^{-i \, a \, k} \, M_1 \, M_2 + C^2 \, e^{i \, a \, k} \, M_1 \, M_2 + C^2 \, M_2^2}}{M_1 \, M_2} \, \, \right\} \text{,}$$

$$\left\{\omega \rightarrow -\sqrt{\frac{C}{M_{1}} + \frac{C}{M_{2}}} + \frac{\sqrt{C^{2} \ M_{1}^{2} + C^{2} \ e^{-i \ a \ k} \ M_{1} \ M_{2} + C^{2} \ e^{i \ a \ k} \ M_{1} \ M_{2} + C^{2} \ M_{2}^{2}}}{M_{1} \ M_{2}} \right\},$$

$$\left\{\omega \to \sqrt{\frac{\,C\,}{\,\text{M}_{1}}\,+\,\frac{\,C\,}{\,\text{M}_{2}}\,+\,\frac{\sqrt{\,C^{2}\,\,\text{M}_{1}^{2}\,+\,C^{2}\,\,\text{e}^{-\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{a}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{2}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{1}\,\,\text{M}_{2}\,+\,C^{2}\,\,\text{e}^{\,\text{i}\,\,\text{k}}\,\,\text{M}_{2}\,\,\text{k}}\,\,\text{M}_{2}\,\,\text{k}_{1}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text{k}_{2}\,\,\text$$

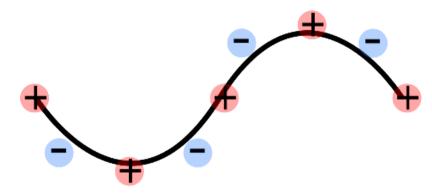
$$\ln[3] = \text{Plot} \left[\left\{ \sqrt{\frac{1}{1} + \frac{1}{0.8} - \frac{\sqrt{1 + 0.8 * e^{-i \cdot k} + 0.8 * e^{i \cdot k} + 0.8 * 0.8}}{0.8}} \right\} \right]$$

$$\sqrt{\frac{1}{1} + \frac{1}{0.8} + \frac{\sqrt{1 + 0.8 * e^{-i k} + 0.8 * e^{i k} + 0.8 * 0.8}}{0.8}}\right], \{k, -3.14, 3.14\}]$$

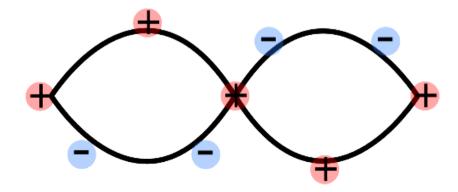


Acoustic and optical modes

Acoustical Mode



Optical Mode



LA = Longitudinal Acoustic

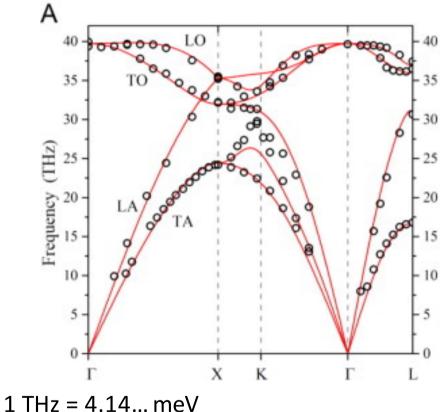
LO = Longitudinal Optical

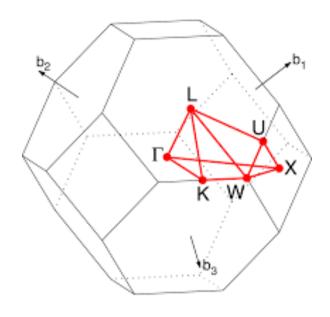
TA = Transversal Acoustic

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][.commatsci.2010.05.010]

1 1HZ = 4.14... meV

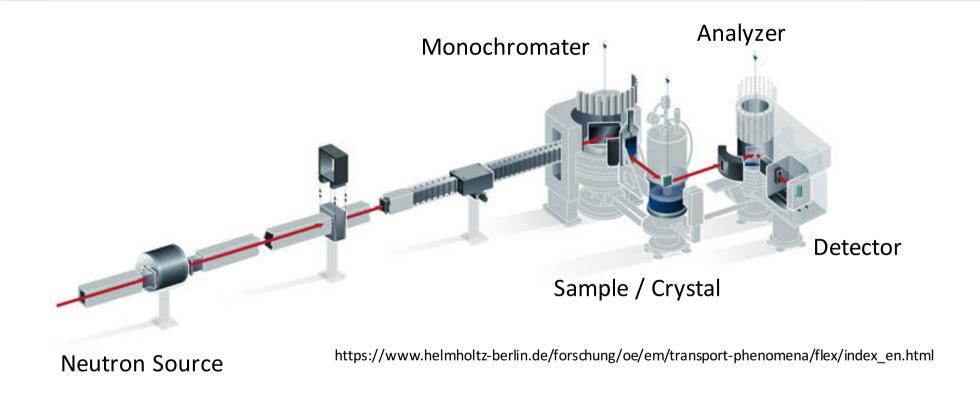
p = number of atoms in the basis of the primitive cell 3xp phonon branches

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

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

Triple axis spectrometer





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

Triple axis spectrometer

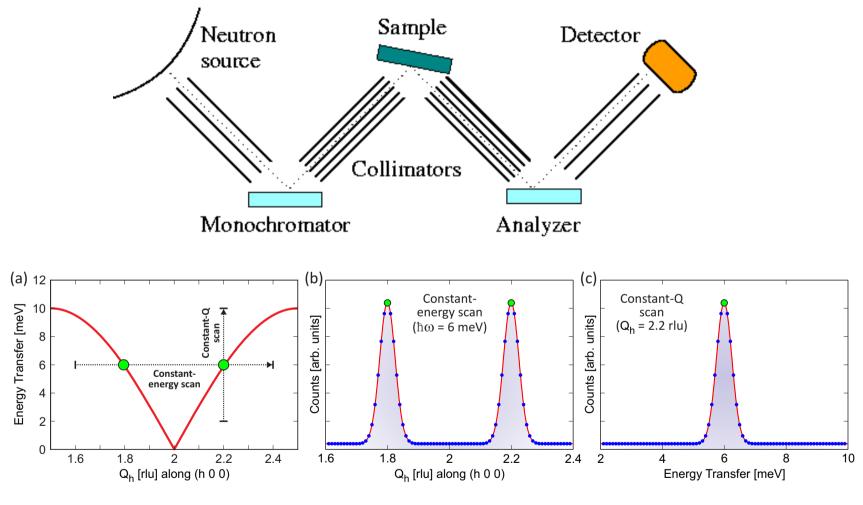


Figure 5: (a) Schematic view of how two points of the phonon dispersion curve can be measured using either (b) constant-energy scan or (c) constant-Q scan. By performing multiple scans it is possible to map out the complete dispersion (see below). https://www.psi.ch/lns/TrainingEN/INS Student Practicum PSI.pdf

Triple axis spectrometer with x-rays

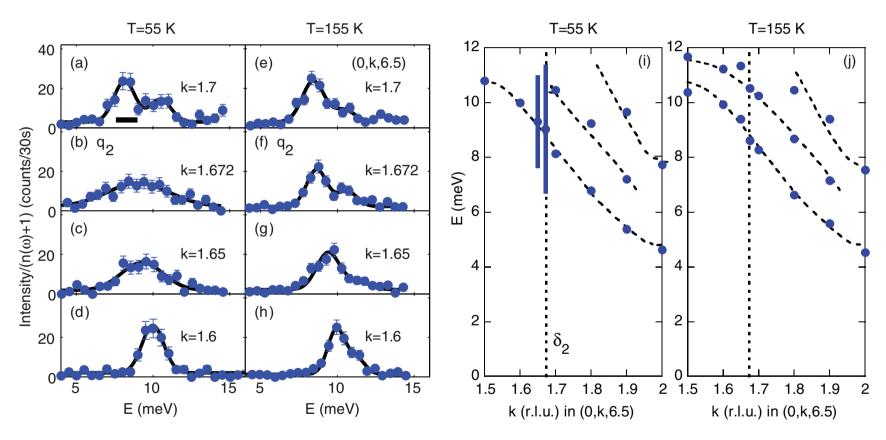
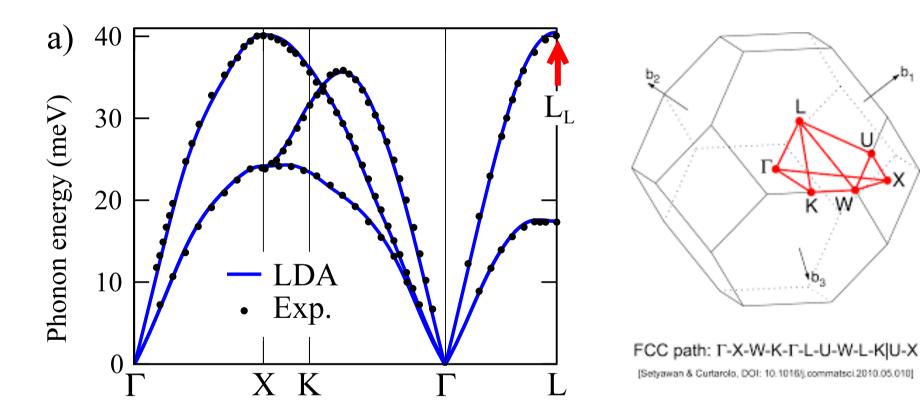


FIG. 5. (Color online) [(a)–(h)] IXS E scans of the low-energy phonons for wave vectors along the (0,k,6.5) line. Solid lines are fits to a sum of Gaussian functions. Data have been multiplied by $1 - \exp[-E/(k_BT)]$ to correct for the Bose factor. The horizontal bar in panel (a) is the instrumental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



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 Detektorkammer Scheiben, so genannten Choppern, gelingt es Forschern, Kryostat-Magnet 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 Probenstab mit Probe 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 Detektorbank 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 ein-Zugsystem fängt. 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 Detektormodule / die Probe. Zählrohre Neutronenstrahl Neutronenleiter Chopper Für große Proben (3x6 cm) Fokussierung im Neutronenleiter Neutronenleiter-Endstück |Chopper Beschichtung Proben (1x1 cm

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

Acoustic Phonon in Sr₂RuO₄

