Solid State Physics
Lecture 8
Laue Equations and Ewald Construction

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After this, let us move onto Laue equations. Laue equations just like Bragg's law are another representation of the diffraction condition. But this representation is useful for single crystal diffraction, finding out the structure of a single crystal and it gives us a lot better sense of the geometry in which the diffraction condition is satisfied. So, let us discuss that. The diffraction condition that is $\Delta\overrightarrow{k}=\overrightarrow{G}$, this may be expressed in another way to give the Laue equations; the geometric representation may be better appreciated from these equations. So, let us take the scalar product of the real axis vectors $\overrightarrow{a_1}$,$\overrightarrow{a_2}$ and $\overrightarrow{a_3}$ with $\Delta\overrightarrow{k}\ and\ \overrightarrow{G}$. So, if we take $\overrightarrow{a_1}\cdot\Delta\overrightarrow{k}$ on this side. So, we are taking, we are taking the scalar product of $\overrightarrow{a_1}$ from the left, also on the right hand side we will do that and that will give us $2\pi v_1$, just by the definition of $\overrightarrow{G}$. Similarly $\overrightarrow{a_2}\cdot\Delta\overrightarrow{k}$, that would yield $2\pi v_1$ from the definition of $\overrightarrow{G}$ and $\overrightarrow{a_3}\cdot\Delta\overrightarrow{k}$ similarly would give us $2\pi v_3$. And these equations have a simple geometric interpretation. The first equation that is this one, if we consider this; this tells us that $\Delta\overrightarrow{k}$ lies on one cone about the direction of $\overrightarrow{a_1}$. Similarly the second one tells that it lies delta k lies on a cone about the direction of $\overrightarrow{a_2}$; third one says similarly the delta k lies on a cone about $\overrightarrow{a_3}$. How is that possible? How can we satisfy all these three conditions? The three conditions can be simultaneously satisfied, if these three cones intersect and give us a common line. So, $\Delta\overrightarrow{k}$ must be that common line. So, three cones intersecting and giving us a common line that is rather a stringent condition, it is not quite common to occur. And it requires a bit of more brainstorming in terms of geometry to be able to appreciate this condition. Let us work out the Ewald construction to better appreciate this stringent condition. So, here I am drawing a sphere; although I am drawing on 2 D, so it looks like a circle, but I am trying to draw a sphere, centered here and I will draw some lattice points using blue color. So, let us put one lattice point here, one lattice point here, like that these are reciprocal lattice points; I can have more lattice points like this, similarly spaced and so on. So, this lattice points, this lattice will certainly extend to infinity. And we have the incident vector, wave vector this that is $\overrightarrow{k}$, the scattered wave vector is this that is $\overrightarrow{k'}$; this is the origin, the angle between them is 2θ and $\Delta\overrightarrow{k}=\overrightarrow{G}$. So, how did we construct this? I have just explained you how I drew the picture; this is not the construction. The construction is the points on the right hand side that is this side here are the reciprocal lattice points of the crystal, and the vector $\overrightarrow{k}$ that is drawn along the direction of the incident wave. So, this is the direction of the incident wave; the we have made this vector end at one of the lattice points. So, the origin is chosen in such a way that, $\overrightarrow{k}$ terminates at one of the reciprocal lattice points. Now, we draw a sphere of radius of this magnitude of this $\overrightarrow{k}$ vector, that is $\overrightarrow{k}=2\pi/\lambda$ of the light that we are shining on it or whatever kind of wave; it can be electronic wave or neutron wave whatever. So, the radius of this sphere is the absolute value of $\overrightarrow{k}$ and we draw that sphere above the origin. Now, a diffracted beam would be formed if the sphere intersects at any other point in the reciprocal lattice. So, here we have considered one point where the sphere intersects; the sphere may intersect say somewhere here, it may intersects on some point outside this plane. So, this is just one plane of the sphere that we are looking at; the sphere is bigger, the lattice is 3 dimensional, so it may intersect in somewhere else. And those are the $\Delta\overrightarrow{k}$ values for which we will have $\Delta\overrightarrow{k}=\overrightarrow{G}$. and this diffraction condition will be satisfied; the Laue equations, all 3 Laue equations will be satisfied. And once everything is satisfied, we will have nonzero scattering factor, nonzero scattering amplitude. And that is the situation where we would get some diffracted wave from this situation. So, the stringent condition is clearly explained by this Ewald condition, Ewald construction. So, this construction is very helpful in understanding, geometrically understanding and making a picture of the diffraction condition in our mind.