

Physics and Materials science

Vibrations of atoms around their equilibrium sites due to the interaction with neighbor atoms

Said Talbaoui

University Soultan Moulay Youssef, faculty of sciences and Techniques, B.P 523, Beni Mellal Morocco

Unlike surface crystallography, which deals with average positions of atoms in a crystal, lattice dynamics (LD) extends the concept of crystal lattice to an array of atoms with finite masses that are capable of motion. This motion is not random but a coherent superposition of vibrations of atoms around their equilibrium sites due to the interaction with neighbor atoms. A collective vibration of atoms in the crystal forms a wave with given wavelength and amplitude. Just as light is a wave motion that is considered as composed of

particles called photons, we can think of the normal modes of vibration in a solid as being particle-like. The quantum of lattice vibration is called the phonon. The problem of lattice dynamics is to find the normal modes of vibration of a crystal and to calculate their energies (or frequencies, ω) as a function of their wave vector k . The relationship $\omega(k)$ is called phonon dispersion. LD offers two different ways of finding the dispersion relation: Quantum-mechanical approach
Semi classical treatment of lattice vibrations

There are two possible polarizations for the vibrations of atoms in a crystal: longitudinal and transverse. In case of longitudinal modes the displacement of the atoms from their equilibrium position coincides with the propagation direction of the wave, whereas for transverse modes, atoms move perpendicular to the propagation of the wave. For one atom per unit cell the phonon dispersion curves are represented only by acoustical branches. However, if we have more than one atom in the unit cell optical branches will appear additionally. The difference between acoustical and optical branches arises because of the options for the vibration of the atoms in the unit cell. For example, atoms A and B of diatomic cell can move together in phase (acoustical branch) or out of phase (optical branch).

Generally, for N atoms per unit cell there will be 3 acoustical branches (1 longitudinal and 2 transverse) and $3N-3$ optical branches ($N-1$ longitudinal and $2N-2$ transverse)