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

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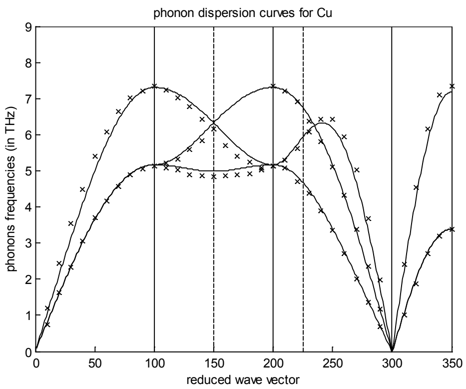
Unlike surface crystallography, which deals with average positions of atoms in a crystal, lattice dynamics (LD) extends the concept of crystal lattice to an array of atoms with finite masses that are capable of motion. This motion is not random but a coherent superposition of vibrations of atoms around 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 ω (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) In the case of 3 dimensions it is important to examine not only the behavior of the frequencies (k) but also the orientation of the polarization vector "(K) ,so we can always choose the directions Of polarization, for a given value "k", so that a direction (Longitudinal mode) is parallel to k, and two directions (transverse modes) are perpendicular to "k".



We give in Fig. the dispersion curves of "Cu" and for values of k oriented along the axes [111] and [100]

Biography

Said Talbaoui is currently at the first year of his PhD studies at the University of Sultan Moulay Slimane Morocco, Department of Physics and he do hold a deep interest in the most fundamental aspects of Physics with a goal to devote my professional career towards understanding them. During his studies he have been introduced and trained on a variety of subjects including Electromagnetism, Special Relativity, and Complex Analysis in addition to two undergraduate courses in Quantum Mechanics and a graduate on Advanced physics and arterials science. He also have self-studied the basics of Quantum Computers and Particle Physics. Finally he can handle myself with the Mathematica software and have some experience with other programming languages, such as Fortran, Matlab,C++.

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