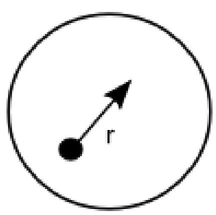
Topic 3-1: General Theory of Diffraction

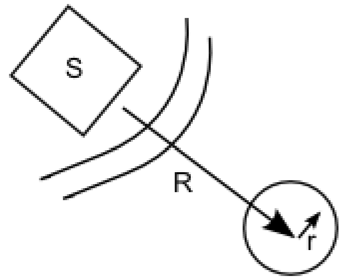
Summary: In this video diffraction is introduced. The goal is to develop a mathematical expression for intensity at the detector of a diffractometer. The first step is to describe the interaction of the source with the sample by finding the amplitude of the wave emitted by the source at one point in the sample. We then repeat this process and find the amplitude of the wave emitted by the sample at the detector. We then extend this equation to include all points in the sample and relate our amplitude expression to intensity.

- <u>Diffraction</u>: the study of how an incident *wave* interacts with matter (the sample)
- Will develop a mathematical expression for wave *intensity* at a detector – practically useful for inferring information about the sample
- Good background knowledge is the interference pattern created by the double slit experiment along with Fourier series and transforms
- Assumptions we can make about diffraction
    - Elastic wave/sample interaction
        - No energy is exchanged between the wave and the sample
    - There exists a scattering density n($\vec{r}$) that depends on the spatial arrangement of atoms
        - This spatial dependence is little $\vec{r}$
        - Below is a figure showing how $\vec{r}$ is used to label points within a sample



- Can define any point in the sample in terms of the vector little $\vec{r}$

Diffractometer

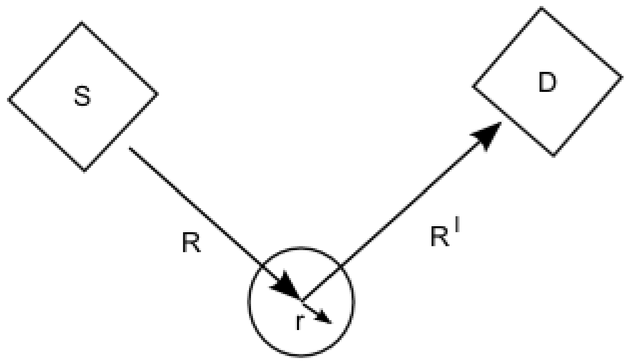


- Above is a figure depicting the first part of a diffractometer: the source, waves emitted by the source and the sample
- The diffractometer begins with the source, which emits incoherent spherical waves, and the sample, with which the sources radiation will interact
- The magnitude of the vector $\vec{R}$ is much greater than the magnitude of $\vec{r}$ so we can assume that the waves incident on the sample are plane waves
    - This means we can treat the wave vector $\vec{k}$ as parallel to $\vec{R}$
- Want to know the amplitude of the wave in the sample at any time t
    - This amplitude expression will need both a spatial and a time component
    - The spatial component begins with the total distance traveled by the wave, that is to say $\vec{R}+\vec{r}$.
    - The time component arises from the frequency of the wave, omega
    - The spatial expression is $e^{i\vec{k}\cdot(\vec{R}+\vec{r})}$ while the time component is $e^{-i\omega t}$
    - Putting this all together we get an expression for the amplitude at the sample

$$F_s(\vec{r},t) = F_o e^{i(\vec{k}\cdot(\vec{R}+\vec{r})-\omega t)} \quad [1]$$

        - This is the amplitude expression we have been after
    - Recall intensity is $F_s{}^*F_s$. Thus, the source wave *intensity* will be constant throughout the sample because the complex exponential term in F_s will drop away due to the complex conjugate. Just the *amplitude* is varying in space and time.
- We can treat the sample as though each point will absorb the incoming radiation and then re-emit it spherically, like the source does
- The tendency for a sample to scatter an incoming wave at any position $\vec{r}$ is determined by the **scattering density**, $n(\vec{r})$

- Now we need to add in a detector to sense the waves scattered off of the sample



Sketch the vectors R+r and R'-r

- We want the amplitude of the scattered wave at the detector
- **Approach:** First, we're going to consider the amplitude at the detector from one little region of sample at $\vec{r}$, then we're going to integrate across the sample to determine the total amplitude at the detector.
- Treat electron density at position $\vec{r}$ as a spherical emitter. Basically, the incident source radiation wiggles the electrons in the sample, and these wiggling electrons act as spherical emitters. For simplicity's sake, we're not going to consider the angular dependence of this re-emission yet.
- Waves from the sample will have a spherical decay in amplitude that goes at $\frac{1}{|\vec{R}'-\vec{r}|}$, where $\vec{R}'$ is the distance from the sample to the detector and $\vec{r}$ once again describes a point in the sample
    - Assuming once again that the magnitude of $\vec{R}'$ is much larger than the magnitude of $\vec{r}$ we can simplify this to $\frac{1}{|\vec{R}'|}$
- We can again treat the wave at the detector as a plane wave
    - This means we can again assume that the wave vector of the wave hitting the detector, $\vec{k}'$ is parallel to $\vec{R}'$ and we can use the same complex exponential from as we did for the amplitude at the sample
- The only difference with this complex exponential is it now has a factor out front that is the scattering density times the spherical decay determined earlier
- This gives:

$$F_r = \frac{F_S n(\vec{r})}{|\vec{R}'|} e^{i\vec{k}'\cdot(\vec{R}'-\vec{r})} \qquad [2]$$

- where we now have an ($\vec{R}$’-$\vec{r}$) term for the path length difference that the scattered wave has traveled

- Talking through the above equation: The amplitude at the detector from a single point $\vec{r}$ within the sample is given by: (a) the incident amplitude at that point $\vec{r}$, (b) the scattering density at that point, (c) a complex exponential term that deals with oscillating amplitude as the wave travels from the sample to the detector and (d) a decay term in the denominator that accounts for the spherical wave decaying in amplitude as it propagates away from point $\vec{r}$ within the sample.

Checking some limits:

- When the source is off, F_s is zero and the wave at the detector has no amplitude.
- When the detector is infinitely far away ($\vec{R}'\rightarrow$ infinity), there is no amplitude at the detector
- When there is no sample at position $\vec{r}$, there is no scattering density. The incident wave does not interact with the sample in this region and no amplitude at the detector is generated from this point.

- Since this equation is rather messy (recall F_s from above) we do some rearranging:

$$F_{\vec{r}} \propto n(\vec{r})e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \qquad [3]$$

  - where $\vec{r}$ and both $\vec{k}$’s are vectors
- $\vec{k}$-$\vec{k}'$ is the change in wave vector which we can combine into one term called delta $\vec{k}$, $\Delta\vec{k}$=$\overrightarrow{k'}$-$\vec{k}$
- This makes our previous equation

$$F_r \propto n(\vec{r})e^{-i(\Delta\vec{k})\cdot\vec{r}} \qquad [4]$$

- This equation is just for one point in the sample, to get all points need an integral across the sample volume

$$F \propto \int_V n(\vec{r})e^{-i\Delta\vec{k}\cdot\vec{r}}d\vec{r} \qquad [5]$$

  - This is an integral over volume of our previous expression

- As we sum over all exit waves from our sample volume, they will constructively or destructively interfere to produce a final *net* amplitude at our detector
- This integral is the Fourier transform of our scattering density with respect to our *change* in wave vector. Whoa.
- Most detectors measure intensity
  - Not a problem because $I=|F|^2$
  - Intensity measurements result in the loss of phase information. This is a big deal! So much for the inverse Fourier transform to back out n(r).

Questions to Ponder

1. What sort of allowed waves can be used for the source?

2. Compare constructive interference and incoherent radiation. Our source tends to produce incoherent radiation, how does that work?

3. Can an inverse Fourier transform give us back our scattering density? Why or why not?

4. What space do $\vec{k}$ and $\vec{k}'$ exist in?

5. Why is it a R^{-1} decay in wave amplitude? Can you argue this from conservation of energy?