Solid State Physics
Lecture 12
Atomic form Factor

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Now, let us deliberate on the Atomic form Factor; let us see how we can understand anything better of it. (Refer Slide Time: 00:33)

If we understand this that will sort of make our understanding of X-ray diffraction or any other wave diffraction in a crystal sort of complete. So, the scattered radiation from a single atom takes into account the interference effect within the atom. So, the form factor f_j that we have considered earlier, that we have defined earlier for j^{th} atom can be written as dV. We have already written this earlier $n_j(\overrightarrow{r})\exp{(-i\overrightarrow{G}\cdot\overrightarrow{r})}$. Now, this integral is extended over the electron concentration associated with a single atom. If we consider that the angle between $\overrightarrow{r}$ and $\overrightarrow{G}$, that is α; then $\overrightarrow{G}\cdot\overrightarrow{r}$ becomes $\overrightarrow{G}\overrightarrow{r}\cos\alpha$. And let us assume that the electron distribution is spherically symmetric, although in case of many orbitals it is not spherically symmetric; but if we assume it to be spherically symmetric, we will not be pretty accurate, but the accuracy level that we will have would be sufficient for describing or qualitatively understanding the diffraction pattern. Now, if we assume the electron distribution to be spherically symmetric; then f_j this can be written as $2\pi\int dr\overrightarrow{r^2}$, this is the volume element in case of spherically symmetric charge distribution, it does not depend on any $\theta or \phi$. Then we have $d(\cos\alpha)n_j(\overrightarrow{r}\exp{(-i\overrightarrow{G}\overrightarrow{r}\cos(\alpha))}$. And this can be written as $2\pi\int dr\overrightarrow{r^2}n_j(\overrightarrow{r})\frac{\exp{(i\overrightarrow{G}\overrightarrow{r})}-\exp{(-i\overrightarrow{G}\overrightarrow{r})}}{i\overrightarrow{G}\overrightarrow{r}}$. So, this we obtain after integrating over $d(\cos\alpha)$ with the range $[-1to1]$ that is the full range of $\cos(\alpha)$ that we have. We have integrated over $d(\cos\alpha)$ using this range and got this quantity now. (Refer Slide Time: 05:01)

Once we have this, then we can write the atomic form factor as f_j can be written a $4\pi\int dG\, n(\overrightarrow{r})\overrightarrow{r^2} = \frac{\sin\overrightarrow{G}\overrightarrow{r}}{\overrightarrow{G}\overrightarrow{r}}$. Once we have obtained this, if the same total electron density; if we assume it to be concentrated at the at $\overrightarrow{r} = 0$, that is at the nucleus which is never true, but we can consider that the electron density is maximum near the nucleus, it tends to the nucleus site. If we consider that kind of a situation, which could be considered in a crystal where most of the space is empty; the electrons are closely bound close to the nucleus and very few roam around and participate in bonding. So, this assumption would also not be very wrong, although in the discussion of electronic states, electron the bonds between two atoms this kind of description will not work at all; but as long as we are using X-ray diffraction for determining the structure, this would still work in this limited context. (Refer Slide Time: 06:48)

So, if we assume something like that, then we will have $\lim_{r\to 0}\frac{\sin\overrightarrow{G}\overrightarrow{r}}{\overrightarrow{G}\overrightarrow{r}}$ within this assumption and that will give us 1. So, we will have $f_j = 4\pi\int$, ok. So, this quantity is actually proportional to this for each electron this is the situation, $4\pi dr\ n_j(\overrightarrow{r})\overrightarrow{r^2}$; this quantity would become the number of electrons, simply from each electron we will have atom contribution to atomic form factor equals 1 and the total atomic form factor would become the atomic number, Z is the atomic number. So, what did we learn from this discussion so far? We have learned that there are, there is a diffraction condition that we can recast in many different forms. We learnt all the various statements of the diffraction condition, we learnt the primitive translation vector in the reciprocal lattice; we developed the concept of Brillouin zone and the scattering amplitude, structure factor and atomic form factor, these are the things that we have developed a concept for.