Megmaradási tételek

Elektromágneses hullám (pl. Röntgen-szórás)

$$E = h\nu \qquad \mathbf{p} = \hbar\mathbf{k}$$

Rugalmas szórás

$$\left.\begin{aligned} E' = E \quad &\Rightarrow \quad |\mathbf{p}'| = |\mathbf{p}| \\ \mathbf{p}' = \mathbf{p} + \hbar\mathbf{G} \quad &\Rightarrow \quad \Delta\mathbf{p}/\hbar = \mathbf{G} \end{aligned}\right\}$$

Bragg-törvény = impulzus megmaradás

Részecske (pl. neutron-szórás)

$$E = \frac{p^2}{2m} \qquad \mathbf{p} = m\mathbf{v}$$

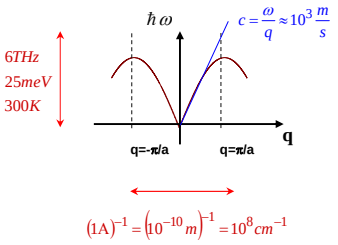
Rugalmatlan szórás

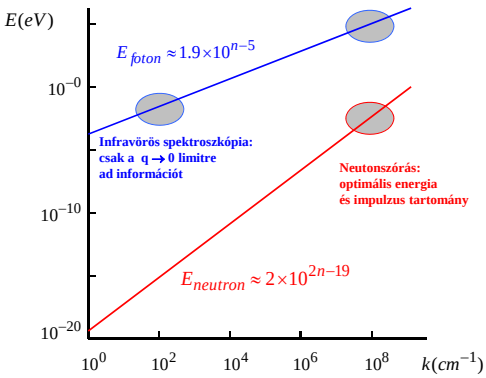
$$\left.\begin{aligned} E' &= E \pm \hbar\omega(\mathbf{q}) \\ \mathbf{p}' &= \mathbf{p} \pm \hbar\mathbf{q} + \hbar\mathbf{G} \end{aligned}\right\}$$

+ fonon abszorbció
- fonon emisszió

Röntgen: keV mellett kell meV-t mérni (többfononos folyamatok)

Mérési tartományok





Neutron szórás

Rugalmatlan szórás

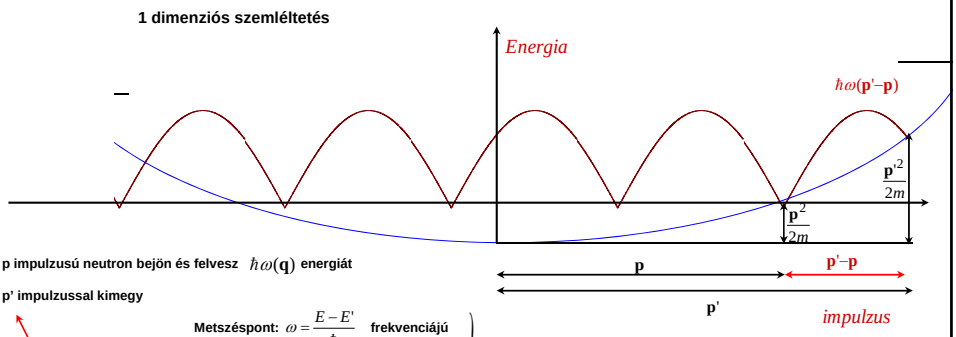
$$\left.\begin{aligned} E' &= E \pm \hbar\omega(\mathbf{q}) \\ \mathbf{p}' &= \mathbf{p} \pm \hbar\mathbf{q} + \hbar\mathbf{G} \end{aligned}\right\} \qquad \left.\begin{aligned} \frac{p'^2}{2m} &= \frac{p^2}{2m} \pm \hbar\omega(\mathbf{q}) \\ \hbar\mathbf{q} &= \mp\mathbf{p}' - \mathbf{p} - \hbar\mathbf{G} \end{aligned}\right\} \qquad \frac{p'^2}{2m} = \frac{p^2}{2m} \pm \hbar\omega\left(\frac{1}{\hbar}(\mp\mathbf{p}' \pm \mathbf{p}) - \mathbf{G}\right)$$

Az $\hbar\omega(\mathbf{q})$ függvény argumentumát átskálázva és kihasználva, hogy $\mathbf{G}$ szerint periódikus

$$\boxed{\frac{p'^2}{2m} = \frac{p^2}{2m} \pm \hbar\omega(\mathbf{p}' - \mathbf{p})}$$

Egy felület egyenlete

1 dimenziós szemléltetés



p impulzusú neutron bejön és felvesz $\hbar\omega(\mathbf{q})$ energiát

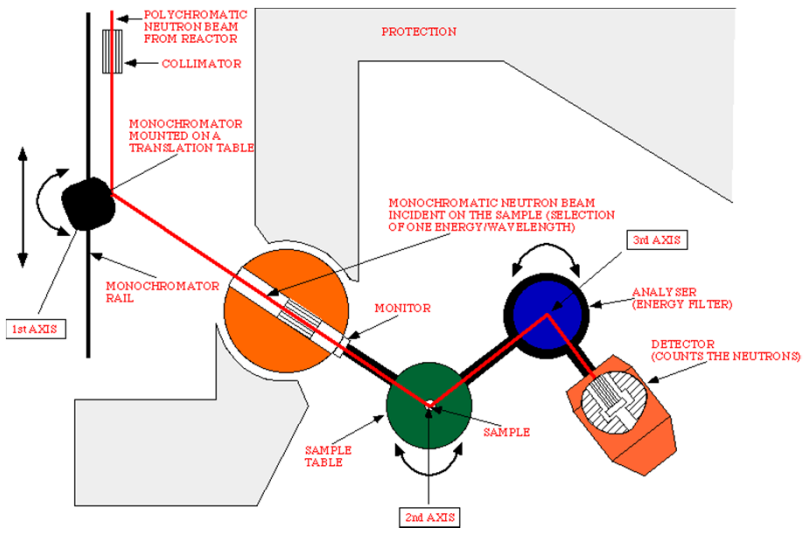
p' impulzussal kimegy

ezt mérjük

Metszéspont: $\omega = \frac{E - E'}{\hbar}$ frekvenciájú

$\mathbf{q} = \frac{\mathbf{p}' - \mathbf{p}}{\hbar}$ hullámszámú

fonon



Egyatomos FCC Neon

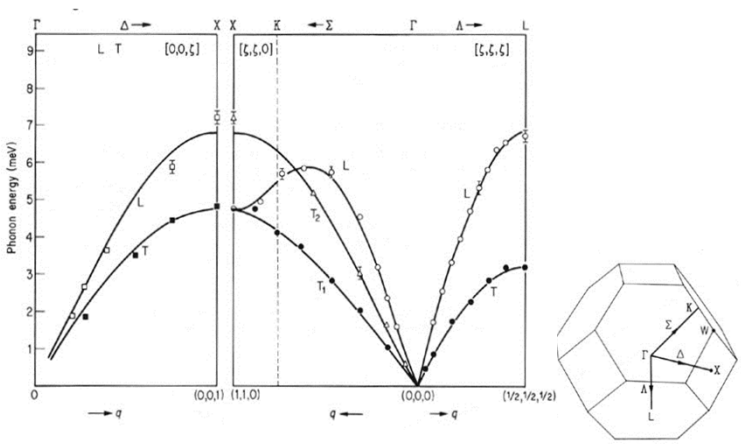
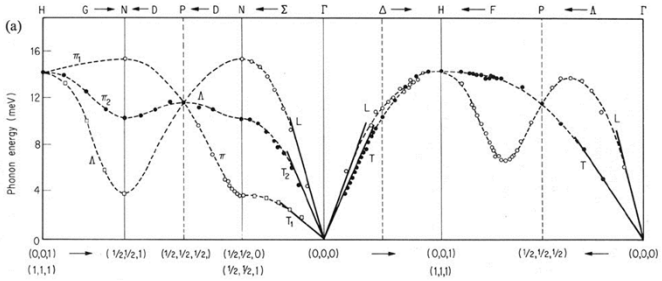


Figure 3.8 Measured vibrational spectrum $\hbar\omega(\boldsymbol{q})$ for various directions in the zone of f.c.c. Ne at 4.7 K (after J. A. Leake *et al.*, *Phys. Rev.* **181**, 125 (1969)). The lines of $\boldsymbol{q}$ depicted are shown in a Brillouin zone, with conventional lettering. $\boldsymbol{q}$ is given in units of $2\pi/a$

Egyatomos BCC Na



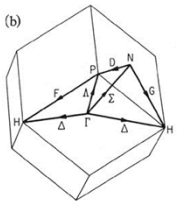
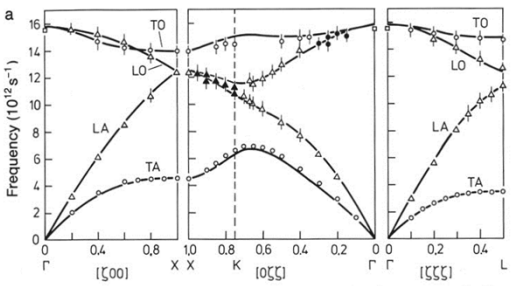


Figure 3.11 (a) Measured vibrational spectrum of b.c.c. Na at 90 K. Modes which are longitudinal and transverse are marked L and T. (b) The lines where $\boldsymbol{q}$ is measured are shown on the Brillouin zone. (After A. D. B. Woods *et al.*, *Phys. Rev.* **128**, 1112 (1962).)

„Kétatomos" Si – gyémánt szerkezet



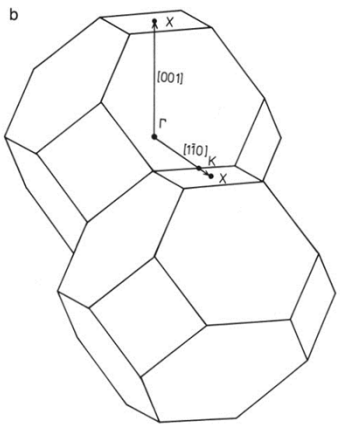


Fig. 4.4. (**a**) Phonon dispersion curves of Si. The circles and triangles are measured points and the full lines are the result of a model calculation by *Dolling* and *Cowley* [4.3]. In place of the wave vector $\boldsymbol{q}$, one often uses the reduced wave vector $\zeta = \boldsymbol{q}(2\pi/a)$ as the coordinate for such plots. The relative lengths of the abscissae correspond to the actual separation of the points in the Brillouin zone. The branches of the dispersion curves carry the notation TA (transverse acoustic), LA (longitudinal acoustic), TO (transverse optical) and LO (longitudinal optical). Along the [100] and [111] directions the transverse branches are degenerate. Concerning the degeneracy of LO and TO at Γ, see also Sect. 11.4. (**b**) A sketch of two neighboring Brillouin zones showing that by moving along [1$\bar{1}$0] from Γ to $\boldsymbol{K}$ one can arrive at $\boldsymbol{X}$ by continuing along the adjoining Brillouin zone boundary. Thus the point $\boldsymbol{X}$ can be described either by the wave vector $\boldsymbol{q} = 2\pi/a$ [001] or by $\boldsymbol{q} = 2\pi/a$ [1$\bar{1}$0]. By studying the fcc lattice (Figs. 2.8, 12), one can convince oneself that these two $\boldsymbol{q}$-vectors describe the same atomic motion