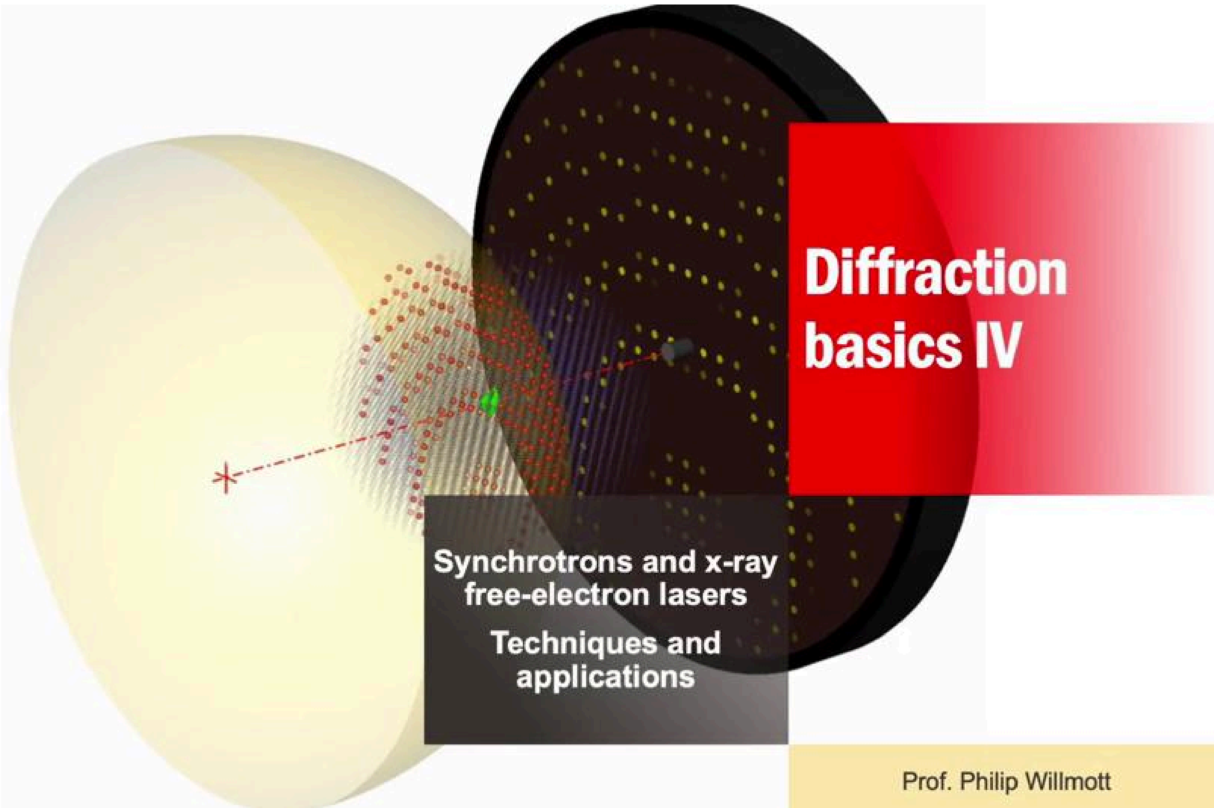
EPFL



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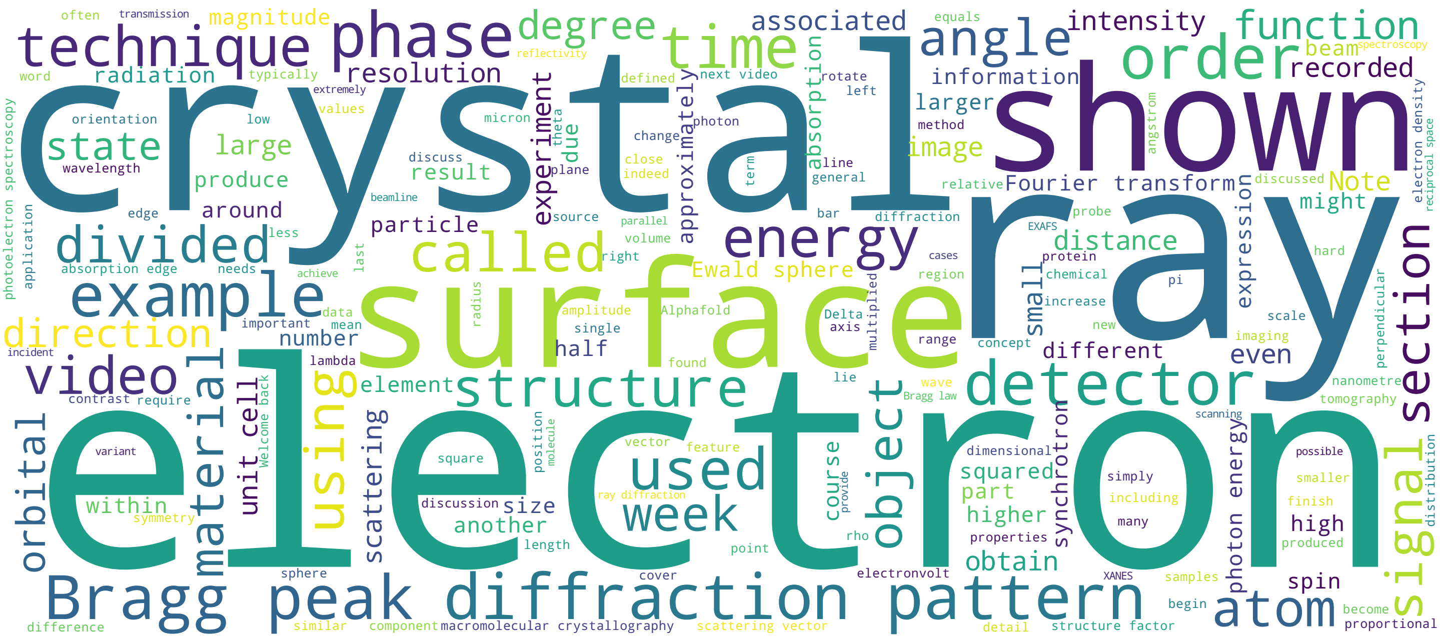

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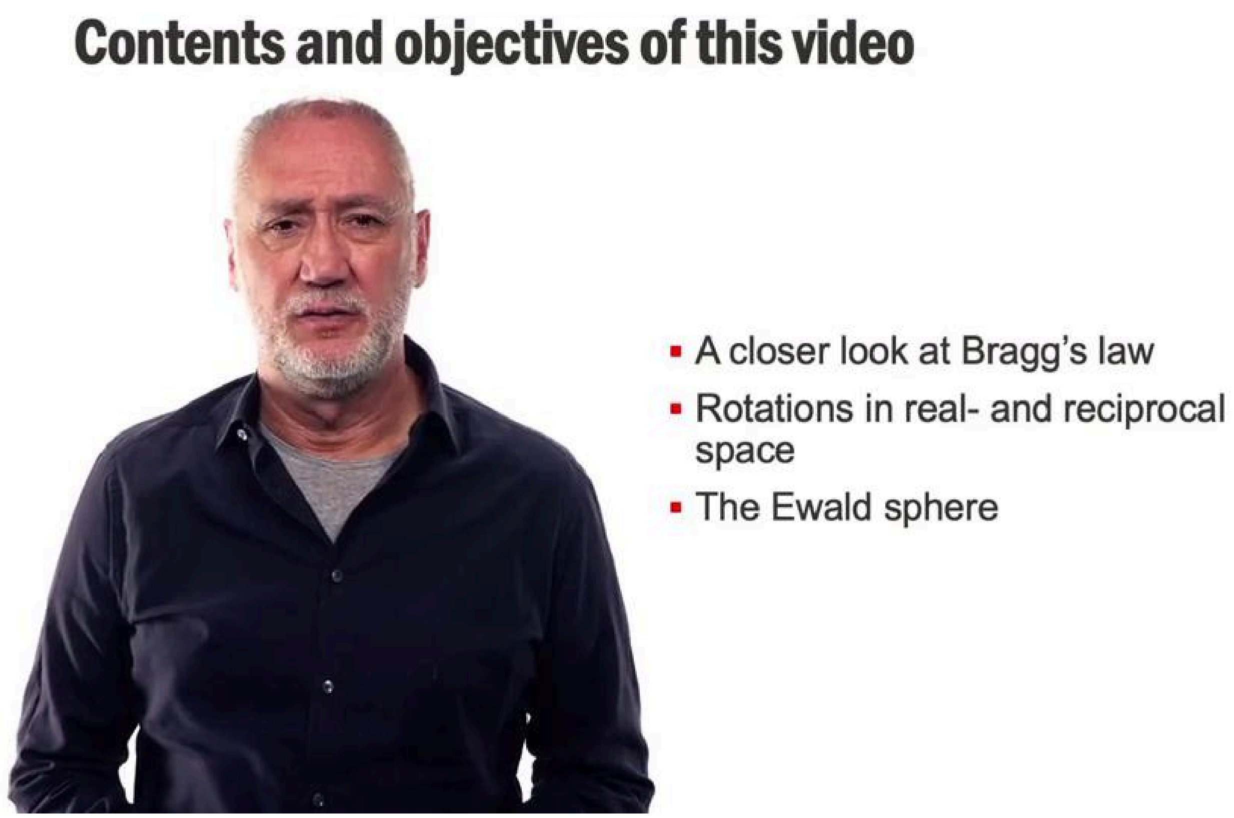
EPFL



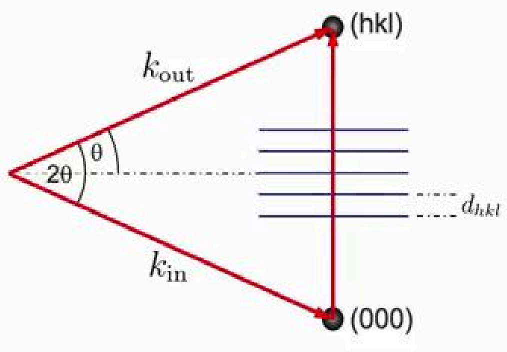
Hello again. In this last video of this section, we will take a closer look at Bragg's law 3 00:00:11,240 --> 00:00:13,229 and what its geometry implies, which will lead us to the concept of the Ewald sphere, a useful mathematical construct for determining the conditions required to record diffraction patterns.

Notes

Summary

0m 05s

Bragg's law in a bit more detail



- Incident wavevector k_{in} points to (000): "direct beam"
- Scattered wavevector k_{out} points to (hkl) Bragg peak
- Q has magnitude $2\pi/d_{hkl}$
- Remember: Q is perpendicular to (hkl) scattering planes
  - Rotate crystal until this condition is met

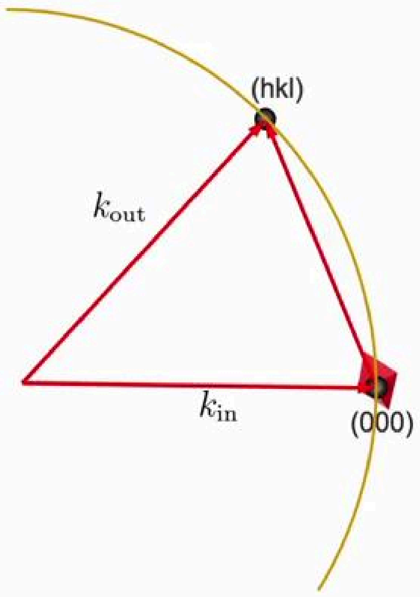
We now return to our graphical representation for X-ray diffraction, whereby the incident wavevector k_{in} points in the direction of the incident X-ray beam, and the scattered wavevector k_{out} points to a Bragg peak, defined by the crystal planes with Miller indices h, k, and l. The vectorial difference between the two is the scattering vector Q, which we have already determined to have a magnitude equal to 2 pi divided by d_{hkl}, whereby d_{hkl} is the interplanar distance of the hkl planes. Remember that Q is perpendicular to the hkl scattering planes. To achieve the Bragg condition, the crystal must be oriented so that this is satisfied.

Notes

Summary

0m 23s

The Ewald sphere



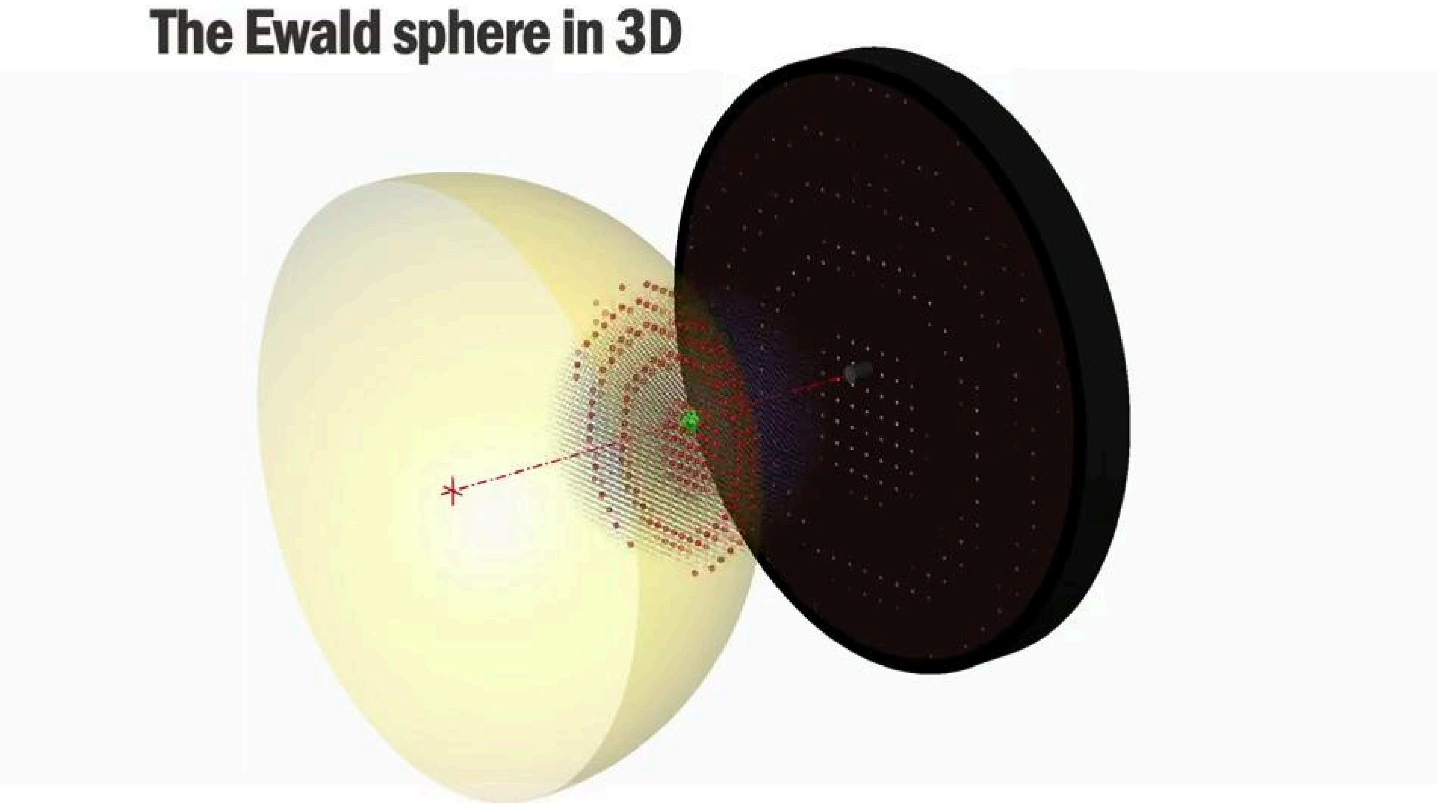
- To see a diffraction peak @ (hkl), the Bragg points (000) and (hkl) must lie on a sphere of radius |k| in reciprocal space (RS)
- To achieve this "Bragg condition", rotate the crystal appropriately

It's hopefully clear that if one rotates a crystal, its diffraction pattern rotates with it. If one thinks just briefly about this, it would be remarkable if this were not the case. Just by tilting your head would cause a diffraction pattern to rotate relative to the crystal, which is patently absurd. Hence, because k_{in} and k_{out} have the same magnitude, in order to see a diffraction spot, the 000 central spot, or direct beam, and the hkl Bragg peak must both lie on a sphere of radius k in reciprocal space. This sphere is called the Ewald sphere. One needs to rotate the crystal appropriately to achieve this so-called Bragg condition.

Notes

Summary

1m 16s



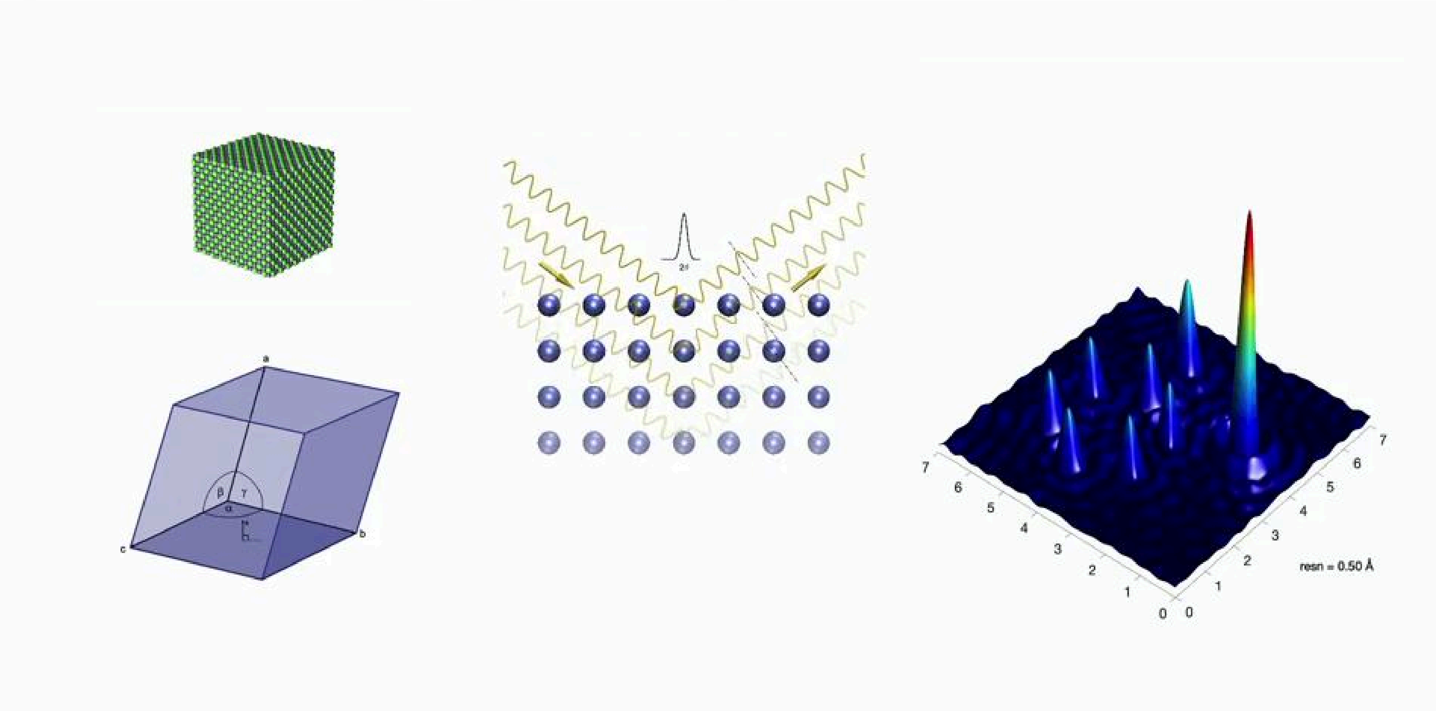
How would this look like on a detector if one rotates a crystal around an axis parallel to the detector plane? We see in this animation that at the beginning, the -1,5 Bragg peak of the two-dimensional diffraction pattern sits almost perfectly on the Ewald sphere. We now rotate the crystal. Every time a Bragg peak passes through the surface of the Ewald sphere, a diffraction spot will light up on the detector. Depending on the symmetry of the crystal, a full diffraction pattern will be recorded after rotating the crystal through a full circle. This animation shows the diffraction pattern as a function of crystal rotation. For those of you familiar with macromolecular crystallography, the progress of the diffraction signal on the detector will be a recognisable and familiar motif.

Notes

Summary

2m 09s

Summary of this section



To summarise this section, we just discussed the properties of crystals and how they are characterised. We were introduced to Bragg's law, and saw how the information encoded in diffraction patterns can allow us to reconstruct the crystalline scattering object that produced it. Lastly, we found out how the geometrical configuration required to obtain a Bragg peak can be understood using the construct of the Ewald sphere.

Notes

Summary

3m 13s

In the next section, we will look more closely at the so-called structure factor, composed of the vector addition of scattering from individual atoms within the unit cell. This prepares us for a discussion about the phase problem in crystallography and how this can be resolved in general, and in particular, the approaches used until very recently in macromolecular crystallography. We finish the next section with a very brief overview of AlphaFold2, a machine learning algorithm presented for the first time in late 2020, which appears to have resolved the phase problem for the large majority of cases in macromolecular crystallography.

Notes

Summary

3m 43s