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Modern Physics

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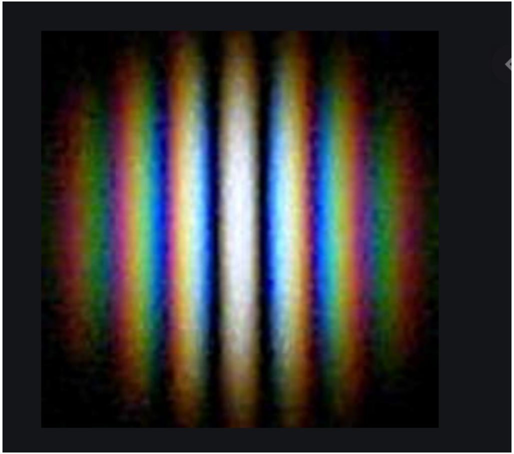
Thomas Young 1802



Diffraction at the double slit 1 — Comment 1

Thomas Young’s double slit experiment has been widely accepted as evidence that light is a wave phenomenon.

The picture shows the result of the experiment.

Daylight falls through a hole in a shutter onto a double slit and colored stripes can be seen on the wall behind the double slit.

This simple experiment created one of the greatest problems in physics in the 19th century.

In 1725, the famous English astronomer James Bradley discovered the aberration of starlight. He found that the angle of observation of stars varies periodically over the course of the year.

Diffraction at the double slit 1 Comment 2

With Newton’s corpuscular theory of light, he was able to trace this effect back to the movement of the earth around the sun.

Knowing the speed of the earth around the sun, Bradley was also able to determine the speed of light.

The speed of light determined by these astronomical measurements agrees well with the terrestrial measurements.

Amazingly, it turned out that the speed of light is the same for all observed stars.

However, in the context of Newton’s corpuscular theory of light, the speed of light should also depend on the speed of the stars.

It was known that stars move at different and high speeds.

Diffraction at the double slit 1 Comment 3

In the context of a wave theory of light it was assumed that light waves propagate in a medium called the ether.

Therefore the speed of light waves is of course independent of the speed of the stars.

In the context of a wave theory, however, it is by no means obvious that the alignment of the wave fronts and thus the direction of propagation should depend on the speed of the earth.

This problem was solved by Augustin-Jean Fresnel in1818.

He assumed that the ether is partly carried along by the earth and thus explained the stellar aberration within the wave theory of light.

Diffraction at the double slit 1 — Comment 4

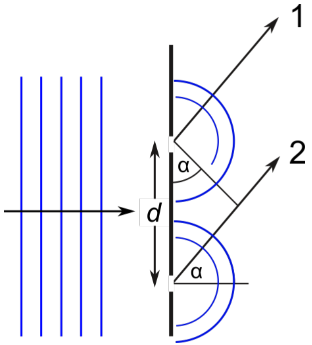
Through Fresnel’s ether theory, the wave theory of light was generally accepted.

However, Fresnel’s theory did not pass all experimental tests.

In the course of the 19th century the ether theory became more and more complicated and contradictory until the problems were solved in 1905 by Albert Einstein within the framework of the special theory of relativity.

Diffraction at the double slit 2

A plane wave comes in from the left and cylindrical waves leave the slits.



Diffraction at the double slit 2 Comment

The figure outlines the situation with a double slit.

The blue lines indicate the wave fronts.

The phase is constant along a wave front.

A plane wave meets the double slit from the left.

After the slits, the light spreads evenly in all directions.

This is indicated by the blue semicircles.

Cylindrical wave fronts leave the slits.

In small areas, the cylindrical wave fronts can be approximated by plane waves, which in turn can be assigned a beam direction.

Diffraction at the double slit 3

Diffraction at the double slit 3 Comment

The illustration shows the superposition of two circular water waves.

The waves interfere and there are directions of contructive and destructive interference.

The parallel beams 1 and 2 can be used when the interference is observed far from the double slit or when a lens is used to focus parallel beams.

This experimental situation is called Fraunhofer diffraction.

Inclined rays must be used to describe diffraction near the slits.

This experimental situation is called Fresnel diffraction.

Diffraction at the double slit 4

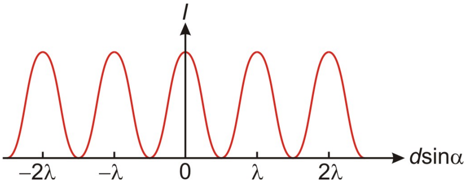
The condition for constructive interference of parallel rays is

$$\boxed{d \sin \alpha_m = m\lambda}$$

and the condition for destructive interference

$$\boxed{d \sin \alpha_m = \left(m + \frac{1}{2}\right) \lambda}$$

with $m = 0, \pm 1, \pm 2 \ldots.$



Intensity after a double slit

Diffraction at the double slit 4 Comment 1

The path difference between ray 1 and 2 results from the product of the distance between the slits multiplied with the sine of the deflection angle.

Constructive interference occurs when the path difference is a multiple of the wavelength.

Destructive interference occurs when half a wavelength is added.

The condition for constructive interference depends on the wavelength.

This is why colored strips can be observed when the gaps are illuminated with white light.

Diffraction at the double slit 4 Comment 2

For red light, the maxima are observed for larger deflection angles than for blue light, since the wavelength of red light is larger than the wavelength of blue light.

The intensity behind a double slit is determined by the square of the cosine function.

This is similar to the interference on thin films.

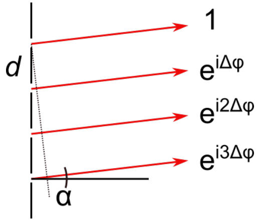
The figure shows the intensity as a function of the path difference between rays 1 and 2.

Grids

Classical wave optics

Diffraction on a grating 1

Grid with four slits



$$\Delta\varphi = \frac{2\pi}{\lambda} d \cdot \sin\alpha$$

The condition for the main maxima is the same as for the double slit

$\boxed{d \sin\alpha_m = m\lambda}$ and $m = 0, \pm 1, \pm 2, \ldots$

Diffraction on a grating 1 Comment 1

Before discussing the case of a grid with many slits, I consider the simple case of a lattice with four slits.

The double slit is supplemented by two additional slits.

As with the double slit, parallel rays are considered that emanate from the slits in different directions.

The phase difference between two adjacent rays results from the same formula that also applies to the double slit.

The condition for constructive interference is the same as for the double slit.

The path difference between two adjacent rays is a multiple of the wavelength for the main maxima of the intensity.

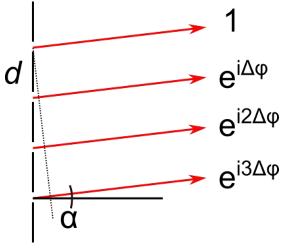
Diffraction on a grating 1 Comment 2

In the sketch of the grating, the additional phase factor is given for each ray.

The additional phase difference between two neighboring rays must be a multiple of 2π for the main maxima.

Diffraction on a grating 2

Minima of the intensity



The phase factors add up to zero if the phase difference between two neighboring rays is $\Delta\varphi = \pi/2$ or the path difference is $\lambda/4$, i.e.

$$1 + e^{i\pi/2} + e^{i2\pi/2} + e^{i3\pi/2} = 1 + i - 1 - i = 0$$

Diffraction on a grating 2 Comment

The phase factor between two neighboring rays is equal to $\pi/2$ if the path difference between two neighboring rays is a quarter of a wavelength.

The four phase factors are 1, i, -1 and $-$i, so that when the four waves overlap, the amplitudes add to zero.

If the path difference is $\lambda/2$, the phase factors are $+1$, -1, $+1$ and -1 so that the amplitudes add up to zero when the four waves overlap.

If the path difference between two neighboring rays is three quarters of the wavelength, the phase factors are 1, $-$i, -1 and $+$i and the amplitudes of the four waves add up to zero when the waves are superimposed.

With four slits there are three intensity minima between two main maxima.

Diffraction on a grating 3: General rules for a grid with N slits

Principal maxima result when the path difference between neighboring rays is an integral multiple of λ

Minima arise when the path difference between two neighboring rays is a multiple of λ/N and not a multiple of λ

The deflection angles for the minima are

$$\boxed{d \sin \alpha_{m'} = \frac{m'}{N}\lambda}$$

with $m' = \pm 1, \pm 2, \ldots$ and m' is not a multiple of N

Diffraction on a grating 3 Comment

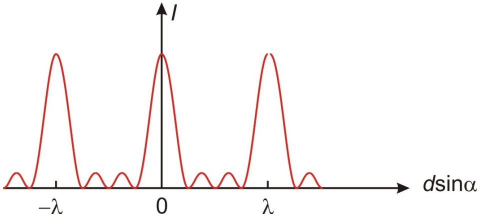
The general rules for the principal maxima and the minima of a diffraction grating are as follows:

For the main maxima, the path difference between two neighboring rays is a multiple of the wavelength λ.

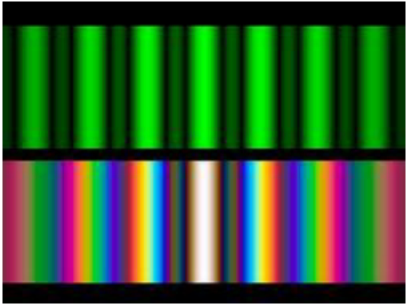
For the minima of the intensity, the path difference between two neighboring rays is a multiple of the wavelength divided by the number N of the slits, as long as this condition does not lead to the condition for the maxima.

Diffraction on a grating 4

Intensity for a grid with 4 slits



Intensity of a grid with 3 slits



Diffraction on a grating 4 Comment

The figure on the left shows the intensity as a function of the path difference of neighboring rays after a grating with four slits.

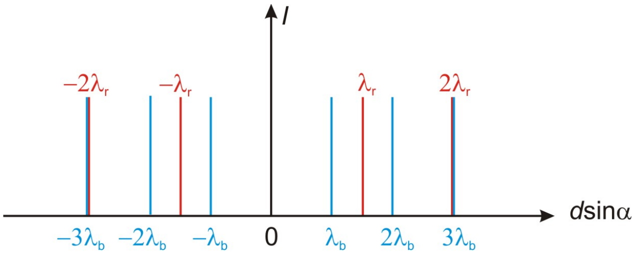
The right figure shows the diffraction on a grid with three slits.

The two minima between the main maxima are clearly visible when almost monochromatic light is used.

When white light is used, the diffraction pattern of the various wavelength overlap.

Diffraction on a grating 5

Diffraction gratings can be used for spectroscopy



The highest spectral resolution of a grid

$$\boxed{\frac{\lambda}{\Delta\lambda} = Nm}$$

Diffraction on a grating 5

Comment 1

Since the width of the main maxima becomes smaller with an increasing number of slits, diffraction gratings can be used for spectroscopy.

The possible resolution of a grid increases with the number of slits.

The figure shows schematically the intensity after a grating with many slits.

The number of slits is so large that only the intensity of the main maxima has to be taken into account.

The intensity is plotted as a function of the path difference between two adjacent rays for two different colors (red and blue).

Diffraction on a grating 5 Comment 2

The path difference between the main maxima increases with the order of diffraction.

The second order path difference is twice as large as the first order path difference.

Therefore the resolution of a grating is also proportional to the diffraction order.

The total resolution of a diffraction grating is therefore determined by the product of the diffraction order m and the number of slits N.

The formula outlined in red indicates the resolution of a diffraction grating.

The figure also shows that different diffraction order can overlap.

In order to avoid this effect, filters must be used that limit the spectral range.

Diffraction on a grating 5 Comment 3

In order to achieve the maximum resolution of a diffraction grating, all slits of the grating must be illuminated.

The light must be parallel in front of the grating.

This is achieved by projecting the light source onto an entrance slit.

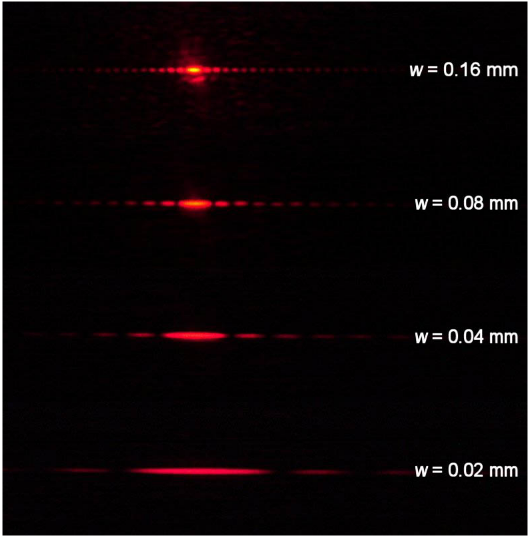
The entrance slit is at the focal point of a second lens that guides the light onto the grating.

Since the entrance slit must always have a finite slit width, this always reduces the ideal resolution of a diffraction grating.

Single silt

Classical wave optics

Diffraction at a single slit 1



Diffraction at a single slit 1 Comment

Similar to the double slit, minima and maxima of the intensity can be observed when light falls on a single slit.

The figure shows the intensity after a single slit that is illuminated with a laser.

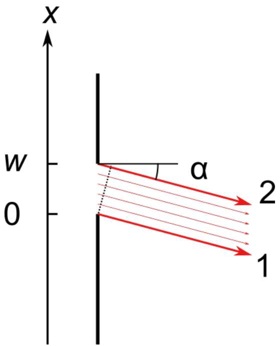
The vertical length of the strips is therefore short.

The width of the slits is reduced from 0.16 mm to 0.02 mm.

The maxima of the diffraction pattern become wider and the distance between the minima increases as the width of the slit is reduced.

Diffraction at a single slit 2

A single slit illuminated by a plane wave



The phase $\Delta\varphi(x)$ of the partial rays depends on the location x

$$\Delta\varphi(x) = \frac{2\pi}{\lambda} x \sin\alpha$$

Diffraction at a single slit 2 Comment 1

The sketch shows a slit perpendicular to the plane of projection.

The coordinate $x = 0$ is assigned to the lower end of the slit and $x = w$ to the upper end.

A coordinate can be assigned to each point within the slit.

A partial beam starts from every point within the slit.

Parallel partial beams can be considered if the diffraction pattern is observed far away from the slit.

Some partial beams are marked by red arrows in the sketch.

The path difference to partial beam 1 is proportional to the coordinate x

Diffraction at a single slit 2 — Comment 2

The formula underlined in red indicates the phase difference of a partial beam, which originates from the location with the coordinate x, to partial beam 1.

The path difference must be multiplied by the wave number $2\pi/\lambda$.

Diffraction at a single slit 3

Integration over the partial beams

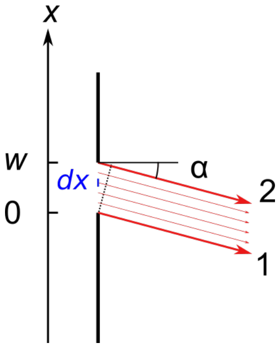
$$\psi = \psi_0 \frac{1}{w} \int_{x=0}^{w} e^{i\Delta\varphi(x)} dx = \psi_0 \frac{1}{w} \left. \frac{e^{i\Delta\varphi(x)}}{i\frac{2\pi}{\lambda}\sin\alpha} \right|_{x=0}^{w}$$

and with $\Delta\varphi = \Delta\varphi(w) = \frac{2\pi}{\lambda} w \sin\alpha$

$$\psi = \psi_0 \frac{e^{i\Delta\varphi} - 1}{i\Delta\varphi} = \psi_0 e^{i\Delta\varphi/2} \frac{e^{i\Delta\varphi/2} - e^{-i\Delta\varphi/2}}{i\Delta\varphi}$$

is the intensity $\psi\psi^*$ behind the single slit

$$\boxed{I = I_0 \left(\frac{\sin \Delta\varphi/2}{\Delta\varphi/2} \right)^2} \quad \text{and} \quad I_0 = \psi_0 \psi_0^*$$



Diffraction at a single slit 3 Comment

The amplitude of each partial beam is proportional to dx/w.

The wave behind the gap results from the integration over all partial beams.

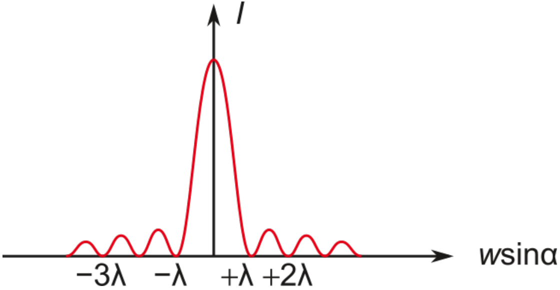
The calculation results in the formula outlined in red for the intensity behind the slit.

The phase difference $\Delta\varphi$ denotes the phase difference between the partial beams 2 and 1.

Diffraction at a single slit 4

Condition for destructive interference

$$m\pi = \frac{\Delta\varphi}{2} = \frac{\pi}{\lambda} w \sin\alpha \quad \rightarrow \quad \boxed{m\lambda = w\sin\alpha} \quad m = \pm 1, \pm 2 \ldots$$



Diffraction at a single slit 4 Comment

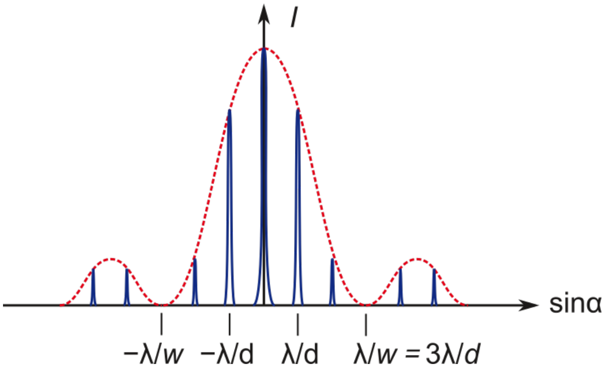
For the diffraction minima, the phase difference $\Delta\varphi/2$ between ray 1 and 2 must be a multiple of π, and the path difference between ray 1 and 2 is a multiple of the wavelength.

In contrast to this, maxima result for a grating when the path difference is a multiple of the wavelength.

The figure shows a sketch of the intensity behind a single slit as a function of the path difference between rays 1 and 2.

Diffraction at a single slit 5

The effect of the single slits on a diffraction grating



Intensity behind a diffraction grating with $w = d/3$

Diffraction at a single slit 5 Comment 1

The slits in a grid always have a finite width.

The intensity behind a grating results from the product of the intensity of the grating and the single slit.

The figure shows the intensity behind a diffraction grating with many slits.

The intensity between the main maxima is negligibly small.

The intensity of the main maxima is modulated by the intensity function of the individual slit.

In the sketch it is assumed that the slit width is one third of the slit distance.

Diffraction at a single slit 5 Comment 2

Therefore, the principal maxima of the third, sixth, etc. order are suppressed by the condition for destructive interference of the single slit.

The intensity function of the single slit can be modified in such a way that the main intensity is shifted from the zero order to another diffraction order.

This is called blazing.

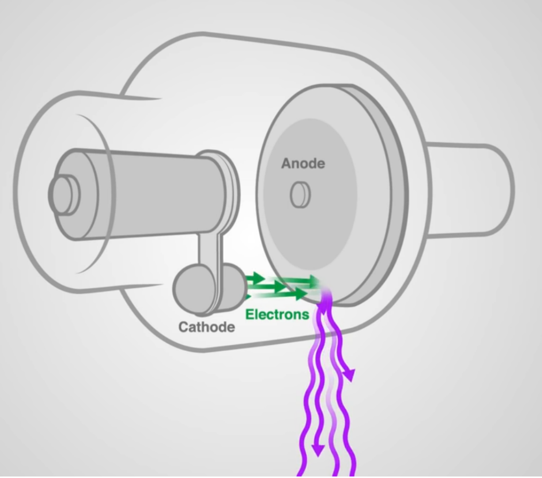
If the intensity function of the individual slits is changed, the intensity of the main maxima changes, but not the respective deflection angle.

Due to blazing, the intensity can be directed to a selected diffraction order.

Bragg

Classical wave optics

Bragg's law 1: X-rays



(XRayTube.mp4)

Bragg's law 1

Comment

X-rays can be produced e.g. in cathode ray tubes.

The video shows an example of an X-ray tube.

Electrons are accelerated and stopped in the anode material.

The slowed-down electrons give off some of their kinetic energy as electromagnetic radiation.

Bragg’s law 2

In 1895 Wilhelm Conrad Roentgen took an X-ray of the hand of his wife Anna Berta Röntgen.

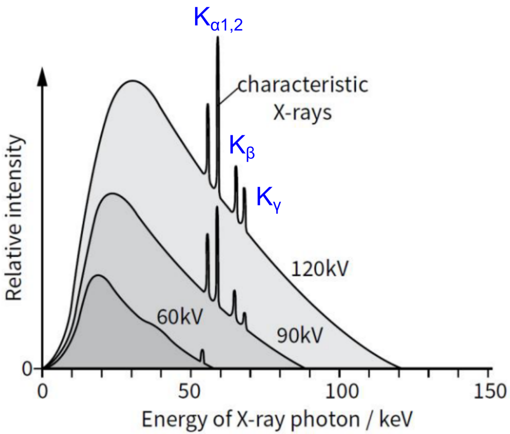
Bragg’s law 2

Comment

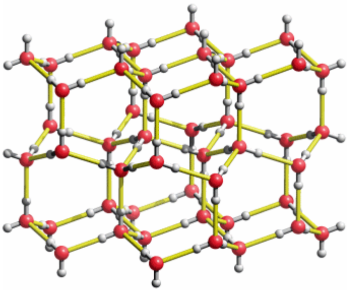
Wilhelm Conrad Roentgen was not the first to experiment with X-rays. But he was the first to recognize the great medical potential of X-rays.

In 1901 he received the first Nobel Prize in Physics „in recognition of the extraordinary service he has acquired through the discovery of the rays named after him“.

Bragg's law 3



Ice crystal



(Eiskristall.mp4)

Bragg's law 3

Comment 1

The figure on the left shows the X-ray spectrum of a tungsten cathode.

The electrons are accelerated with voltages of 60, 90 and 120 kV.

The figure shows the broad spectrum of bremsstrahlung, which results from the deceleration of electrons in the cathode.

The sharp spectral lines of the characteristic X-ray radiation rise above the broad spectrum of bremsstrahlung.

William Henry and William Lawrence Bragg in England and Max von Laue in Germany discovered that the diffraction of the radiation of the sharp characteristic X-ray lines can be used to determine crystal structures.

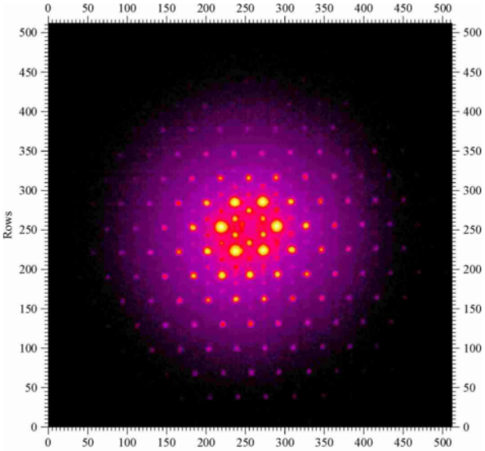
Bragg's law 3 Comment 2

The Nobel Prize was awarded to Max von Laue in 1914: ”For his discovery of the diffraction of X-rays by crystals”, an important step in the development of X-ray spectroscopy”.

The Nobel Prize war awarded to William Henry Bragg and William Lawrence Bragg in 1915: ”For their services in the analysis of crystal structure by means of X-rays, an important step in the development of X-ray crystallography”.

Bragg’s law 4

The wavelength of the X-rays is in the range of about 10^{-10} m and is therefore comparable to the distances between atoms in crystal lattices



Bragg's law 4

Comment

The wavelength of X-rays is comparable to the distances between atoms in molecules and crystal lattices.

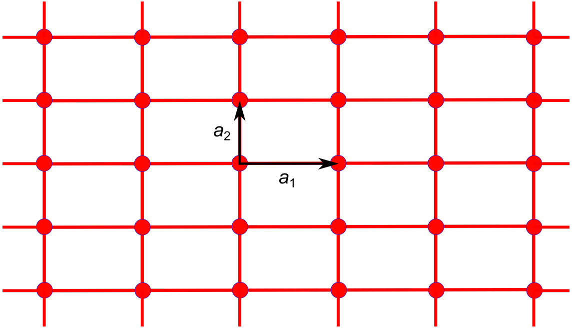
Electromagnetic waves are scattered on the atoms.

The scattered waves interfere, so that a diffraction pattern results.

By analyzing these diffraction patterns, the symmetry of the crystal lattice and the position of the atoms can be determined.

Bragg's law 5

X-rays are scattered at centers that are arranged in a crystal lattice. The distances between these centers are determined by the three vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$. The vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ span the primitive cell of the crystal lattice.



$$\vec{R}_{n_1,n_2,n_3} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Bragg’s law 5 Comment 1

X-rays are scattered at centers usually made up of many atoms.

In the figure, each center is marked with a red dot.

The arrangement of the centers is determined by the three vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$.

These vectors span the primitive cell of a crystal lattice.

The crystal lattice results from the translation of the primitive cells.

Each primitive cell contains one center for the diffraction of X-rays.

The relative location of the primitive cells is determined by the vectors $\vec{R}$ and the three numbers n_1, n_2 and n_3.

Bragg’s law 5 Comment 2

The one-dimensional analog of a crystal lattice is a diffraction grating.

The distance between the slits determines the deflection angles of the main maxima.

In the case of a crystal lattice, the deflection angles are determined by the arrangement of the primitive cells.

The phase function of a single slit determines the intensity of the main maxima of a diffraction grating.

In a crystal lattice, the intensity of the diffraction maxima is determined by the atoms and their arrangement within the primitive cell, i.e. there is a phase function that is determined by the arrangement of atoms within the primitive cell.

Bragg’s law 5 Comment 3

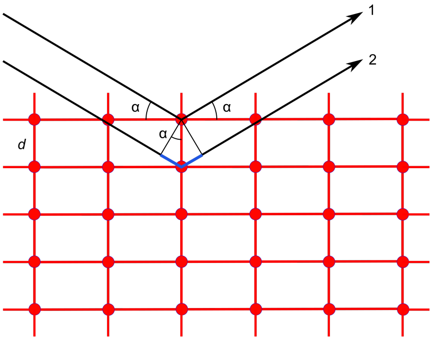
The positions of the primitive cells in a crystal lattice can therefore be determined with the deflection angles of the maxima.

This corresponds to the red dots in the figure.

The intensity of the diffraction maxima is determined by the location and type of atoms within the primitive cell.

Bragg’s law 6

Diffraction on a lattice plane with distance *d*



path difference between ray 1 and 2

$$\boxed{\Delta s = 2d \sin\alpha}$$

Bragg’s law 6

Comment

Bragg’s law assumes that the light is reflected on lattice planes.

These planes are called Bragg planes.

Bragg planes planes are formed by the primitive cells.

The distance between two neighboring Bragg planes is *d* and it is not difficult to calculate the path difference between the two rays 1 and 2.

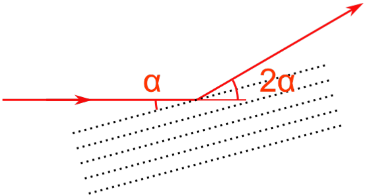
The formula outlined in red indicates the path difference between ray 1 and 2.

Bragg's law 7

The condition for constructive interference is

$$\boxed{m\lambda = 2d \sin \alpha_m}$$

with $m = 1, 2, \ldots$



Bragg's law 7

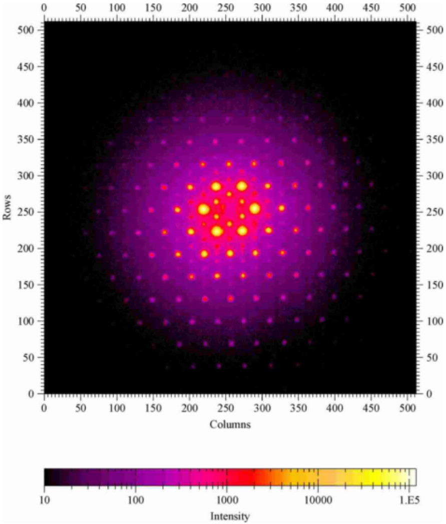
Comment

Constructive interference occurs when the path difference is a multiple of the wavelength.

There are sharp diffraction maxima, since the interference is due to many rays.

The sketch shows that the angle α of Bragg's law is half the deflection angle of the X-ray beam.

Bragg's law 8


0 50 100 150 200 250 300 350 400 450 500
Rows
Columns
10 100 1000 10000 1.E5
Intensity

Bragg's law 8 Comment

The figure shows again the X-ray diffraction on a crystal lattice.

Each diffraction maximum determines the orientation and the spacing of a set of lattice planes.

Note that the intensity of the diffraction maxima is very different.

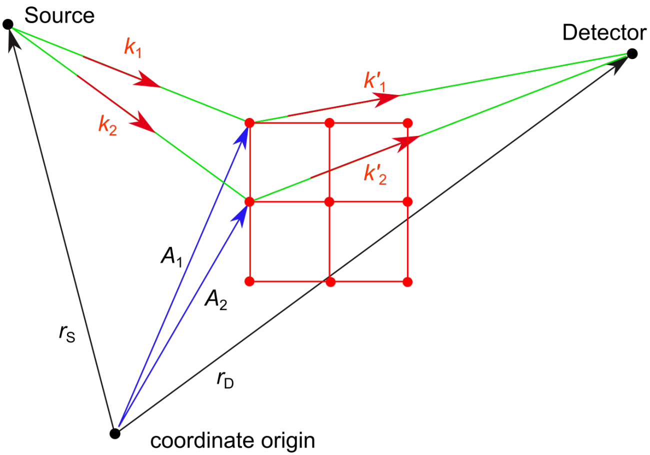
The intensity of the maxima depends on the atoms within the primitive cell.

Laue

Classical wave optics

Laue equations 1

Max von Laue considers the diffraction of X-rays on the primitive cells



Laue equations 1

Comment

It is not obvious how the structure of the crystal lattice and the arrangement of the atoms within the primitive cells can be determined with Bragg's law.

This problem can be solved using the Laue equations.

To describe X-ray diffraction, Max von Laue starts out directly from the scattering of X-rays on the primitive cells.

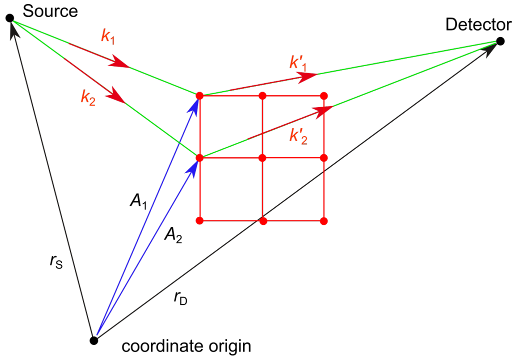
As before, the primitive cells are marked by red dots in the figure.

The position of two primitive cells is given by the vectors $\vec{A}_1$ and $\vec{A}_2$.

The location of the X-ray source and the location of the detector are given by the vectors $\vec{r}_S$ and $\vec{r}_D$, respectively.

The orientation of the wave vectors is given by the rays that connect the source with the primitive cells and the primitive cells with the detector.

Laue equations 2



parallel beams can be used because the crystals are small and the distances in the x-ray diffractometer are large

$$\vec{k}_1 = \vec{k}_2 = \vec{k}$$
$$\vec{k}'_1 = \vec{k}'_2 = \vec{k}'$$

$$\boxed{\begin{aligned}\varphi_1 &= \vec{k}_1(\vec{A}_1 - \vec{r}_S) + \vec{k}'_1(\vec{r}_D - \vec{A}_1) \\ \varphi_2 &= \vec{k}_2(\vec{A}_2 - \vec{r}_S) + \vec{k}'_2(\vec{r}_D - \vec{A}_2)\end{aligned}}$$

$$\Delta\varphi = \varphi_1 - \varphi_2 = \vec{k}(\vec{A}_1 - \vec{A}_2) + \vec{k}'(\vec{A}_2 - \vec{A}_1) = (\vec{k} - \vec{k}')(\vec{A}_1 - \vec{A}_2)$$

Laue equations 2 Comment 1

The phase of the two beams on their way from the source to the detector is indicated by the formulas in the box.

These formulas are simplified considerably if parallel rays are assumed.

The assumption of parallel rays is plausible because the crystals are small compared to the distances in an x-ray diffractometer.

An important additional assumption is that the scattering does not change the wavelength of the X-rays.

If this condition is met, one speaks of elastic scattering.

Laue equations 2 Comment 2

The X-rays do not transmit or receive energy from the crystal.

The wave vectors change their direction due to the diffraction, but not the absolute value.

If the wavelength changes due to the scattering, one speaks of inelastic scattering.

Inelastic scattering is dealt with in the sixth chapter of this lecture.

With these conditions, the phase difference between the two beams can be calculated.

The phase difference depends on the difference in the wave vectors of the incident and the scattered wave, as well as on the difference between the locations of the primitive cells.

Laue equations 3

The difference between the vectors $\vec{A}_1$ and $\vec{A}_2$ is

$$\vec{R}_{n_1,n_2,n_3} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

The condition for constructive interference is

$$\boxed{2\pi m = (\vec{k} - \vec{k}\,')\vec{R}_{n_1,n_2,n_3}}$$

with $m = 0, \pm 1, \pm 2, ...$

Laue equations 3 Comment

The formula underlined in red gives the difference vector *R* between the positions of two primitive cells.

Constructive interference occurs when the phase difference is a multiple of 2 π.

The formula outlined in red indicates the condition for constructive interference.

That is an important interim result, but not the end of the discussion.

Laue equations 4

In addition to the vectors $\vec{a}_i$, a second set of vectors $\vec{b}_i$ is defined by the scalar product

$$\boxed{\vec{a}_i \vec{b}_j = 2\pi\delta_{ij}}$$

The vectors $\vec{b}_i$ form the reciprocal lattice

$$\boxed{\vec{K}_{hk\ell} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3}$$

The indices $h, k, \ell = 0, \pm 1, \pm 2...$ are the Miller indices.

Laue equations 4 Comment

In addition to the three vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$, which span the primitive cell, Laue defines a second set of three vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$.

These vectors are defined by the framed scalar product.

The three vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ also span a special type of primitive cell in analogy to the vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$.

The translation of these primitive cells forms a lattice called the reciprocal lattice.

The second equation outlined in red gives the vectors $\vec{K}$ of the reciprocal lattice.

The indices h, k, ℓ are called the Miller indices.

Laue equations 5

Due to the condition

$$\vec{a}_i \vec{b}_j = 2\pi\delta_{ij}$$

the vectors $\vec{b}_i$ are

$$\boxed{\begin{aligned} \vec{b}_1 &= \frac{2\pi}{V_{\text{Cell}}}(\vec{a}_2 \times \vec{a}_3) \\ \vec{b}_2 &= \frac{2\pi}{V_{\text{Cell}}}(\vec{a}_3 \times \vec{a}_1) \\ \vec{b}_3 &= \frac{2\pi}{V_{\text{Cell}}}(\vec{a}_1 \times \vec{a}_2) \end{aligned}}$$

V_{Cell} denotes the volume of the primitive cell

$$\boxed{V_{\text{Cell}} = \vec{a}_1(\vec{a}_2 \times \vec{a}_3)}$$

Laue equations 5 Comment 1

Due to the definition of the vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$, these three vectors can easily be calculated with the cross product of the vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$.

The cross products must be divided by the volume of the primitive cell.

The volume of the primitive cell is calculated with the scalar triple product of the vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$.

You can also simply reverse the formula and write

$$\boxed{\begin{aligned} \vec{a}_1 &= \frac{2\pi}{V_{\mathrm{BZ}}}(\vec{b}_2 \times \vec{b}_3) \\ \vec{a}_2 &= \frac{2\pi}{V_{\mathrm{BZ}}}(\vec{b}_3 \times \vec{b}_1) \\ \vec{a}_3 &= \frac{2\pi}{V_{\mathrm{BZ}}}(\vec{b}_1 \times \vec{b}_2) \end{aligned}}$$

Laue equations 5 — Comment 2

The primitive unit cell of the reciprocal lattice is called the 1st Brillouin zone. V_{BZ} denotes the volume of the 1st Brillouin zone

$$\boxed{V_{\mathrm{BZ}} = \vec{b}_1(\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{V_{\mathrm{Cell}}}}$$

Laue equations 6

Why is it useful to calculate the reciprocal lattice?

$$\underline{\vec{K}_{h,k,\ell}\vec{R}_{n_1,n_2,n_3}} = (h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3)(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)$$
$$= \underline{2\pi(n_1 h + n_2 k + n_3 \ell)}$$

Comparison with the condition for constructive interference

$$\underline{(\vec{k} - \vec{k}')\vec{R}_{n_1,n_2,n_3} = 2\pi m}$$

shows

$$\boxed{\vec{k} - \vec{k}' = \vec{K}_{h,k,\ell}}$$

Laue equations 6 Comment

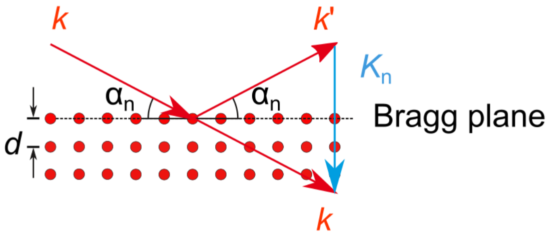
The first formula gives the scalar product of a vector of the reciprocal lattice multiplied by a lattice vector $\vec{R}$, which describes the position of the primitive cells.

Due to the definition of the vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$, this scalar product always results in a multiple of 2 π.

The comparison with the condition for constructive interference shows that the difference between the wave vectors of the incident and the scattered beam is always a vector of the reciprocal lattice.

Laue equations 7

Comparison of the conditions for constructive interference by Bragg and Laue



$$n\lambda = 2d \sin \alpha_n$$

$$\vec{k} - \vec{k}' = \vec{K}_n$$

$$\boxed{k \sin \alpha_n = \frac{K_n}{2}}$$

Laue equations 7

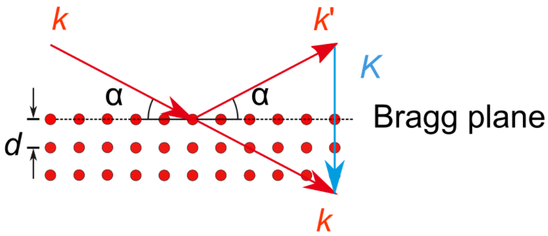
Comment

If the Laue condition is drawn into the picture with which the Bragg condition was derived, one sees that the vectors of the reciprocal lattice are perpendicular to the Bragg planes.

The amount of the wave number vector multiplied by the sine of the diffraction angle α results in half the length of a reciprocal lattice vector.

Laue equations 8

especially for first order diffraction maxima



$$\underline{k \sin \alpha = \frac{K}{2}} = \frac{2\pi}{\lambda} \sin \alpha$$

$$\underline{\lambda = 2d \sin \alpha}$$

Distance between the Bragg planes

$$\boxed{d = \frac{2\pi}{K}}$$

Laue equations 8

Comment 1

If the diffraction maxima of the first order are considered and the indices are omitted, then the formula outlined in red results for the distance between the Bragg planes.

The distance between the Bragg planes is inversely proportional to the length of the reciprocal lattice vectors.

Laue equations 8 — Comment 2

With the vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ that determine the position of the primitive cells, the basis vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ of the reciprocal lattice can be calculated.

With that all reciprocal lattice vectors are known, and the distances of all Bragg planes can be calculated.

With the wavelength of the X-ray radiation used and the Bragg formula, all possible scattering angles then result.

Conversely, it is possible to determine the reciprocal lattice from the scattering angles.

If the vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ are known, the lattice vectors $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ can be calculated.

Laue equations 9

Influence of the atoms in the primitive cell

$$\varphi_1 = \vec{k}_1(\vec{A}_1 + \vec{d}_1 - \vec{r}_Q) + \vec{k}'_1(\vec{r}_D - \vec{A}_1 - \vec{d}_1)$$
$$\varphi_2 = \vec{k}_2(\vec{A}_2 + \vec{d}_j - \vec{r}_Q) + \vec{k}'_2(\vec{r}_D - \vec{A}_2 - \vec{d}_j)$$

Phase difference between ray 2 and ray 1 is

$$\underline{\Delta\varphi = \varphi_2 - \varphi_1 = (\vec{k} - \vec{k}')(\vec{A}_2 - \vec{A}_1) + (\vec{k} - \vec{k}')(\vec{d}_j - \vec{d}_1)}$$

The wave function of the diffracted wave

$$\psi = \psi_0 \sum_{\vec{R}} e^{i(\vec{k}-\vec{k}')\vec{R}} \cdot \left(\sum_{j=1}^{N} e^{i(\vec{k}-\vec{k}')(\vec{d}_j-\vec{d}_1)} f_j \right)$$

Laue equations 9 — Comment 1

The intensity of the diffraction maxima is determined for a crystal lattice by the atoms in the primitive cell.

The phase of rays 1 and 2 is determined not only by the location of the primitive cells, but also by the location of the atoms within the primitive cell.

In the first two equations, the position vectors of the atoms are written in blue.

The vectors d_j indicate the position of the atoms in relation to the primitive cell.

The phase difference contains a contribution that depends on the difference in the position of the primitive cells, and an additional contribution that depends on the difference in the atomic positions.

This additional contribution is marked in blue in the underlined formula.

Laue equations 9

Comment 2

For the diffracted wave one has to add up the contribution of all primitive cells that are illuminated by the X-ray beam.

As before, the first sum determines the deflection angle of the diffraction maxima.

The brackets written in blue determine the intensity of the diffraction maxima.

The contributions of all atoms within the primitive cell are added up.

Laue equations 9 Comment 3

The additional factor f_j is the atomic structure factor.

The scattering power of an atom increases with the number of electrons in the atom.

Therefore, the scattering power of hydrogen with atomic number 1 is extremely small compared to the scattering power of calcium with atomic number 20.

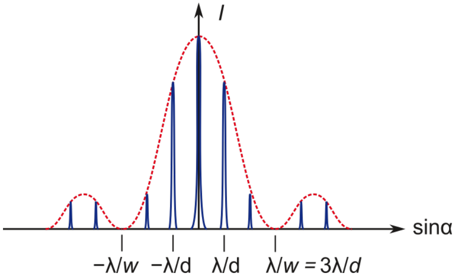
The blue bracket is the structure factor of X-ray diffraction.

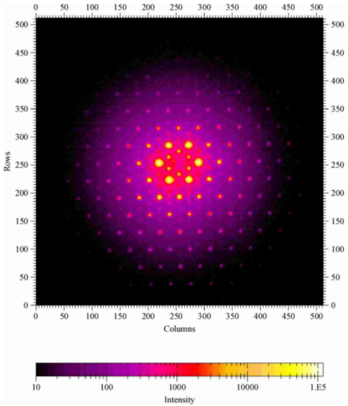
If there is only one atom in the primitive cell, the structure factor is given by the atomic structure factor.

Only in this case do the red dots in the previous figures correspond to the atoms.

Laue equations 10

Comparison of diffraction on the diffraction grating and diffraction on the crystal lattice





Laue equations 10 Comment

Finally, note the analogy of X-ray diffraction and diffraction on a grating.

The first sum written in black corresponds to the sum over the slits.

The second sum written in blue corresponds to the contribution of a single slit.

Just as the intensity of the interference maxima of a grating is modulated due to the single slit, the intensity of the maxima of X-ray diffraction is modulated due to the atoms in the primitive cell.

It turns out that the reciprocal lattice is fundamental for the description of crystalline solids (compare chapter 6: Solids).

Revision

Summary in questions

1. What is the interference condition for constructive interference with a double slit?
2. Sketch the intensity after a double slit as a function of the path difference of the rays.
3. What is the interference condition for constructive interference for a grid with N slits?
4. What is the condition for destructive interference for a grid with N slits?
5. Sketch the intensity of a grid with 5 slits as a function of the path difference of neighboring partial beams.
6. How big is the spectral resolution $\lambda/\Delta\lambda$ for a grid with N slits.

Summary in questions

7. Why does the resolution depend on the diffraction order?
8. Sketch the intensity after a single slit as a function of the path difference of the peripheral rays.
9. Sketch the intensity after a grid with 4 slits as a function of the path difference of neighboring rays, if the slit openings are a quarter of the slit distance.