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Lecture – 47 Experimental determination of Phonon dispersion curves

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In the previous lecture we introduced the idea of normal modes, their energies and most importantly the concept of phonon, which is specified by k; the crystal momentum and the corresponding energy h cross omega k. And the dispersion that we have derived earlier under simple assumptions is that there is a relationship between omega and k, and in the simplest form it looks like this; k and k goes up to pi by a here, minus pi by a here, which now I can call phonon dispersion relation.

Question is, how do we determine it? For that let us again have a look at the energies and the momenta that we are talking about; a is of the order of 1 Angstrom, corresponding k comes out to be 10 raised to minus 24 to 10 raised to minus 23 kg meter second inverse and the energy of a phonon h cross omega k comes out of the order of 0 to 10 meV. So, if I want to study in a crystal what is the frequency and what is k, I should be able to excite a mode with k and see the energy loss or energy gained during the process.

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range $10^{-24}-10^{-23}$ kg m s⁷

So, to study omega versus k curve with a particle or EM wave scattered by phonons; you see I am already using this language these vibrations are now am going to call phonons.

So, these photons are scattering this wave, I should detect an energy difference of meV range and momentum of range 10 raised to minus 24 to 10 raised to minus 23 kilogram meter second inverse. Keep in mind that this momentum corresponds to a of the order of 1 Angstrom. So, the lambda of incoming light or wave a particle should be of the order of 1 Angstrom. Let us see how do we do it.

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So, question 1; can we study omega versus k using ordinary light. And the answer is no, because lambda light is of the order of 5000 Angstrom and that is 5000 spacings of the crystal. So; obviously, I cannot actually think of very very large momentum that is being transferred. The momentum corresponding momentum for this light would be very small. So, momentum h cross k, light will be much much much smaller than that required or equivalently the crystal momentum of phonon. So, I cannot really use light to excite the phonon which has a momentum corresponding to a lambda equals 1 Angstrom; so ordinary light is out.

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Let us ask a next question. Can we use X rays? Because X rays after all have, have lambda equals 1 Angstrom or 2 Angstroms that I used to study the crystal structure. So, lambda is of the order of 1 Angstrom. And therefore, which is 10 raised to minus 10 meters and therefore, the frequency of X rays is of the order of 10 raised to 18. So, h f corresponds to this frequency which is much much much larger than omega phonon right. Omega phonon was of the meV range.

So, h f is of the order of let us say h is 10 raised 6 times 10 raised to minus 34 times 10 raised to 18 divided by 1.6 times 10 raised to minus 19 eV which is of the order of 1000 eV. Whereas, h cross omega phonon, we calculated in the previous lecture is of the order of meV. So, I should be able to detect a difference of meV in 1000 eV. So, my instrumentation has to be very very sophisticated if I want to use X rays to study phonons, it is done, it is doable. So, we can do it except my, my detector has to be such that out of 1000 eV if there is a difference of meV range; I should be able to detect it.

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Third option, can we use electrons. So, these electrons should be of the order of, lambda electron should be of the order of 1 Angstrom. And if you calculate the corresponding energy p squared over 2 m, it comes out to be of the order of 100 eV.

So, again I need instrumentation that should be able to detect a change of meV range in this 100 eV. I can use electrons, but there is one more trouble with electrons. Electrons carry charge and this implies they interact with other electrons in a solid. And if they do then; obviously, they are not interacting just with the phonons, but other electrons also and therefore, the information that we get will not be only about phonon, so electrons certainly are out. So, we need a particle which is non interacting and gives energy in the range of meV with wavelength 1 Angstrom.

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So, let us look at neutrons. If I look at a neutron of wavelength of the order of 1 Angstrom and calculate its energy p square over 2 m, it comes out to be about 50 meV. So, these seem to be right. I gave 50 meV take away 10 15 meV. So, we are in the right range, the difference will be substantial. So, neutrons are used, quite a lot in studying dispersion relations. And these neutrons if the energy is of the order of 50 meV, it corresponds to, if I equate this to k T, the T comes out to be about 600 Kelvin equals T.

So, these are known as thermal neutrons. These neutrons are obtained from reactors, thermalized; that is brought down the energy is brought down and then are used to study dispersion relations of phonons.

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So, what we learn in this, is I can use X rays, requires sophisticated instrumentation in terms of resolution, because out of 1000 eV I got to detect a change of meV milli electron volts, and I can use thermal neutrons right. This also requires a reactor and things like those, but rest of the energy and momentum and energy are comparable to those of phonons and therefore, they are used quite extensively in studying omega versus k behavior.

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90H-P40096 $\frac{\overrightarrow{p}}{\overrightarrow{p}'+\overrightarrow{h}k}=\overrightarrow{p}$

Energy conservation
 $E_{neutrino}$ (coming m)

= $E_{neutrino}$ (going out)

+ $\overrightarrow{h} \omega(k)$

So, what is done in these experiments is, if I have a sample which could be a crystal where I want to study the phonon relationship. I let a particle or neutron come in with momentum p, and when it goes out, it goes out with momentum p prime. As we said in the previous slide, then p prime plus h cross k will be equal to p. And the energy conservation, then gives that energy of neutron coming in should be equal to energy of neutron going out plus h cross omega k for the photon. So, by measuring the momentum of incoming neutron, outgoing neutron. from the difference I can make out.

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So, from the difference p minus p prime, I can make out what h cross k is; that is what the momentum of the phonon excited is. And from the energy difference E in minus E out, I can make out what the frequency of that mode is and then plot them, and this is how the experiments are done. More subtleties are whether you take constant energy neutrons coming in and measure at different angles what energy is going out and so on, but this is how the experiment is performed.

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And finally, I owe you an explanation of momentum conservation for crystal momentum of phonons; that is p out of the neutrons which are scattered should be equal to p n of neutrons plus h cross k of phonon. This also I will write a supplement and give it with this lecture.