Quantized lattice vibrations -Phonons

Atoms are in permanent oscillation around their mean position within the crystal lattice. The collective part of atomic oscillations can be described as phonons. Assuming a linear chain of identical ? atoms and assuming the elastic interaction between neighbours obeying Hook´s law, the equation of motion of an individual atom, *n*, with neighbours, *p*, is

$M\frac{d^2u}{dt^2} = \sum_p C_p(u_{n+p} - u_n)$, where *u* is the displacement of the respective atoms from their equilibrium positions and C_p are the respective force constants. This equation of motion can be solved using an ansatz of a plane wave:

$u_{n+p} = u_o \exp(i[(n+p]\vec{q}\vec{a} - \omega t)$ with $\vec{a}$ – lattice vector and $\vec{q}$ wave vector. After some algebra one obtains a dispersion relation $\omega^2 = function(\vec{q})$. For a next neighbour interaction only (p=1) this relation in a one-dimensional chain is $\omega^2 = \frac{4C_1}{M}\sin^2(\frac{qa}{2})$. This function is periodic in q, all information is contained inside the 1st Brillouin-zone: $-\frac{\pi}{a} < q < \frac{\pi}{a}$. For small q one finds a linear relation ω=~q, the slope measures the sound velocity $v = \frac{\omega}{q}$, $\omega(q=0) = 0$, and measures a wave with wavelength equal to the macroscopic size of the crystal, the maximum $q_{\max} = \frac{\pi}{a}$ is reached at the zone boundary and measures a wave length $\lambda = 2a$,here the maximum frequency is $\omega_{\max} = 2\sqrt{\frac{C_2}{M}}$.

Next we assume a linear chain of two atoms with mass M_1 and M_2. The equations of motion of both sublattices are a system of two coupled differential equations which result in a dispersion relation $\omega^2 = C(\frac{1}{M_1} + \frac{1}{M_2}) \pm C[(\frac{1}{M_1} + \frac{1}{M_2})^2 - \frac{4\sin^2 qa}{M_1 M_2}]^{1/2}$. This equation provides always 2 solutions for one *q*. For *q=0*: $\omega_1^2 = 0$ and $\omega_2^2 = 2C(\frac{1}{M_1} + \frac{1}{M_2})$; for *q* close to zero there is a linear relation between ω and *q* again. For $q_{\max} = \frac{\pi}{2a}$ (note 2a!) there are two solutions $\omega_1^2 = \frac{2C}{M_1}$ and $\omega_2^2 = \frac{2C}{M_2}$, between which is a frequency gap ("energy gap") where no solution exists. The branches of both classes of the solution describe two different kinds of oscillations: the optical branch (solution 2) has nonzero solutions for all q. Here atoms of different masses oscillate against each other (optical phonons). Solutions of the acoustical branch provide the sound velocity (small *q*) and correspond to collective oscillations of all atoms together. -At the zone boundary, only one of the sublattices is in oscillation, the other one is at rest. (know these solutions qualitatively)

Expanding this approach to 3D lattices with *s* different kinds of atoms, we have to consider the three degrees of freedom of motion for each atom. Assuming the crystal has a size of Pa_1, Pa_2 and Pa_3 there are $3sP^3$=3sN displacements in a crystal. The individual displacement $u_n = A\exp(i[\vec{Q}'\vec{a}_n - \omega t])$ is composed by $\vec{Q}' = \vec{Q} + \vec{G}$ where $\vec{Q}$ is a wave vector within the1st BZ and $\vec{G}$ is a reciprocal lattice vector. This results in 3sN differential equations with 3sN solutions. The direction of wave propagation is given by the wave vector $\vec{Q}$ where all physics is compiled in the 1st BZ within the range $-\pi < \vec{Q}\vec{a} < \pi$, leading to 3s solutions. These 3s equations describe 3s branches $\omega_j(\vec{q})$ with j=1,2,3. Considering each atom having 3 degrees of freedom (1 longitudinal, 2 transverse), there a 3 acoustic branches (1 LA + 2 TA) which are the elastic waves providing a certain sound velocity. In addition there are 3(s-1) optical branches.

The energy of lattice vibrations is quantized = PHONON: the energy of an elastic oscillation state is $\hbar\omega_j(\vec{q}) = (n+1/2)$ where n is an integer number and the population of a certain energy level can be calculated by Bose- Einstein statistics. Phonons can interact with photons, neutrons and other "particles" via energy and momentum transfer. Phonons have no "true" momentum , because in average the whole lattice is fixed. → Pseudo-momentum $p = \hbar\vec{q}$.

The complete phonon dispersion curves of a 3D crystal contain all information about collective oscillation modes in a crystal.

Method to measure phonon dispersion are

1. Inelastic neutron scattering(entire ω(q))
2. Inelastic x-ray scattering
3. Raman scattering (optical phonons)
4. Brillouin scattering (acoustic phonons)