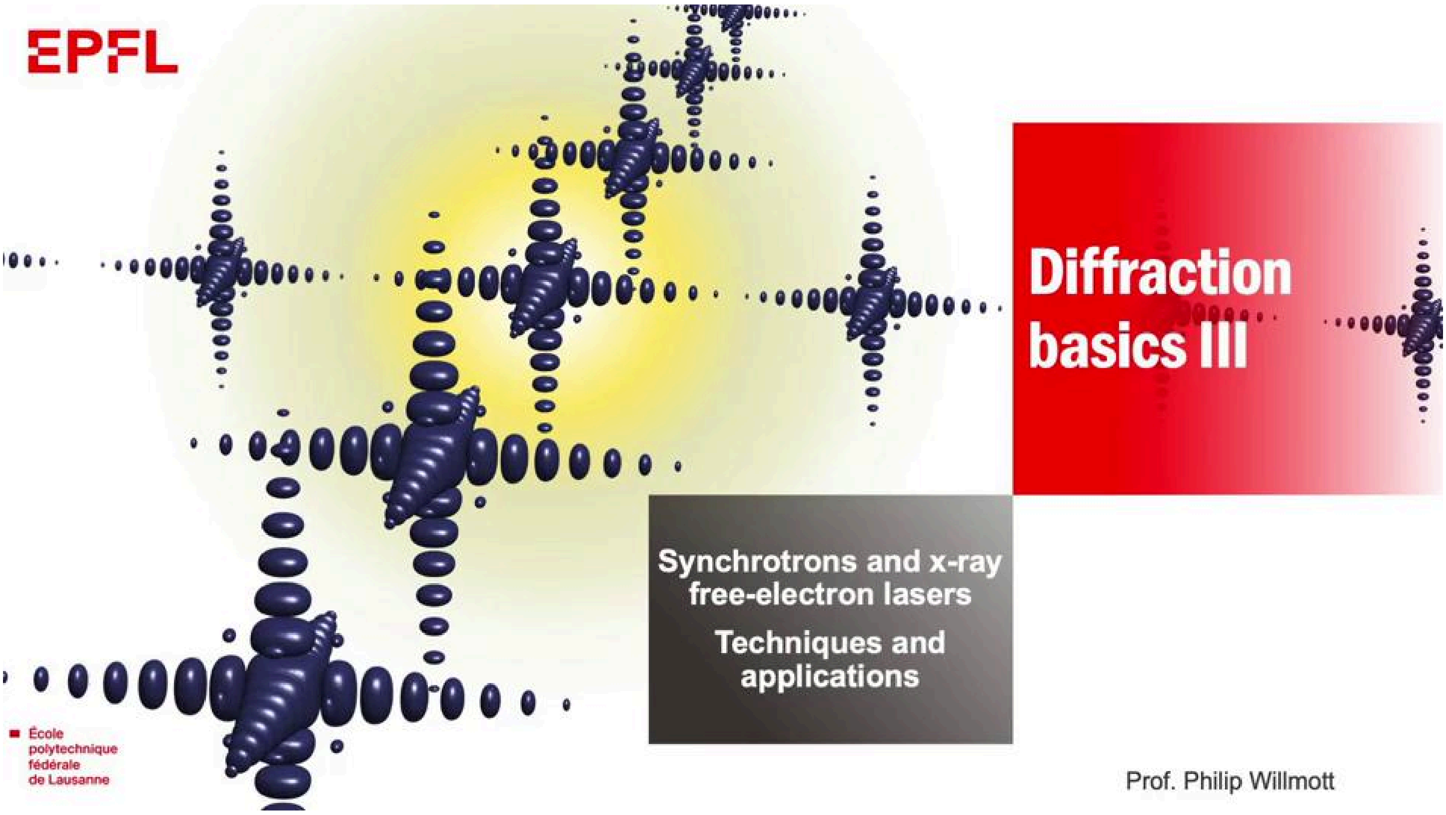

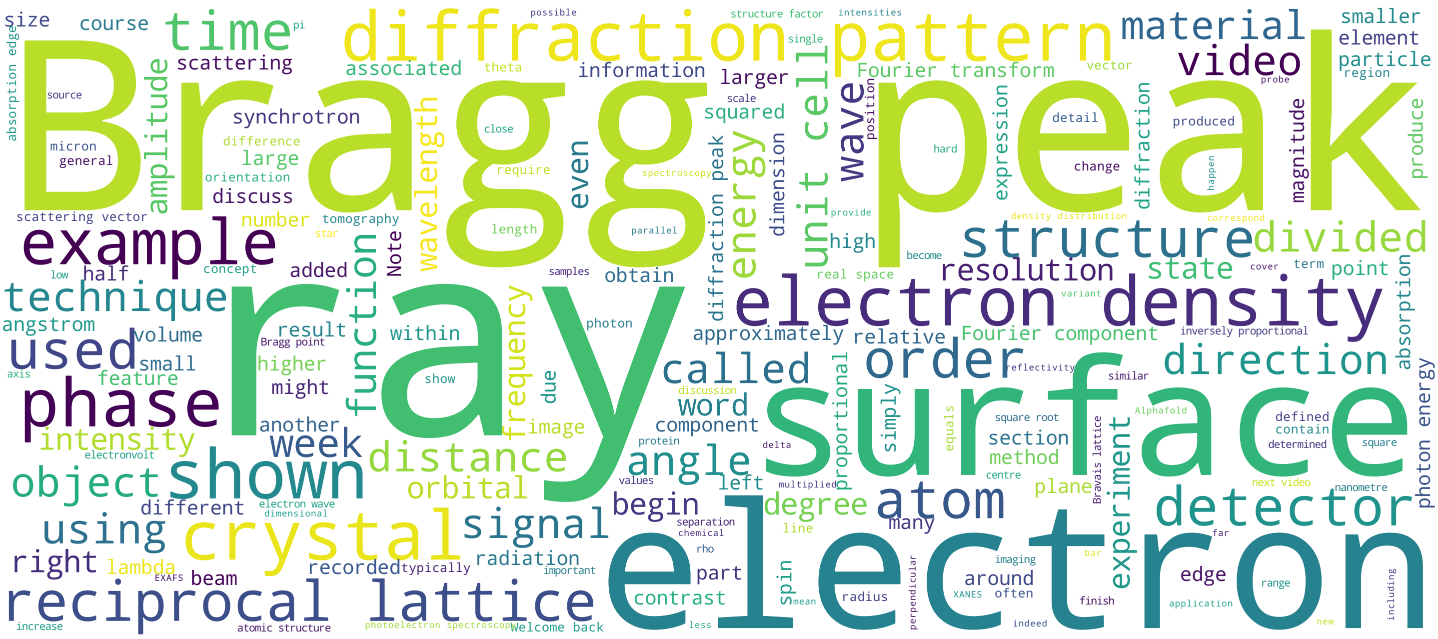

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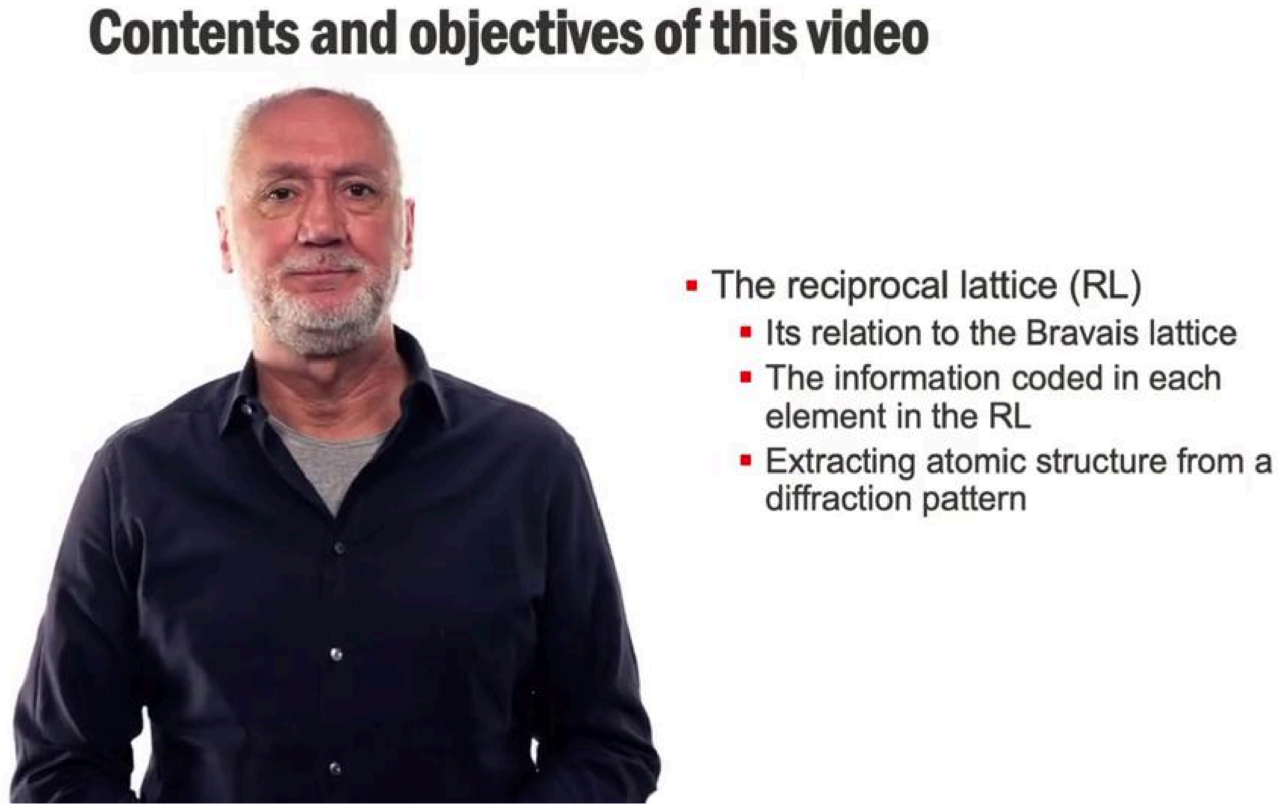
Video



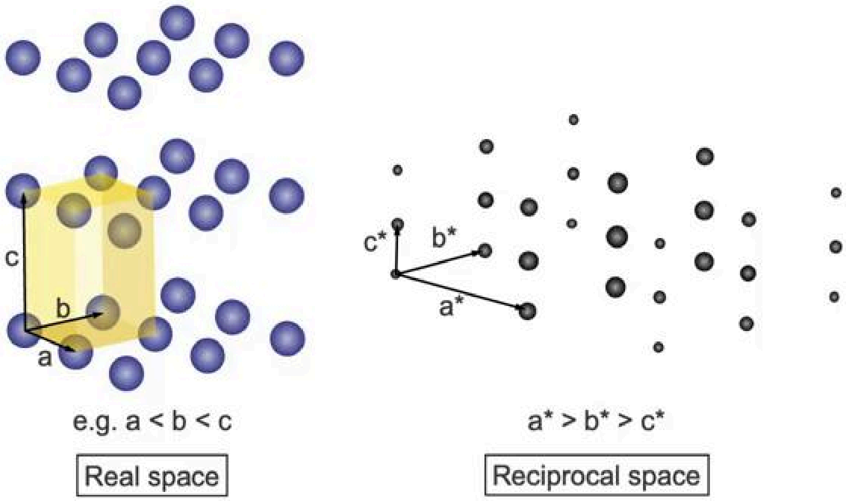
Welcome back. In this video, we will review the concept of the reciprocal lattice and its relationship to the Bravais lattice. Information is encoded in the reciprocal lattice, which we will see allows us to reconstruct the atomic structure within the crystal's unit cell that produced the diffraction pattern.

Notes

Summary

0m 05s

First thoughts about the reciprocal lattice



- The reciprocal lattice (RL) represents the framework and components of the diffraction pattern
  - A “reciprocal Bravais lattice” with regularly spaced peaks
  - Intensities associated with each point in RL are not the same (c.f. the basis associated with the Bravais lattice in real space)
  - The spacings between peaks in RL (a*, b*, c*) are inversely proportional to the corresponding dimensions in real space (a, b, c)
    - Why? RL is volume of *frequencies*
    - $\nu \propto 1/\lambda$
    - $m\lambda = 2d\sin\theta$
    - $\Rightarrow \nu \propto 1/d$

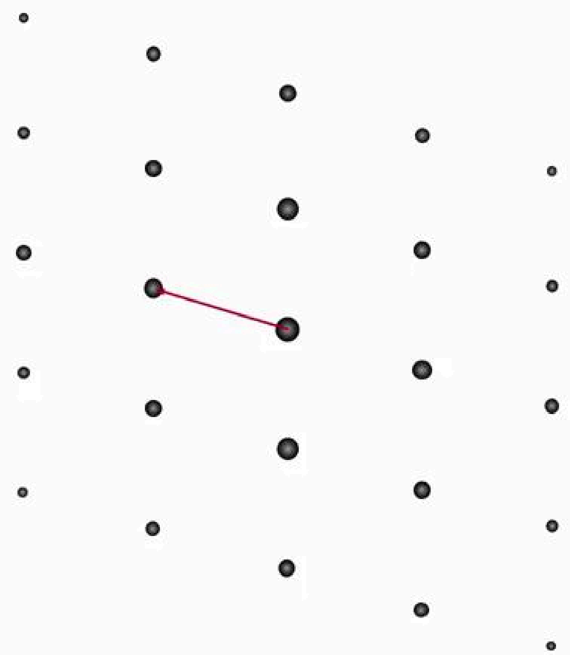
The reciprocal lattice consists of a set of evenly spaced diffraction peaks, each one corresponding to a unique set of scattering planes. In contrast to the mathematical construct of the Bravais lattice, which consists of evenly spaced delta functions or infinitely narrow points, the Bragg peaks in the reciprocal lattice have different intensities and are only infinitely narrow in the simplified model of an infinitely large and infinitely weak scattering crystal. The spacings between peaks in the reciprocal lattice denoted by a star, b star and c star are inversely proportional to their corresponding real space lattice constants a, b, and c. Now, why is this so? The reciprocal lattice is a volume of frequencies associated with waves. These are so-called Fourier components of the electron-density distribution within the crystal's unit cell, which, when added together, reproduce that electron distribution. Any given Bragg peak in the reciprocal lattice has a frequency that is inversely proportional to the wavelength. And thus the wavelength is proportional to the lattice spacing d, the frequency must be inversely proportional to d. Now let's unpack this rather confusing statement step by step.

Notes

Summary

0m 26s

First thoughts about the reciprocal lattice



- Remember: a diffraction pattern is the FT of the object that produces it
  - Each point in the RL is therefore a "Fourier component" of the diffraction pattern
  - The position of each point in the RL defines the frequency and direction of a sinusoidal wave of electron density
  - The intensity at each point defines the amplitude of the wave
  - The phase ϕ of that wave is fixed for that wave relative to all the other waves but cannot be measured directly

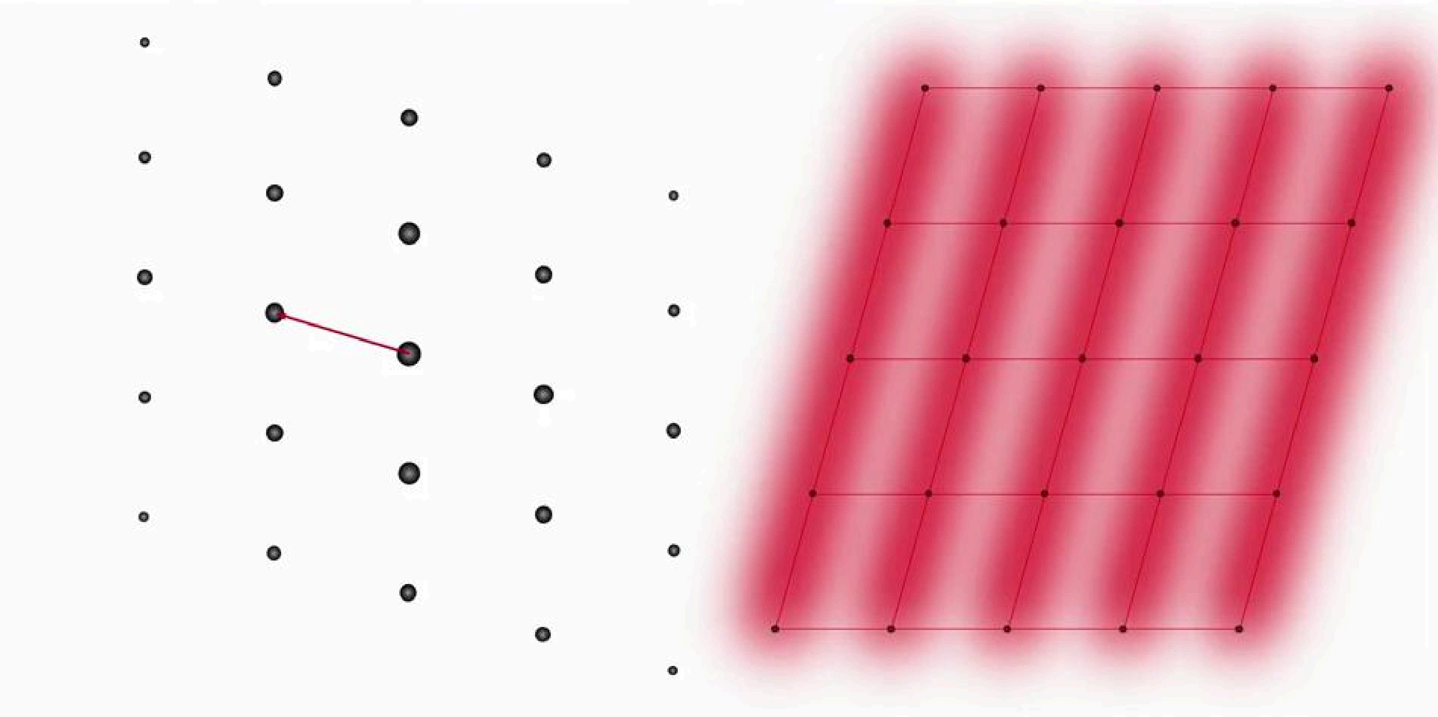
We begin by recognising that the diffraction pattern is the Fourier transform of the scattering object that produced it. This object being the electron cloud within the unit cell. Each point or Bragg peak in the reciprocal lattice is therefore a Fourier component of the diffraction pattern. Each Bragg peak defines the frequency and direction of a sinusoidal wave of electron density. Let's focus on a single Bragg peak. Let's say this one.

Notes

Summary

2m 02s

First thoughts about the reciprocal lattice



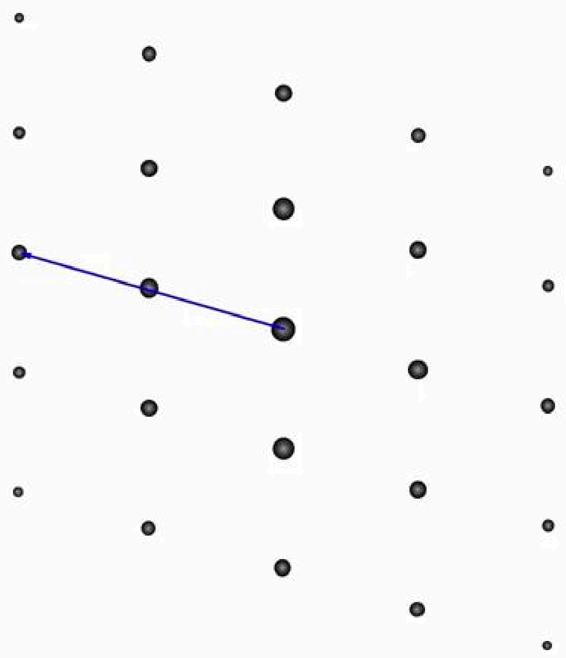
On the right is the real space Bravais lattice associated with the diffraction pattern on the left. The Bragg peak is one reciprocal lattice constant away from the centre of the diffraction pattern in the direction defined by the arrow. Hence this corresponds to a wave of electron density in the same direction and a periodicity equal to the separation of the crystal planes that are perpendicular to the arrow revealed here.

Notes

Summary

2m 40s

First thoughts about the reciprocal lattice



- Remember: a diffraction pattern is the FT of the object that produces it
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  - The intensity at each point defines the amplitude of the wave
  - The phase ϕ of that wave is fixed for that wave relative to all the other waves but cannot be measured directly

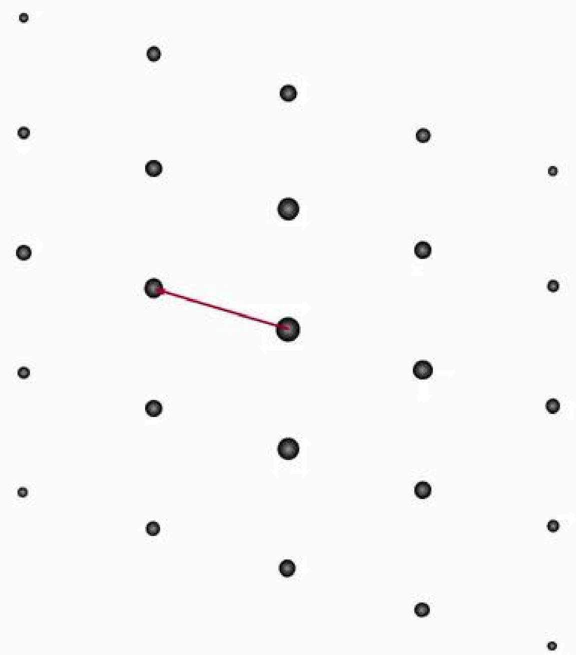
If we now consider this diffraction peak, which is in the same direction from the diffraction peak centre as the first one, but has twice the distance or length, the corresponding electron wave will have double the frequency shown here.

Notes

Summary

3m 14s

First thoughts about the reciprocal lattice



- Remember: a diffraction pattern is the FT of the object that produces it
  - Each point in the RL is therefore a “Fourier component” of the diffraction pattern
  - The position of each point in the RL defines the frequency and direction of a sinusoidal wave of electron density
  - The intensity at each point defines the amplitude of the wave
  - The phase ϕ of that wave is fixed for that wave relative to all the other waves but cannot be measured directly

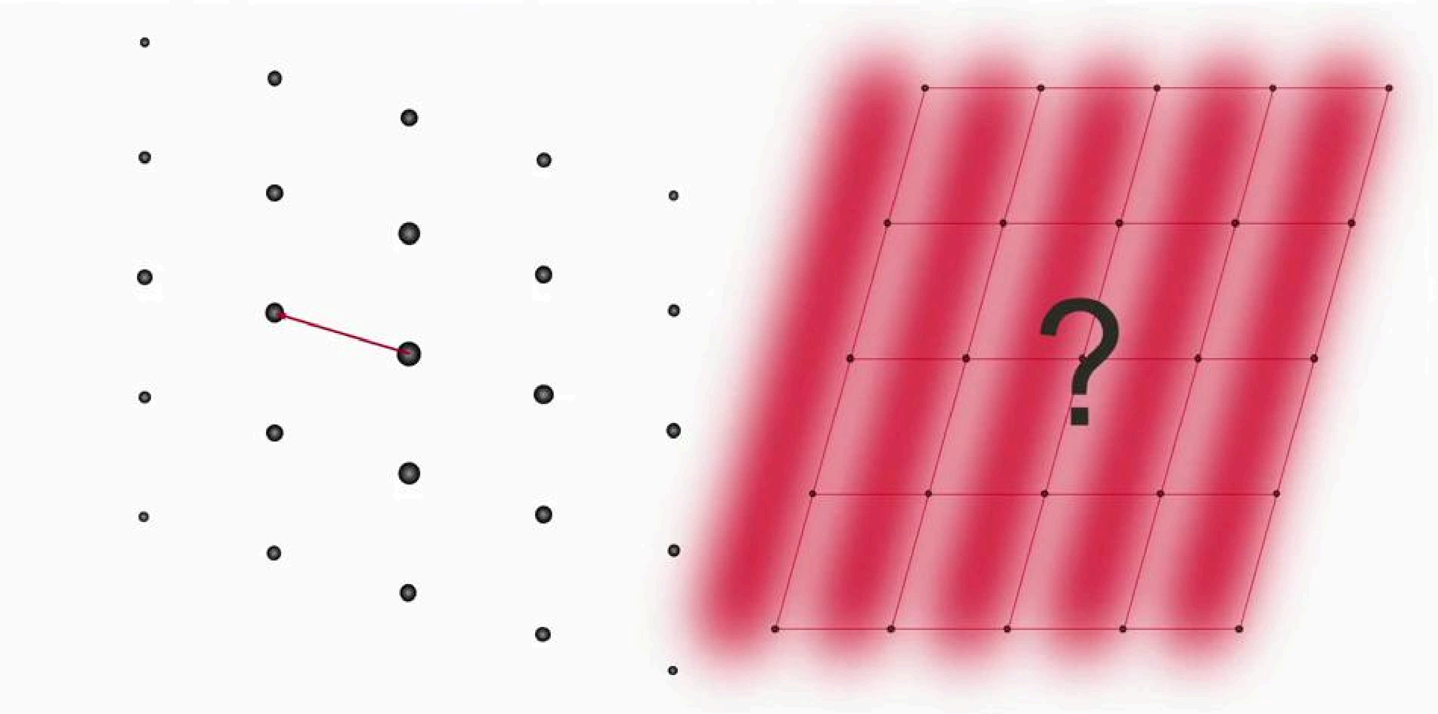
The intensity of each Bragg peak defines the amplitude of the associated sinusoidal electron wave. Precisely, the amplitude is proportional to the square root of the Bragg peak intensity illustrated schematically here. What remains missing in the definition of each Fourier component or wave is its phase. We don't know where the peaks and troughs lie within the unit cell.

Notes

Summary

3m 33s

First thoughts about the reciprocal lattice



This is the phase problem.

Notes

Summary

4m 05s

First thoughts about the reciprocal lattice

- So, what happens if you…
  - … take the information provided by each diffraction point in the RL
    - The direction (angle) of the wave relative to the origin of the RL
    - The frequency (given by the distance from origin of the RL, proportional to $1/\lambda$)
    - The amplitude of the wave, given by the square root of the intensity
  - … by some clever trick, work out the phase ϕ associated with each of these points (more on this later… MUCH more!!)
  - … draw the corresponding wave $W(A,\lambda,\phi)$ in real space
  - … and add them all together?

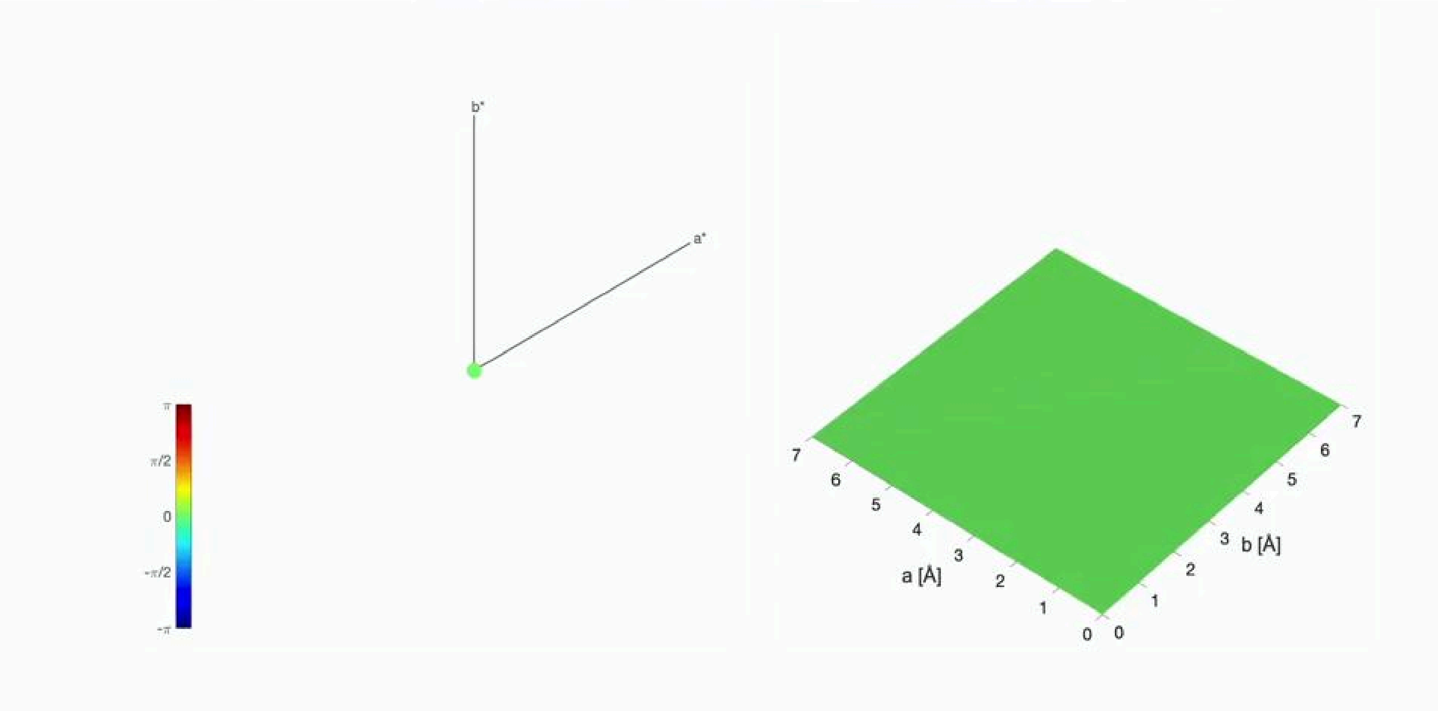
So what happens if you take the information provided by each diffraction point in the reciprocal lattice, The direction or angle of the wave relative to the origin of the reciprocal lattice, The frequency given by the distance from the origin of the reciprocal lattice proportional to one upon lambda, The amplitude of the wave given by the square root of the intensity, And by some clever trick, work out the phase fi associated with each of these points? Then draw the corresponding wave w as a function of a, lambda and phi in real space and add them all together.

Notes

Summary

4m 07s

First thoughts about the reciprocal lattice



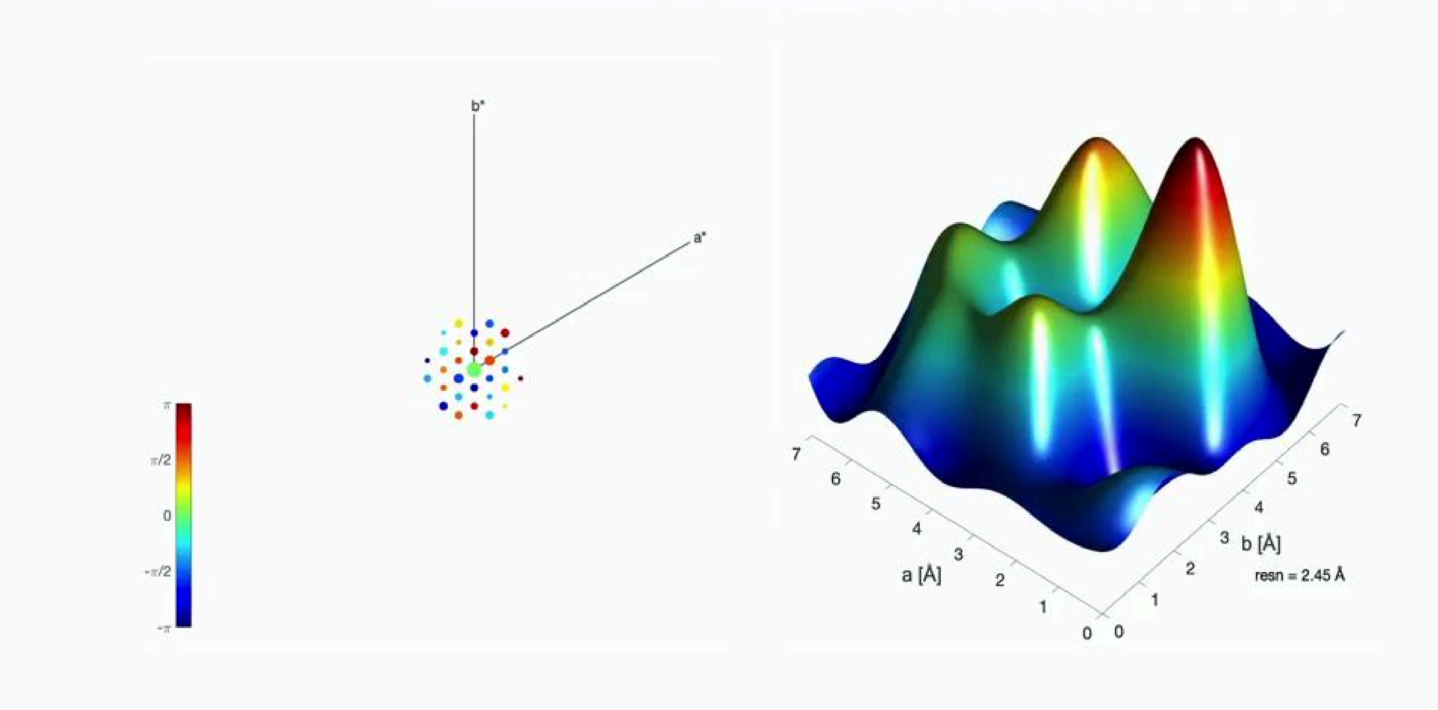
Well, if you've been following the argument thus far, you will guess that what happens is that the electron density within the unit cell will be generated. In other words, the atomic structure will come out. In this animation, we show this for a planar molecule with a crystal that has two lattice parameters, 120 degrees relative to one another. The diffraction pattern thus contains only Bragg points in two dimensions. On the left, we show the Bragg points as they are added one by one, each one representing a wave. The radius of each Bragg point corresponds to the amplitude of the corresponding wave. Its distance from the origin indicates the frequency, while the colour indicates the phase of the wave. The waves are added up in two dimensional space on the right. We begin with the central diffraction spot. This is no distance from the centre and therefore has zero frequency, or in other words, it has an infinitely large wavelength and is therefore simply a constant.

Notes

Summary

4m 55s

First thoughts about the reciprocal lattice



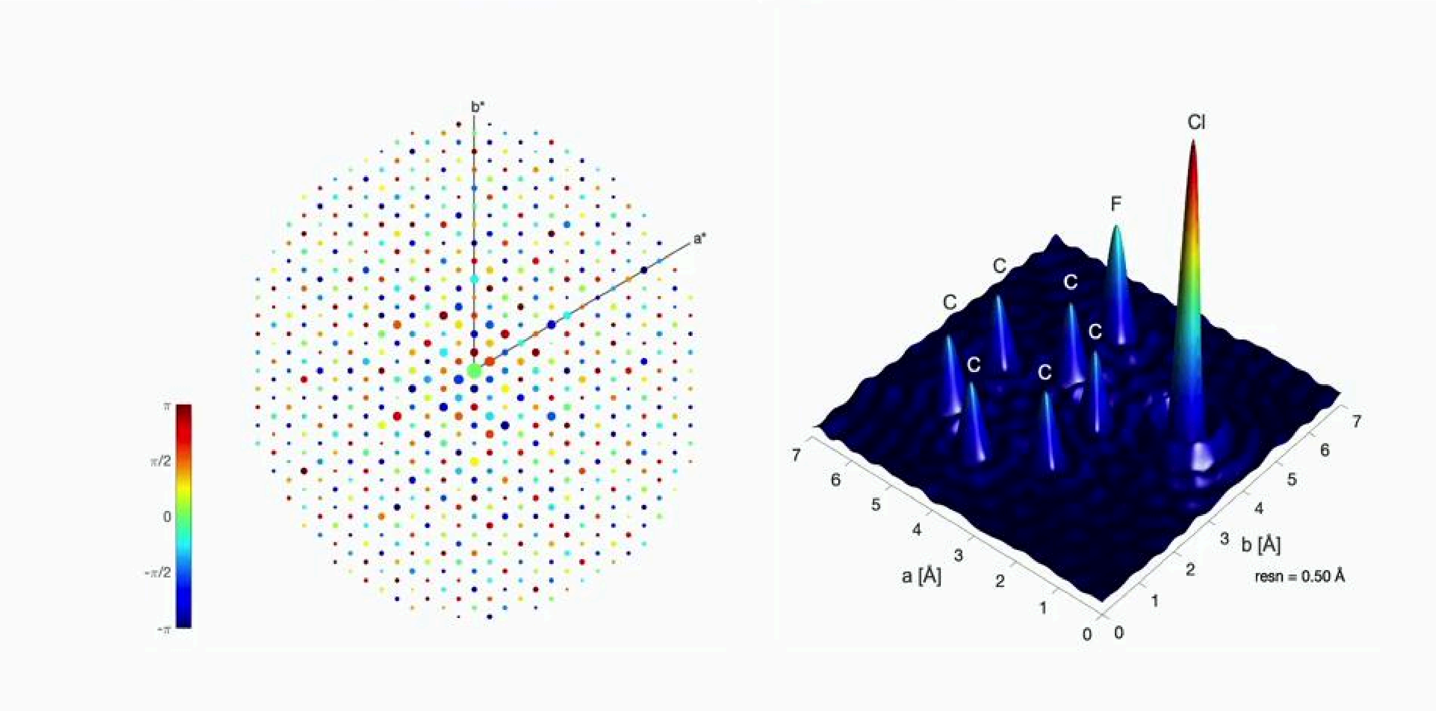
We now add Fourier components one after the other with ever increasing distance from the diffraction pattern origin, in other words, with ever increasing scattering vector Q and electron wave frequency.

Notes

Summary

6m 15s

First thoughts about the reciprocal lattice



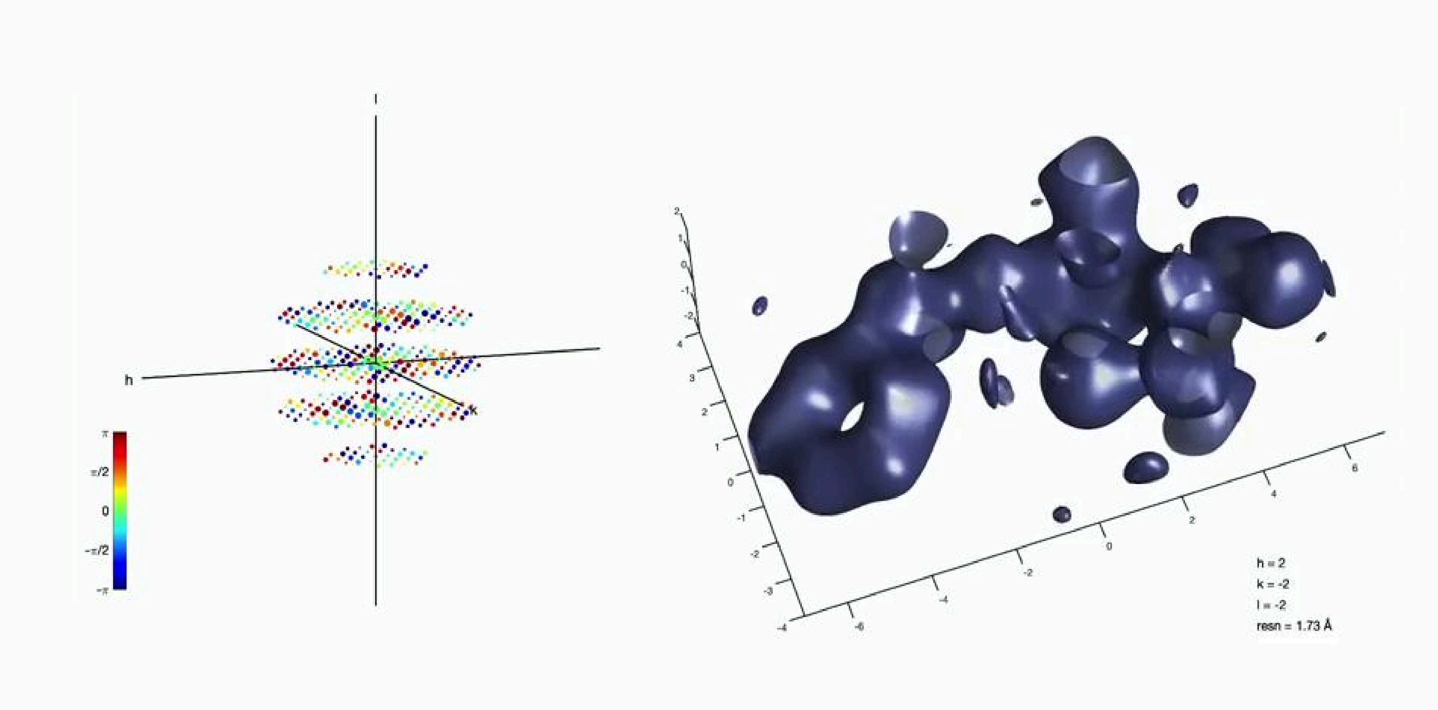
As Bragg peaks are added that are further away from the diffraction origin, more and more detail emerges as we are adding sine waves with increasing frequency or in other words, decreasing wavelength. This defines the resolution at any one moment in the reconstruction of the electron density. Don't make the common mistake of thinking that these wavelengths are the wavelengths of the x-rays, that is the lambda used in the Bragg equation. No, these are the wavelengths associated with the sine waves of the Fourier components of the electron density distribution or Bragg peaks of the diffraction pattern. We continued adding these components until we obtain a resolution of 0.5 angstroms. This corresponds to Bragg peaks that have scattering vectors Q, that are 2 pi divided by 0.5, which is approximately equal to 12.5 reciprocal angstroms in magnitude. The final electron density distribution consists of a hexagonal carbon ring and two heavier atoms, one being fluorine, the other chlorine.

Notes

Summary

6m 34s

... and in 3D



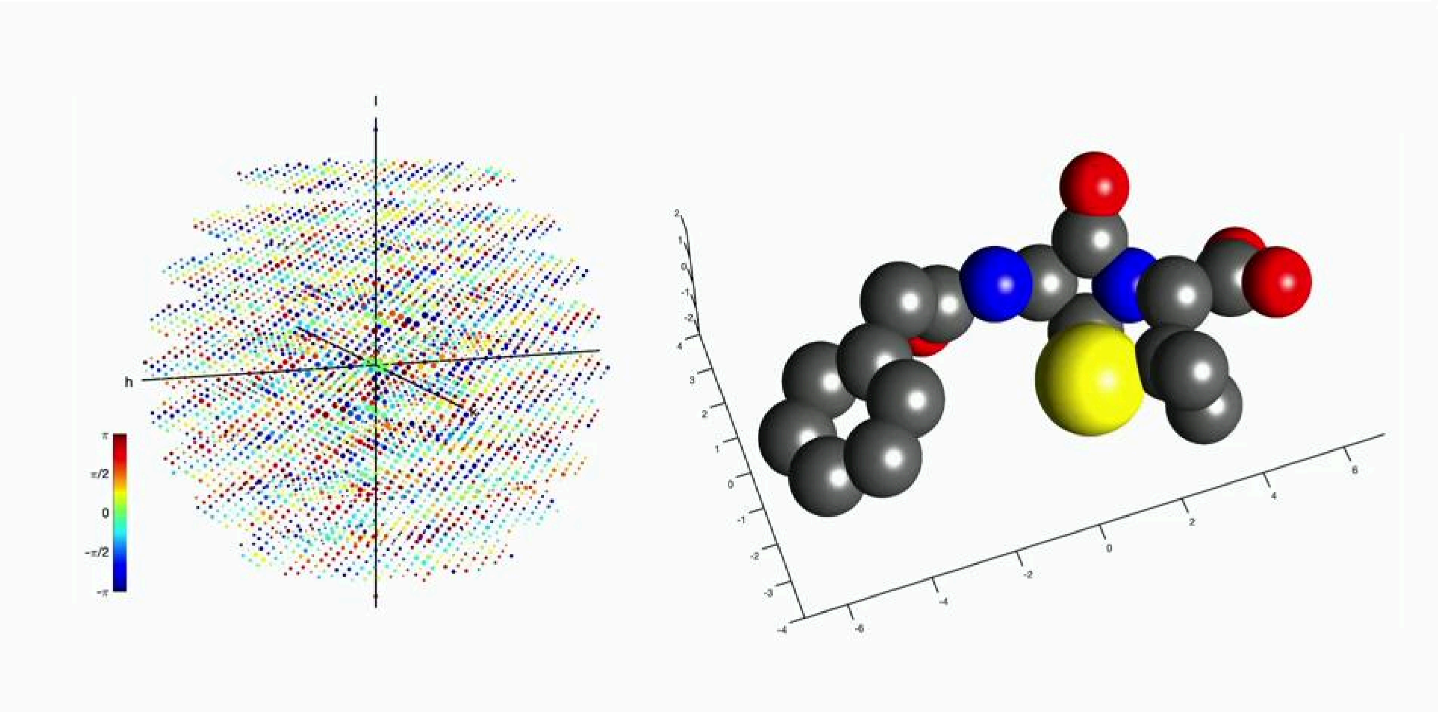
Now just to demonstrate the beauty of diffraction patterns and the information they contain, I now show another example in three dimensions. Here on the right, the electron density is represented by isosurfaces, that is, surfaces of equal electron density. Note that the first few diffraction peaks that are added are all in the hk plane on the left, meaning that to begin with there is no variation of electron density in the vertical direction.

Notes

Summary

7m 47s

... and in 3D



Only when Fourier components are added that lie above or below the hk plane, does the electron density begin to show features in the vertical direction. The final electron density is of benzyl penicillin, the structure of which was determined by Dorothy Crowfoot Hodgkin in 1945, in a scientific tour de force which would reveal the mechanism by which penicillin destroyed bacteria.

Notes

Summary

8m 20s

In the last video of this section, we will be introduced to the Ewald sphere, the mathematical construct based on the Bragg law, which helps us understand how to record diffraction data.

Notes

Summary

8m 51s