X – Ray Diffraction

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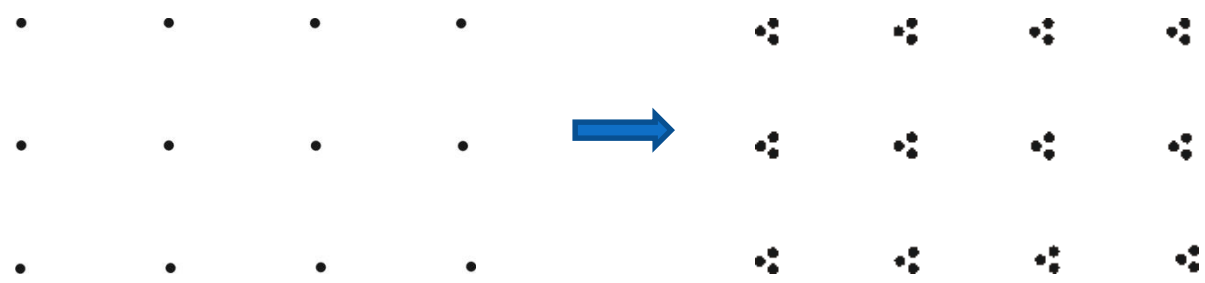
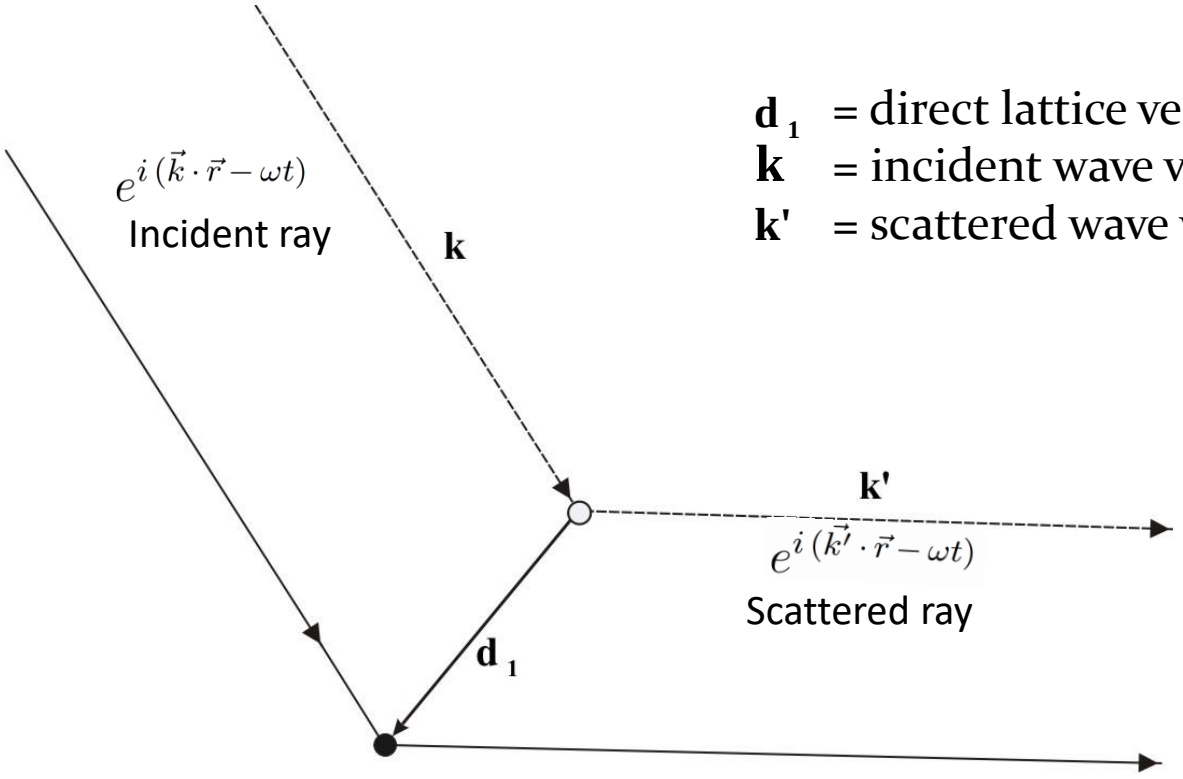
Outline

1. Mono-atomic Basis
2. Poly-atomic basis – *Geometrical Structure Factor*
3. Charge distribution – *Atomic Form Factor*
4. Conclusions

First we will consider a cubic crystal lattice with mono-atomic basis and then, we will consider the case where basis consists of more than two atoms/ions.



Mono-atomic basis



$\mathbf{d}_1$ = direct lattice vector
$\mathbf{k}$ = incident wave vector
$\mathbf{k'}$ = scattered wave vector

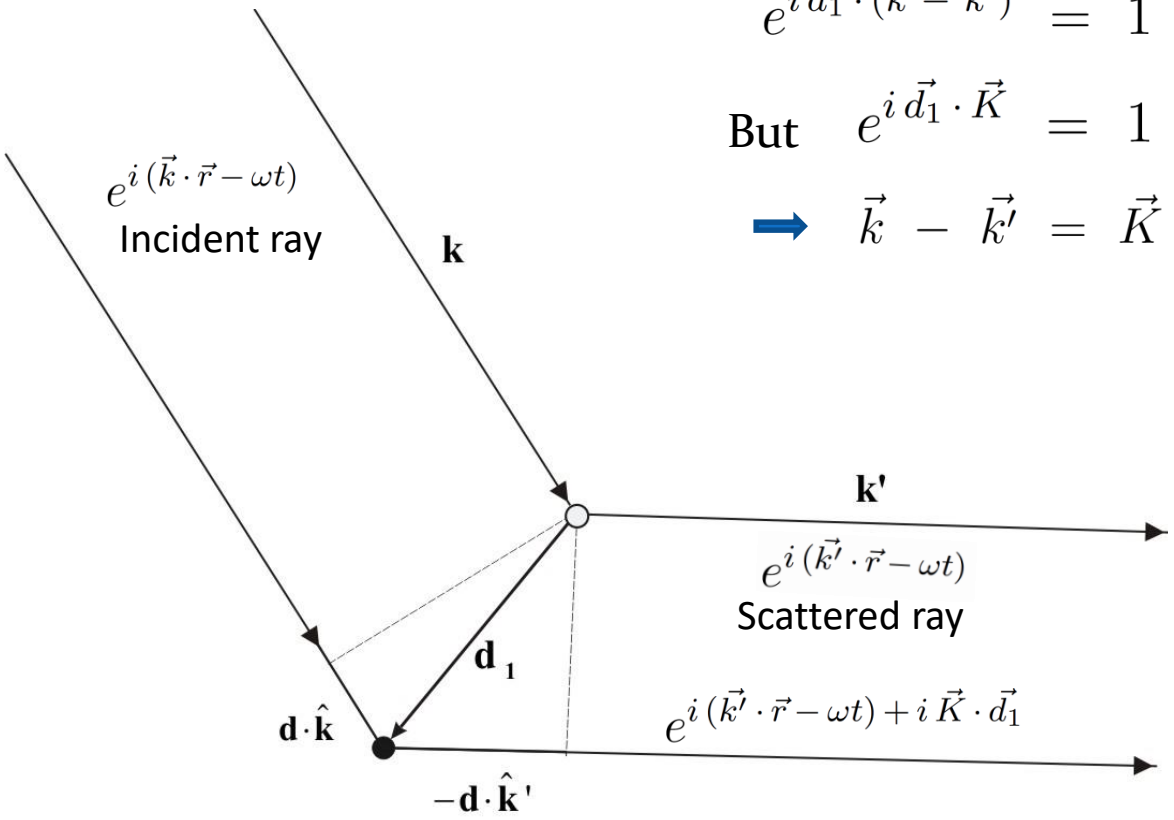
The path difference = $\vec{d_1} \cdot \hat{k} - \vec{d_1} \cdot \hat{k'} = m\lambda$

$$\vec{d_1} \cdot (\vec{k} - \vec{k'}) = 2\pi m$$

$$e^{i\,\vec{d_1} \cdot (\vec{k} - \vec{k'})} = 1$$

But $e^{i\,\vec{d_1} \cdot \vec{K}} = 1$

➡ $\vec{k} - \vec{k'} = \vec{K}$ Reciprocal lattice vector



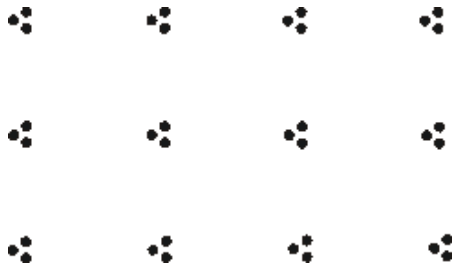
Thus, $$e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_j}} = e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)}$$

$$e^{i\,\vec{K}\cdot\vec{d_j}} = 1$$

This is the condition for constructive interference along ***k'*** direction.

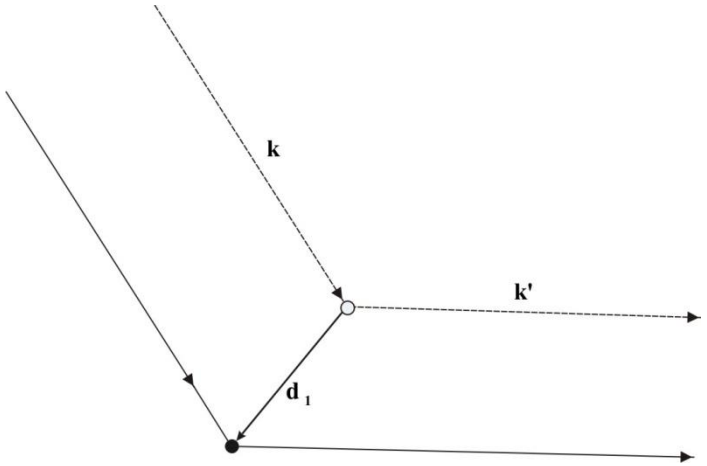
What happens if the basis has more than one atom / ion ?

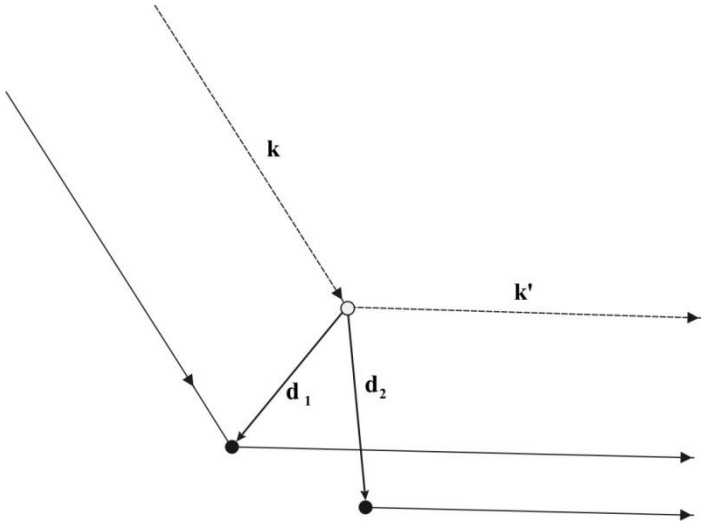
- The interference will depend on how the X – rays are scattered by the basis atoms / ions.
- The atoms in the basis may be placed in such a way that they result in destructive interference for certain $\vec{K}$ directions.



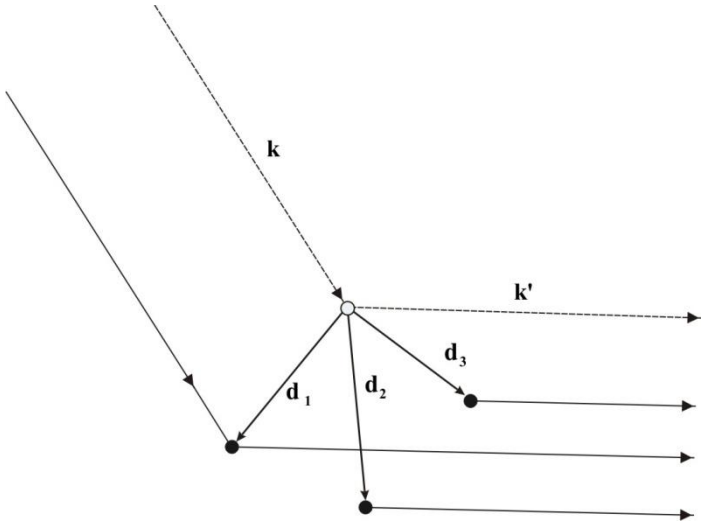
Poly-atomic basis

$$y = e^{i(\vec{k'} \cdot \vec{r} - \omega t) + i\vec{K} \cdot \vec{d_1}}$$

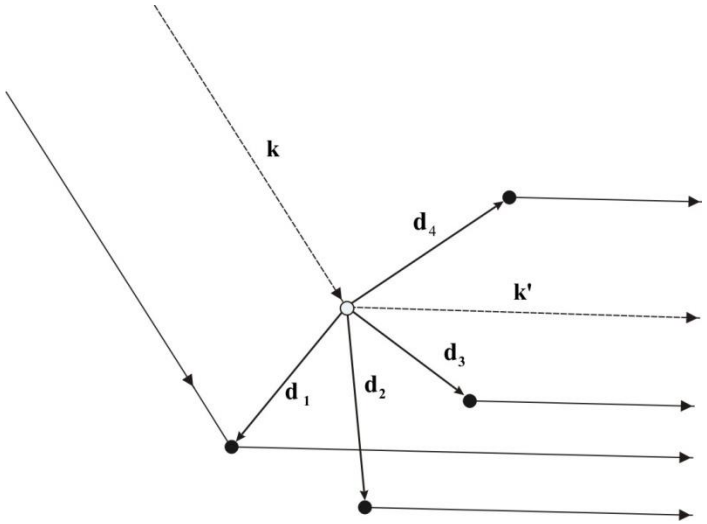




$$y = e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_1}} + e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_2}}$$



$$
\begin{aligned}
y \;=\; & e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_1}} \\
& + \\
& e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_2}} \\
& + \\
& e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_3}}
\end{aligned}
$$



$$
\begin{aligned}
y \;=\; & e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_1}} \\
& + \\
& e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_2}} \\
& + \\
& e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_3}} \\
& + \\
& e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)+i\,\vec{K}\cdot\vec{d_4}}
\end{aligned}
$$

This can be written in a more compact form as :

$$
y \;=\; e^{i\,(\vec{k'}\cdot\vec{r}-\omega t)} \left(\sum_{j=1}^{4} e^{i\,\vec{K}\cdot\vec{d_j}} \right)
$$

Thus, if the basis consists of *n* atoms / ions, the scattered X – rays will be of the form :

$$y = e^{i(\vec{k'} \cdot \vec{r} - \omega t)} \left(\sum_{j=1}^{n} e^{i \vec{K} \cdot \vec{d_j}} \right)$$

$$= e^{i(\vec{k'} \cdot \vec{r} - \omega t)} \, S(\vec{K})$$

The function $S(\vec{K})$ contains the information about how the atoms /ions are placed in the basis and is known as the ***Geometrical Structure Factor***.

If $S(\vec{K})$ vanishes for some value of $\vec{K}$ then the peak corresponding to $\vec{K}$ will be absent from the diffraction pattern. Such absences are known as *systematic absences*.

Atomic form factor

In the above treatment, it was assumed that ions scatter x – rays equally in all directions.

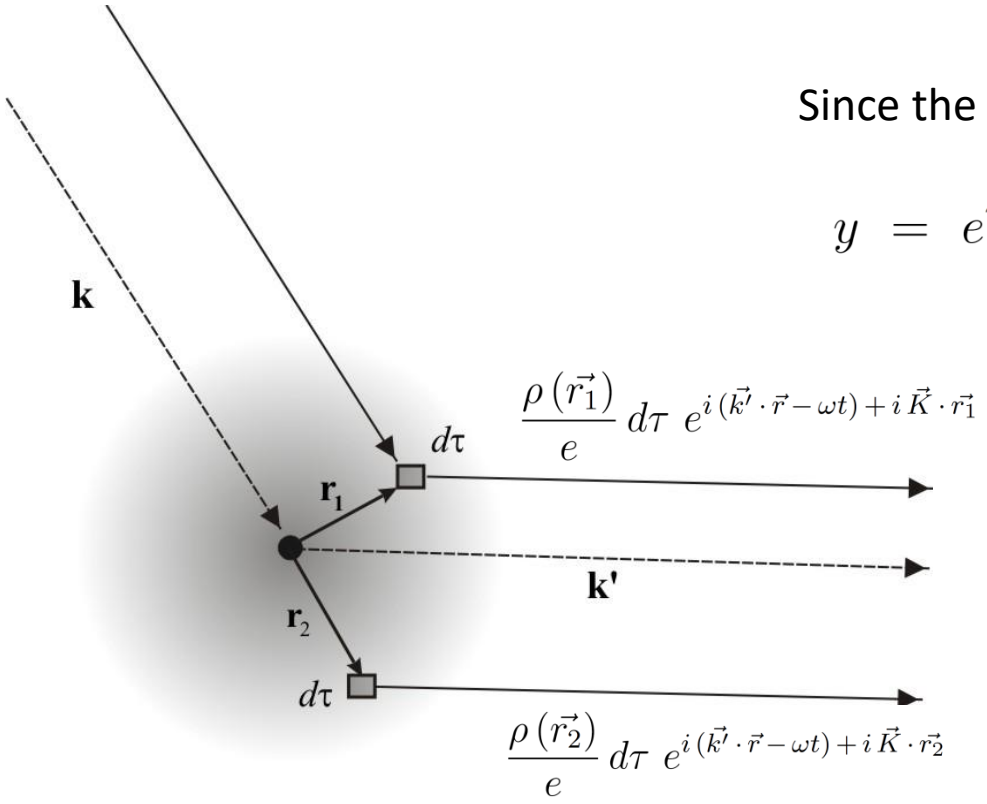
However, the amplitude of the scattered rays will depend on the charge distribution of charge in each ion and will also have angular dependence via $\vec{K}$

Thus, the proper form of the resultant scattered rays must be :

$$y \;=\; e^{i\,(\vec{k'}\,\cdot\,\vec{r}\,-\,\omega t)} \left(\sum_{j\,=\,1}^{n} \; f_j \; e^{i\,\vec{K}\,\cdot\,\vec{d}_j} \right)$$

where $\qquad f_j \;=\; f_j\,(\vec{K})$

$$y = \frac{\rho(\vec{r_1})}{e} d\tau \; e^{i(\vec{k'}\cdot\vec{r}-\omega t)+i\vec{K}\cdot\vec{r_1}} + \frac{\rho(\vec{r_2})}{e} d\tau \; e^{i(\vec{k'}\cdot\vec{r}-\omega t)+i\vec{K}\cdot\vec{r_2}}$$



Since the charge distribution is continuous

$$y = e^{i(\vec{k'}\cdot\vec{r}-\omega t)} \int \frac{\rho(\vec{r})}{e} d\tau \; e^{i\vec{K}\cdot\vec{r}}$$

The factor $\int \frac{\rho(\vec{r})}{e} d\tau \; e^{i\vec{K}\cdot\vec{r}}$ is known as the ***Atomic Form Factor*** and contains information about the electronic charge distribution in an atom/ion.

Conclusions

Thus the resultant scattered X – rays are given by

$$y = e^{i(\vec{k'} \cdot \vec{r} - \omega t)} \left(\sum_{j=1}^{n} f_j \, e^{i \vec{K} \cdot \vec{d}_j} \right)$$

1. If in a crystal, the basis consists of only one ion, a peak will be observed corresponding to every possible reciprocal lattice vector.

2. More than one ion in a basis results in absence of certain peaks which would have been observed in the above case. This is given by *Geometrical Structure Factor* – contains information about location of ions in the basis.

3. Amplitude of the scattered waves depend on the electronic charge distribution within the ions. This is given by the *Atomic Form Factor*.

Thank You