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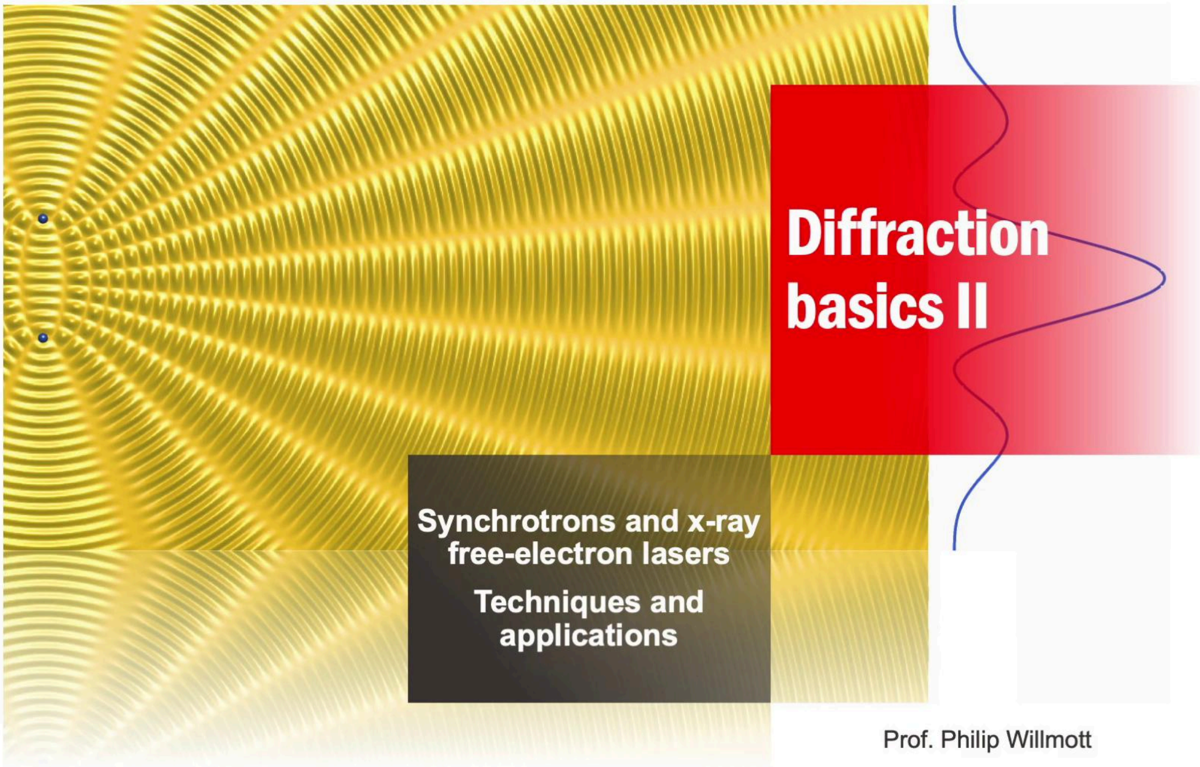


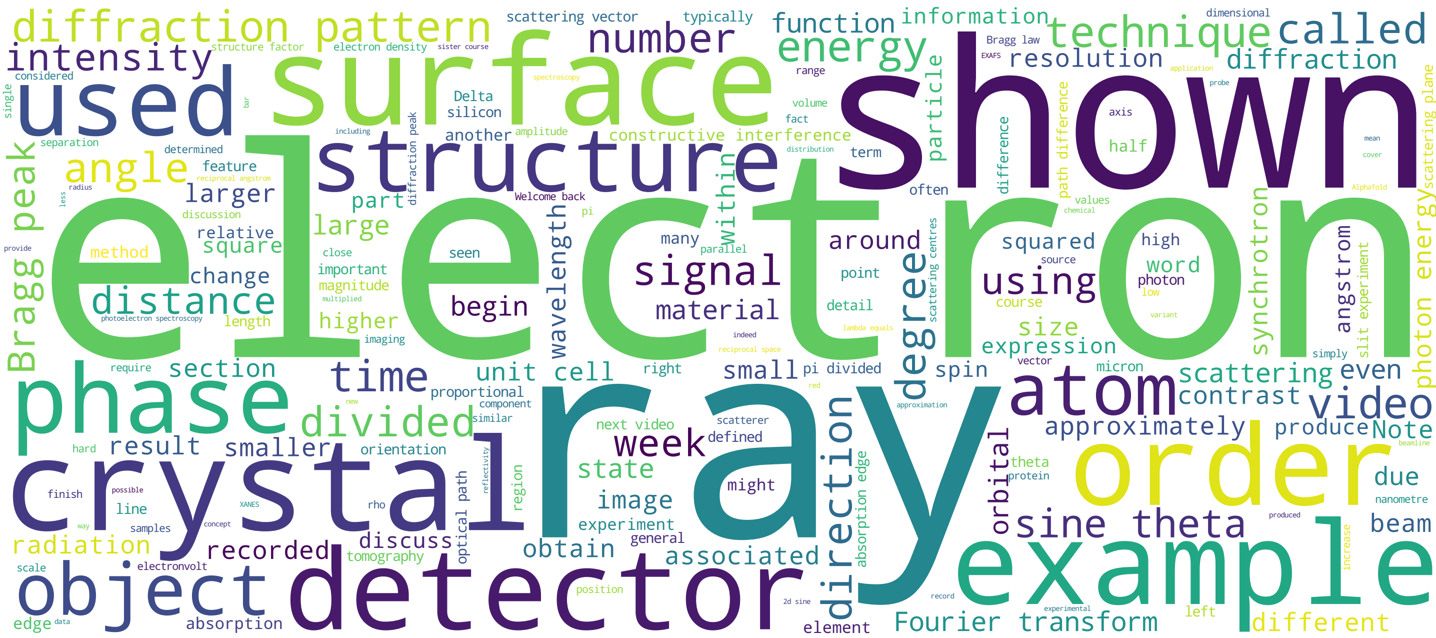
# Diffraction basics II

## Synchrotrons and x-ray free-electron lasers

## Techniques and applications

École polytechnique fédérale de Lausanne

Prof. Philip Willmott

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Video

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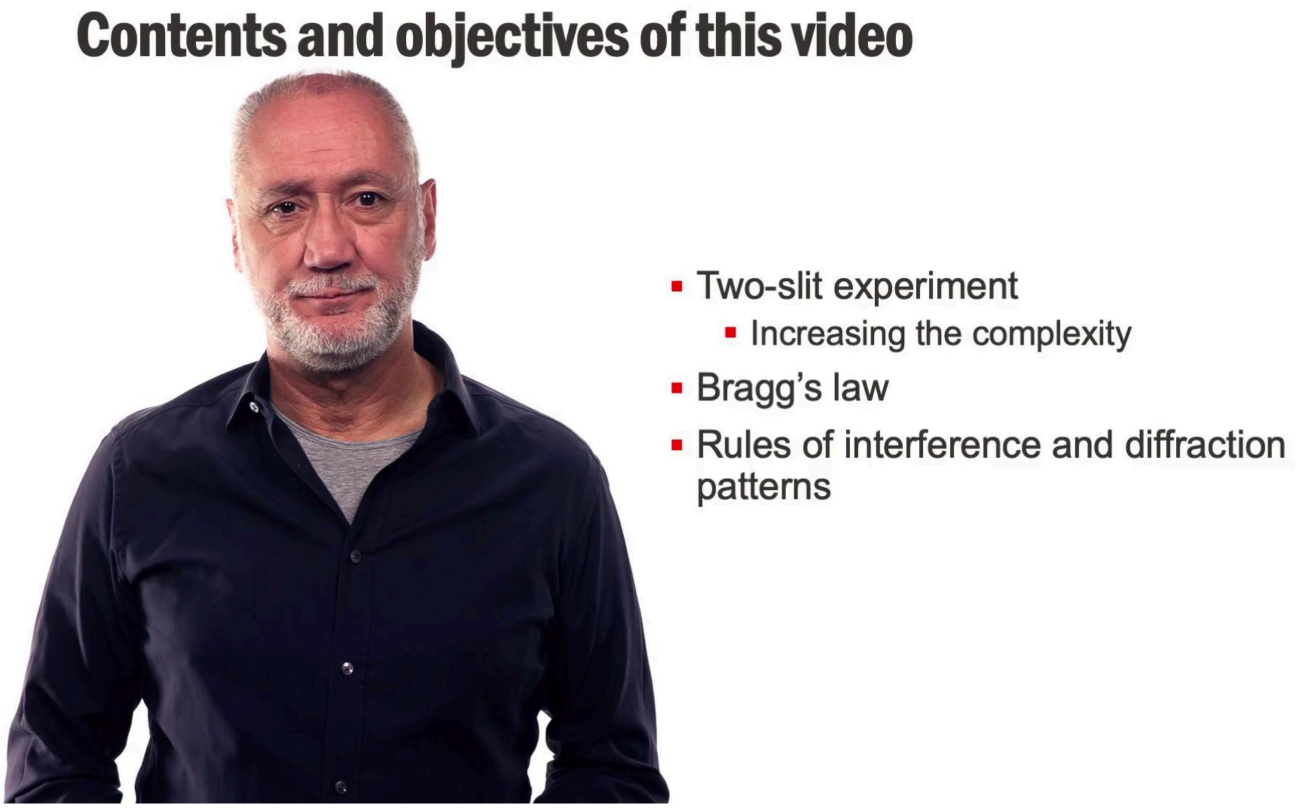
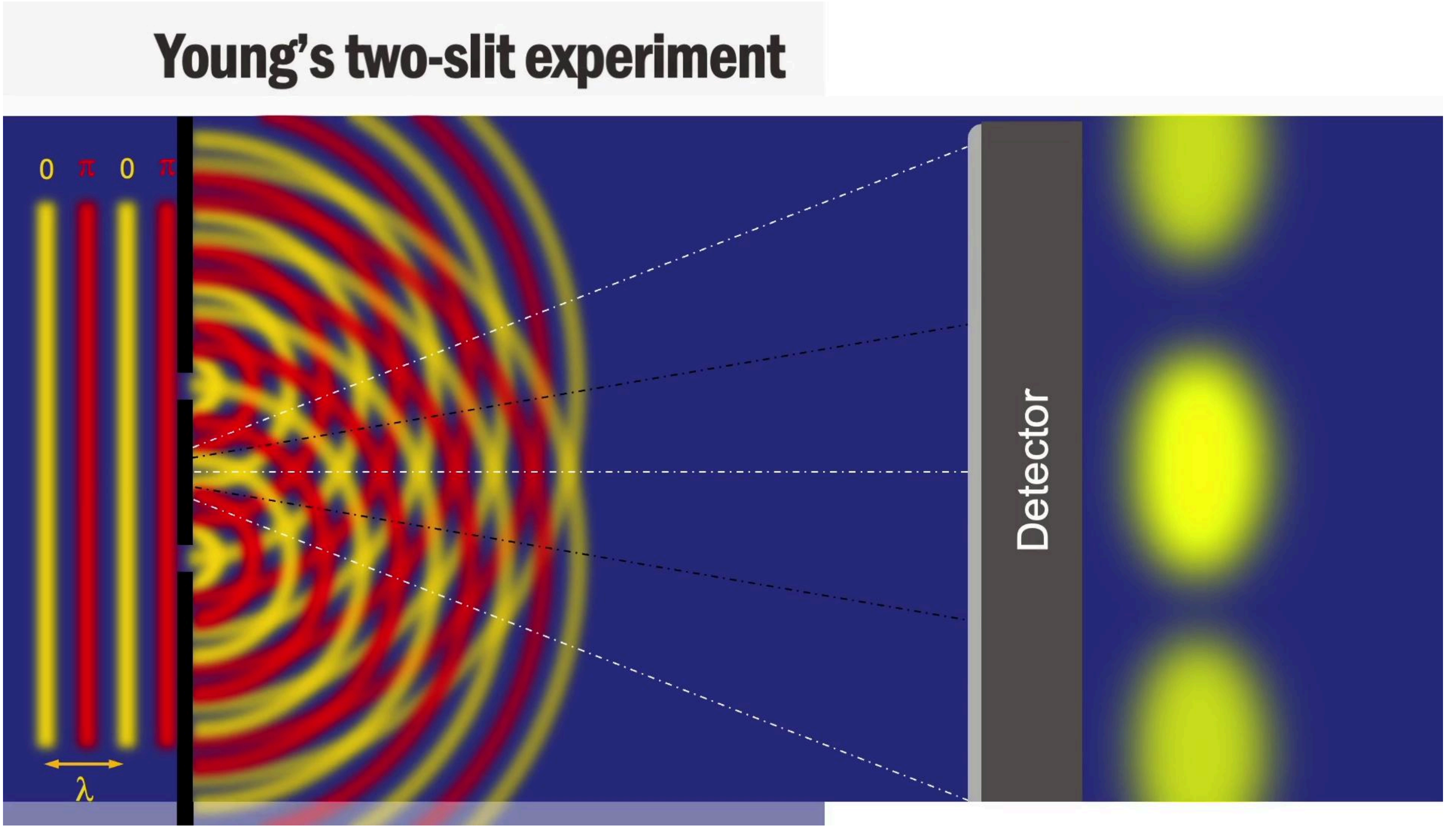



In this video, we will first look at the famous Young's two slit experiment using wave optics and extend this to cases where there are more than two scattering centres. This will prepare us for a description of Bragg's law and the general rules associated with it.

Notes

Summary

0m 05s



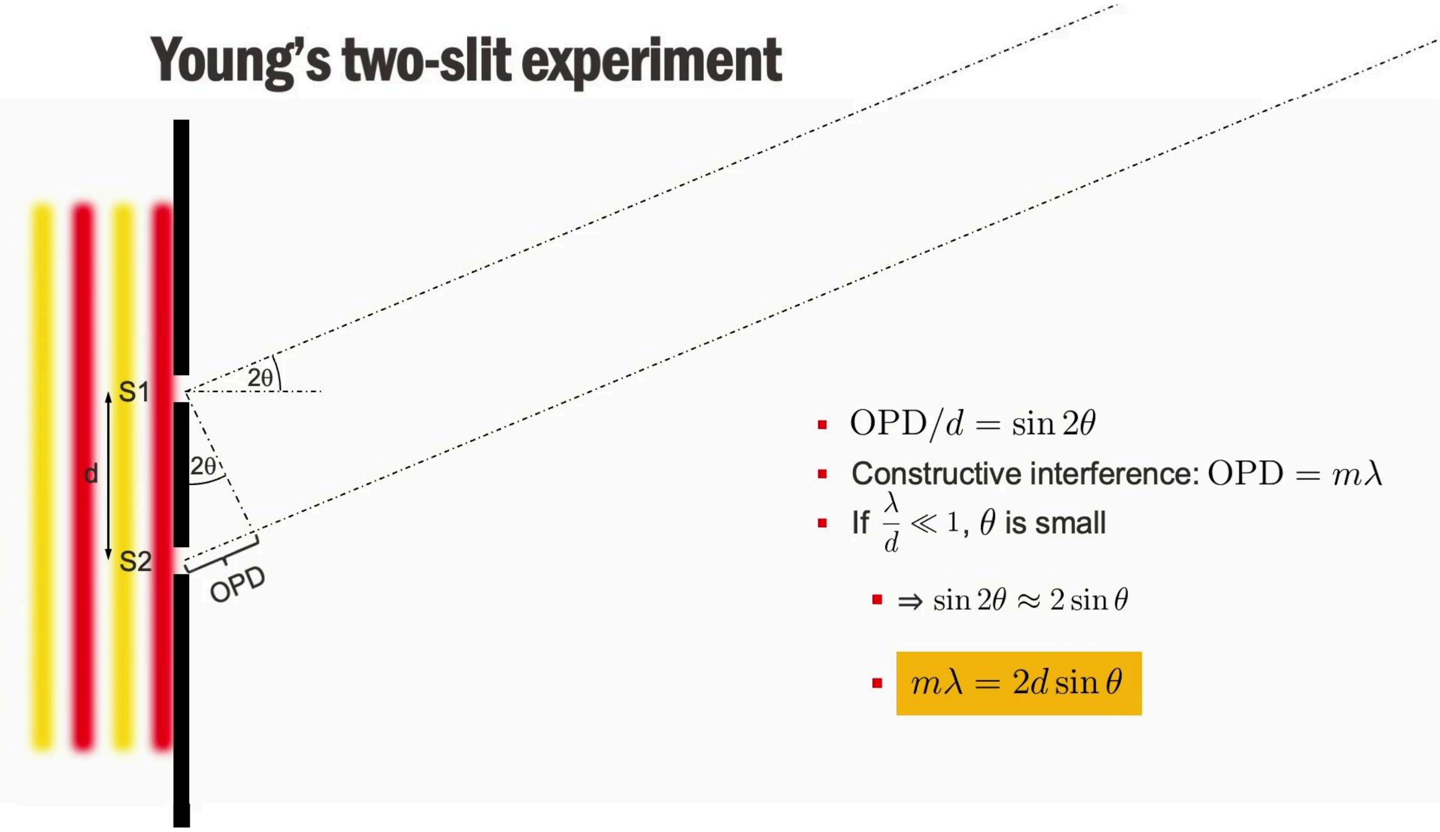

So let's begin with the Young's two slit experiment. A plane wave impinges on an opaque screen containing two narrow openings. The wave has a wavelength lambda. Wave peaks are shown in yellow, troughs in red. The light that passes through the two openings spreads out due to diffraction. A detector is placed downstream of the waves. In the forward direction, it can be seen that peaks overlap with peaks and troughs overlap with troughs, resulting in constructive interference. In contrast, at another angle shown here with the black dot-dashed line, the peaks overlap with troughs, resulting in destructive interference. The next maximum where constructive interference occurs is highlighted here. The same effect occurs, obviously, on the other side. As a result, a pattern of bright spots emerges on the detector.

Notes

Summary

0m 24s

## Young's two-slit experiment




- $\text{OPD}/d = \sin 2\theta$
- Constructive interference: $\text{OPD} = m\lambda$
- If $\frac{\lambda}{d} \ll 1$, $\theta$ is small
  - $\Rightarrow \sin 2\theta \approx 2\sin\theta$
  - $\boxed{m\lambda = 2d\sin\theta}$

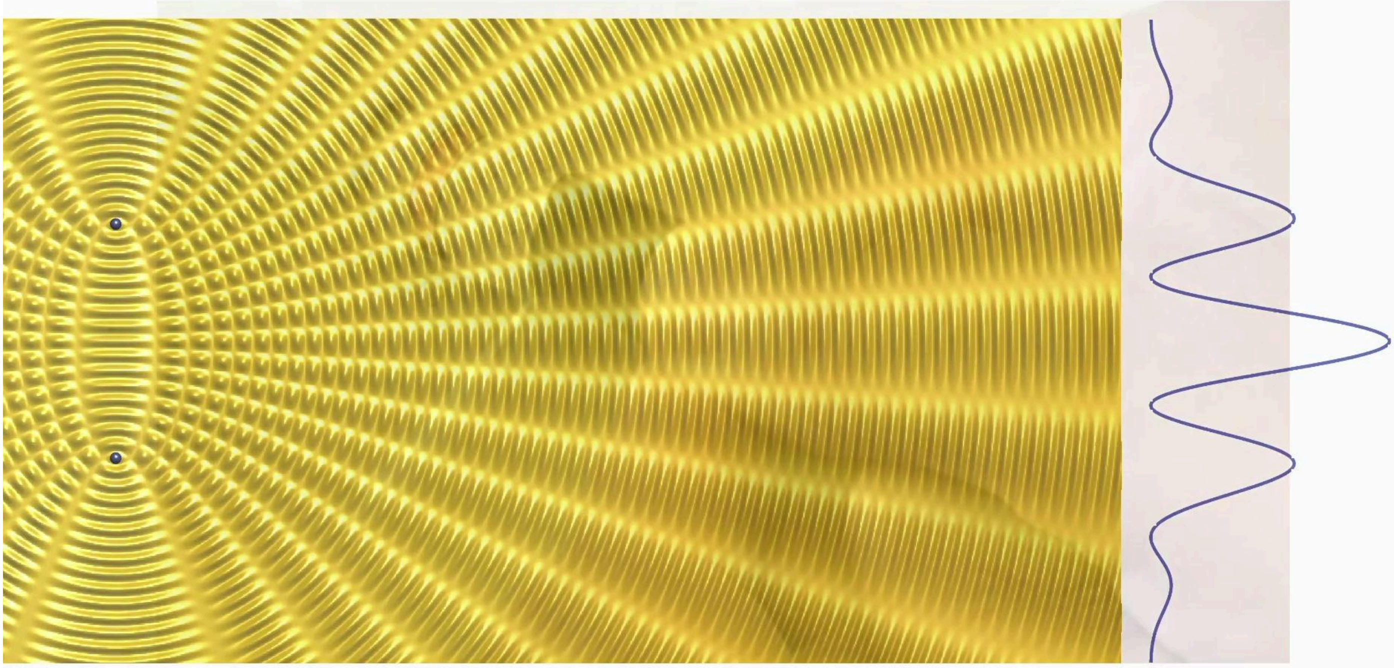
We now derive a mathematical expression for the condition for constructive interference, that is, for a diffraction maximum. We begin again with the incident beam on two slits S1 and S2 in an otherwise opaque screen separated by a distance d. Let us consider the intensity at a point P. The line connecting S1 to P, we label path 1, and from S2 to P, path 2. The difference in length between paths 1 and 2 is the optical path difference or OPD. We now simplify this situation by assuming that P is far away from the slits, given by the condition that paths 1 and two are much larger than the slit separation d. In this case, we can make the approximation that paths 1 and 2 are parallel at an angle 2 theta to the normal of the screen. We immediately see that sine 2 theta is equal to the optical path difference divided by d. Now, if the optical path difference is equal to an integer multiple of wavelengths, constructive interference will occur. Now, if we also assume that the wavelength is much smaller than the slit separation, theta will be a small angle, and we can make the approximation that sine 2 theta is approximately equal to 2 sine theta. We therefore come to our final expression for constructive interference that m Lambda is equal to 2D sine theta, where m is an integer.

Notes

Summary

1m 48s

# Distance makes the fringes grow narrower



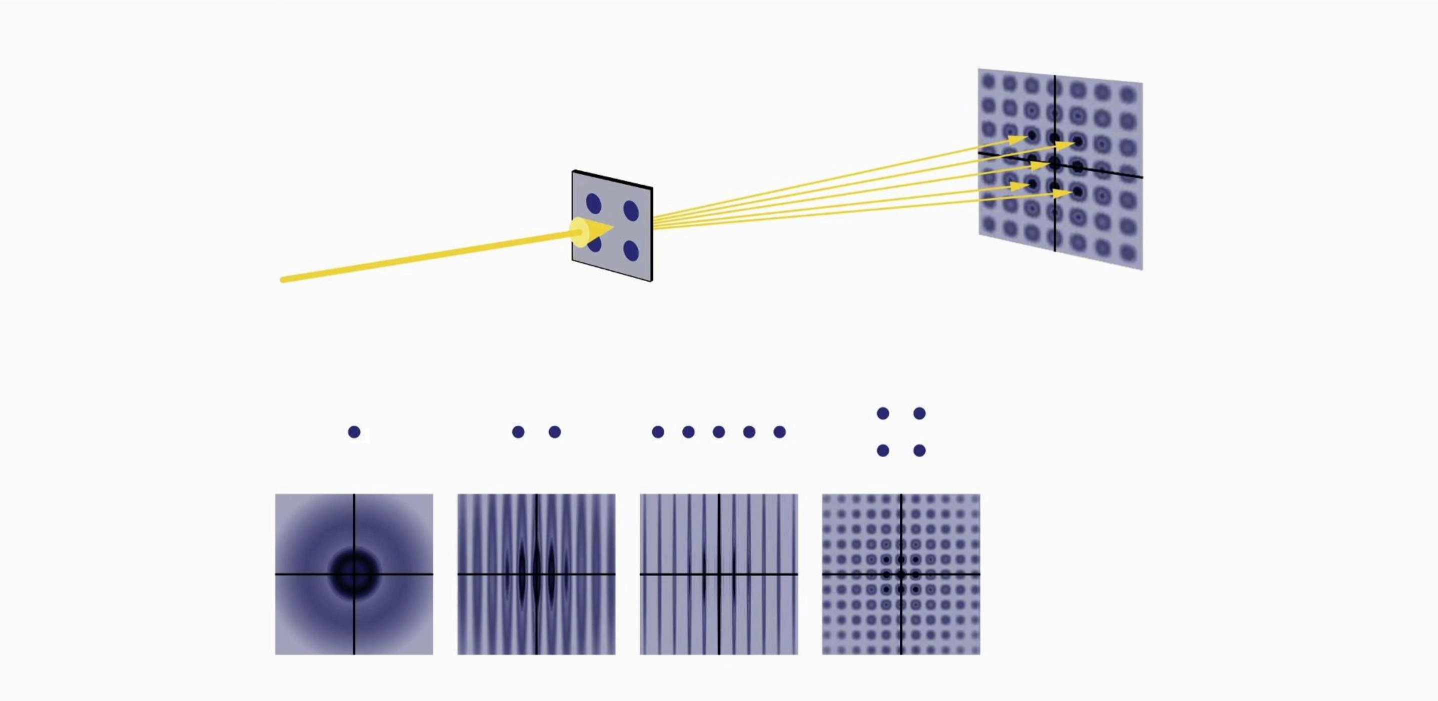
From this expression, we can predict that as the distance between two scattering centres or slits increases the angle between maxima and the diffraction pattern becomes narrower. Watch this video carefully.

Notes

Summary

3m 50s

# Blinging up Young



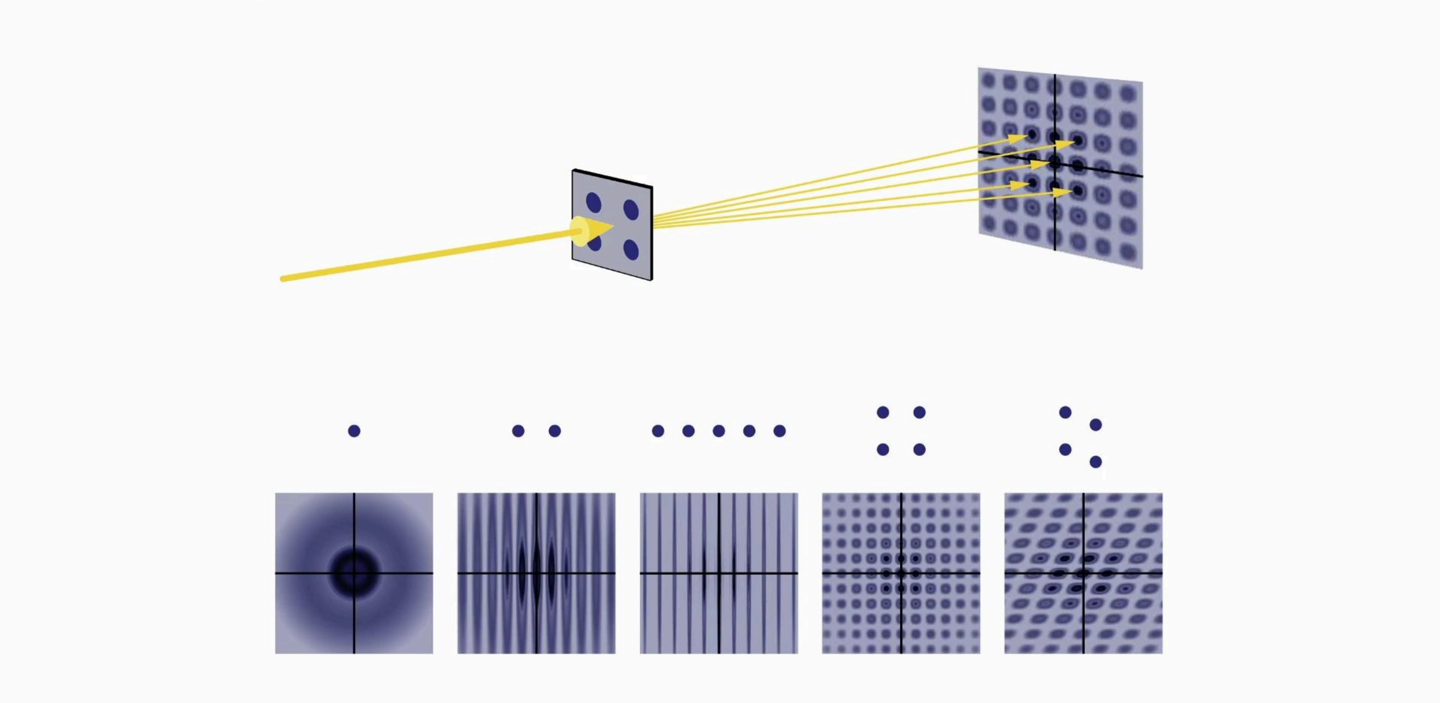
One can observe diffraction of visible coherent light, such as produced by laser pointers, from a regularly spaced set of scatterers, such as the millimetre pattern on a plastic ruler. The scattering centres here are the reflecting surfaces between the black millimetre lines. Now we have described crystals, we should see how X-rays scattered from them look like. Let's begin with a single point scatterer. The far field pattern, remember this is the Fourier transform of the object, is a modulated Gaussian. Interference between scattering from two adjacent spots results in interference fringes much like those seen in the famous Young's double slit experiment. Increasing the number of evenly spaced scatterers will sharpen that interference signal, just like the maximum of a grating monochromator sharpened with the number of scattering facets described in the sister course. Extending this motif to a second dimension causes the pattern to change from being a set of fringes to being a set of spots, while the angle between scatterers is reflected at 90 degrees in the interference or diffraction pattern. Also importantly, the larger the separation between the scatterers, the smaller their angular separation or separation in reciprocal space and vice versa.

Notes

Summary

4m 10s

# Blinging up Young



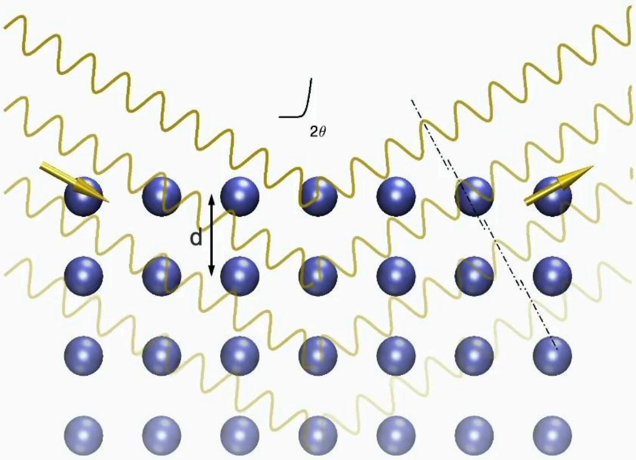
Hence, crystals with small unit cells such as sodium chloride have widely spaced diffraction features, while protein crystals which have characteristic repeat dimensions of two orders of magnitude larger than sodium chloride, have very crowded diffraction patterns.

Notes

Summary

6m 01s

# Bragg's law



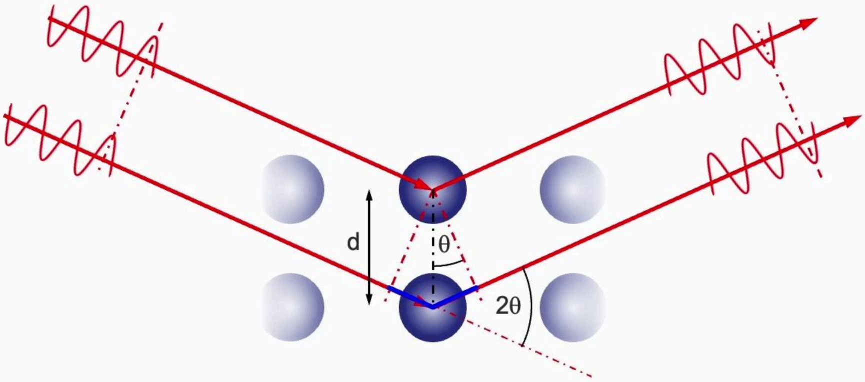

We now discuss Bragg's law, the famous equation describing diffraction of X-rays by crystalline substances via the relationship between the wavelength of the X-rays, the angle of incidence, theta, and the separation d, between crystal planes.

Notes

Summary

6m 19s

# Bragg's law




Again, $m\lambda = 2d\sin\theta$ or $\lambda = 2d_{hkl}\sin\theta$

Using arguments essentially identical to those we considered for interference in Young's double slit experiment, we first identify the optical path difference between X-rays scattered through an angle 2 theta from adjacent planes and obtain the equation for a diffraction maximum defined as the geometry in which the scattered radiation is in phase. Once more, it is given by m Lambda equals 2d sine theta. Or, for a given crystal plane defined by the Miller indices h, k and l, we can re-express this as lambda equals 2d_hkl sin theta.

Notes

Summary

6m 40s

# Rules of interference and diffraction patterns

- (1) The larger the separation between elements in a scattering (diffracting/interfering) array ($d_{real}$), the closer the distance between diffraction features $d_{rec}$
  - $d_{rec} \propto 1/d_{real}$
- (2) The scattering vector Q, i.e. the vector joining up the incoming beam $k_{in}$ and the diffracted beam $k_{out}$, always lies perpendicular to the scattering planes of a crystal

In the sister course, we described Thomson scattering and the scattering vector Q, that is the vector difference between the incoming and the elastically scattered wave vectors. In crystal diffraction, the direction of Q is always at right angles to the scattering planes responsible for the scattered signal in the direction of k_out while its magnitude can be expressed in a variety of ways. We determined Q to be equal to 4 pi divided by lambda sine theta. And combining this with Bragg's law, lambda equals 2d sine theta, we see that Q is equal to 2 pi divided by d_hkl. So for example, Q for the silicon-004 reflection has a value of 2 pi divided by d_004 for silicon. But d_004 for silicon is equal to 1.3578 angstroms. Hence Q is equal to 4.628 reciprocal angstroms. A convenient practical expression for Q in reciprocal angstroms is also given and is equal to 1.0135, in other words, close to unity, times the photon energy in kiloelectronvolts multiplied by sine theta. We consider now rules that are always met in crystal diffraction. First, the larger d_real, the size of the scattering units in a scattering array, or in other words, a crystal, the closer the distance d_rec between the diffraction features.

Notes

Summary

7m 29s

# Rules of interference and diffraction patterns

- (3) The sharpness (or width) of the diffraction signal is inversely proportional to the number of scattering elements that are involved
  - $FWHM_{rec} \propto 1/N_{real}$
- (4) The intensity of a diffraction peak is proportional to the square of the number of scattering elements that contributed to it (assuming they are all equally illuminated)
  - $I_{rec} \propto N^2_{real}$

Here, the subscript "rec" is short for reciprocal. The second rule is, as mentioned just before, that the scattering vector Q lies perpendicular to the scattering planes of a crystal. The third rule is that the width of the diffraction peak, assuming perfectly parallel and coherent incident radiation and ignoring any experimental or sample broadening effects is inversely proportional to the number of scattering planes. The fourth rule states that the diffraction peak intensity is proportional to the square of the number of scattering planes.

Notes

Summary

9m 32s

## Rules of interference and diffraction patterns

- (5) The most important rule for a deep understanding of diffraction. But one you can probably get away with not understanding for this course. Probably…

**The diffraction pattern of a homogenously illuminated system is the square of the Fourier transform of that system**

$$I_{\mathrm{rec}}(\mathrm{system}) \propto [\mathcal{FT}(\mathrm{system})]^2$$

Now, the last rule, or more accurately, it's a fact, is perhaps the most important for those of you who will use diffraction on a regular basis, namely, that the diffraction pattern produced by elastic scattering of an object is equal to the square of the Fourier transform of that object.

Notes

Summary

10m 19s

# In the next video...

In the next video, we will discuss the so called reciprocal lattice, the information encoded within a diffraction pattern, and how one can extract the atomic structure from that.

Notes

Summary

10m 41s