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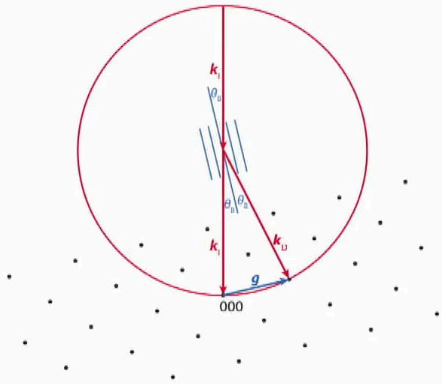

Basics of electron diffraction: the Ewald sphere

Transmission Electron Microscopy

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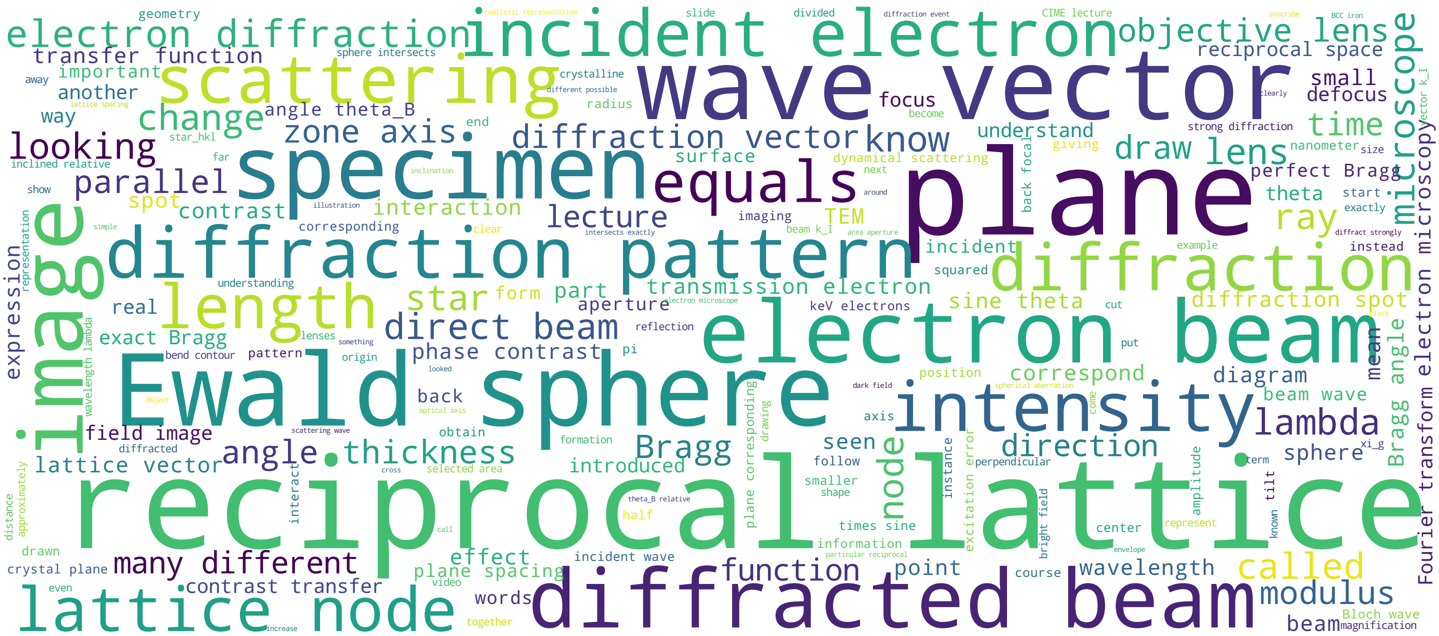

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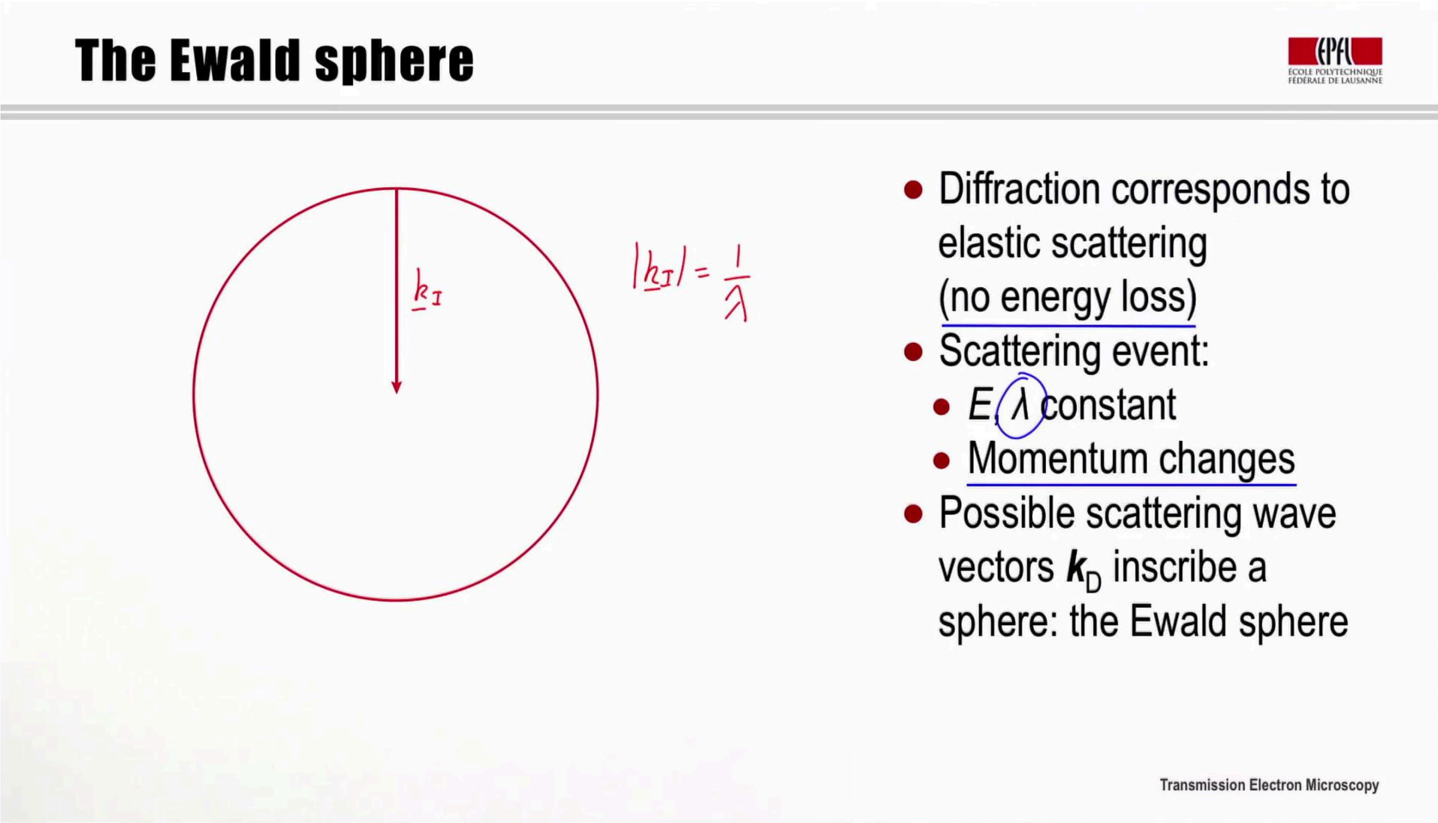
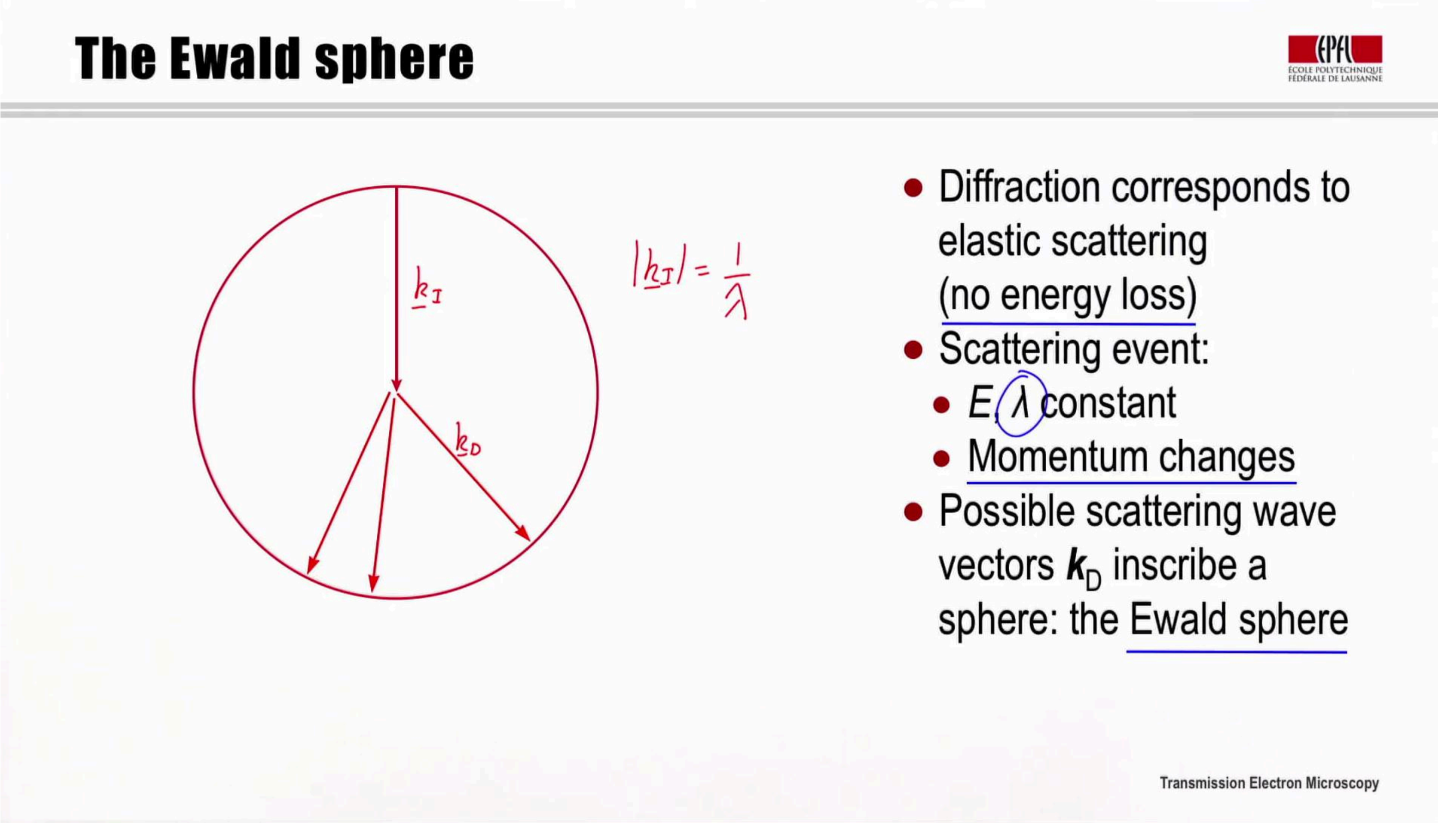


Welcome to CIME's lectures on transmission electron microscopy and the lecture on the Ewald sphere. In the last lecture, I introduced the concept of the reciprocal lattice: a lattice of nodes in reciprocal space, where each node corresponds to a possible diffraction vector from a plane with Miller indices (h k l). This reciprocal lattice forms the first half of our framework for understanding and interpreting electron diffraction. In this lecture, I'm going to introduce the second half of the framework, namely, the Ewald sphere. To understand the Ewald sphere, we are going to consider that electron diffraction corresponds to elastic scattering. The incident electron beam is diffracted by the Coulomb field of the sample and during this diffraction event, there is no energy loss. Therefore, at this scattering event, the energy of the electron beam, and hence its wavelength, both remain constant. However, as we have already seen, there is a momentum change during diffraction. We can describe this on a wave vector diagram. So here, I have a wave vector for the incident electron beam: k_I, where, as we have previously seen, the length of k_I – its modulus – equals one over lambda; the wavelength of the electron beam.

Notes

Summary

0m 05s

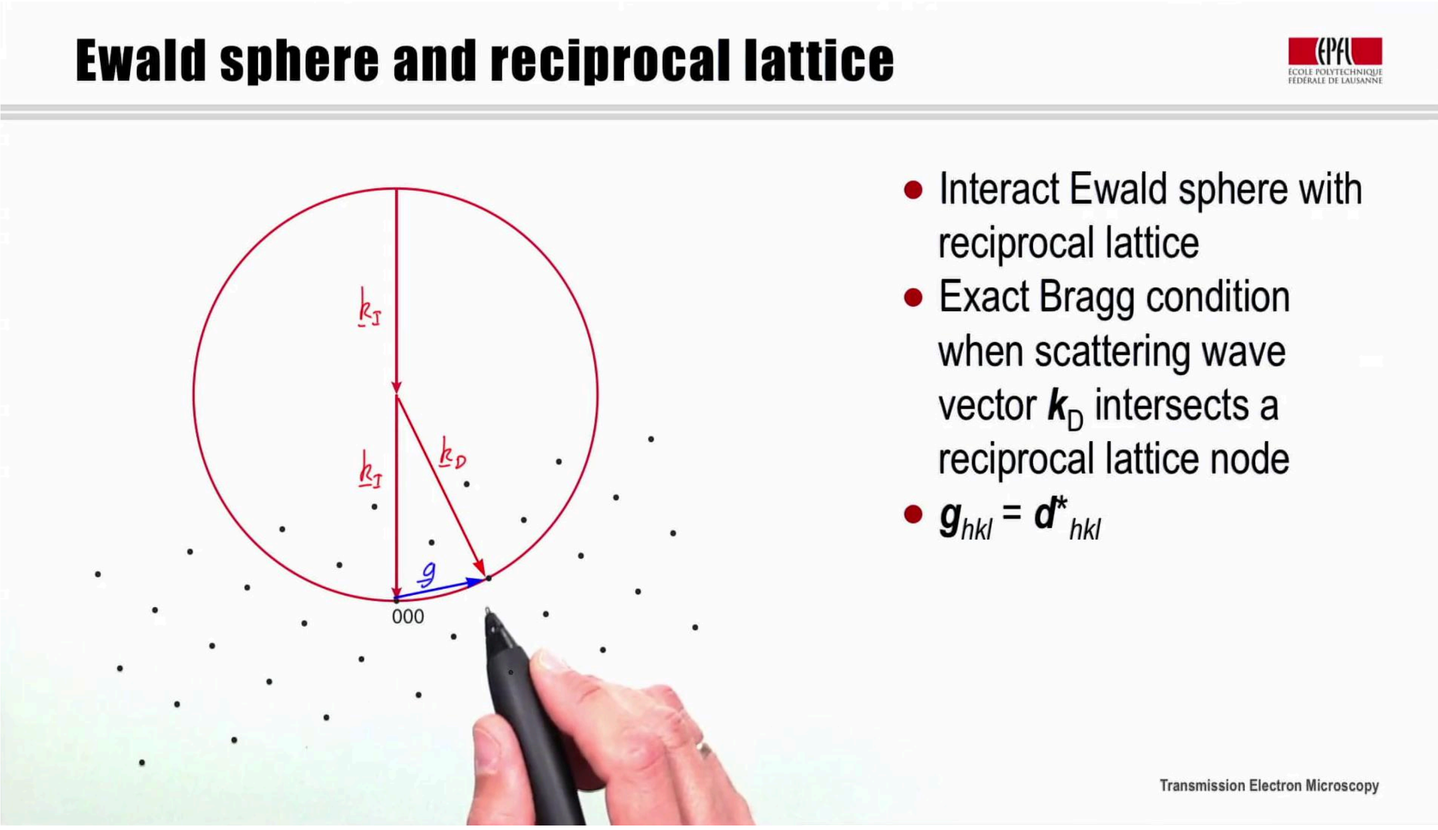


I'm going to say that here, I have some diffraction event. Now the scattering from this event could occur in one of many different directions. So, for instance, we could have a diffracted wave vector here. Equally, we could have diffraction in this direction, or this direction, or one of many different possible directions. Now, while the angle of scattering may change, of course the length of these diffracted beam wave vectors cannot change. They all have the same length as that of the incident electron beam: one over lambda. So, looking just at this plane of scattering, we can see that all these different possible scattering wave vectors will inscribe a circle. That is just looking at one plane. However, we could also have diffraction out of plane. And if you consider the out of plane scattering wave vectors, we can see that, together, they will inscribe a sphere. And this sphere of possible diffracted beam wave vectors is called the Ewald sphere. Since the radius of the Ewald sphere has a length of one over lambda, we can see that the Ewald sphere has reciprocal dimensions. And we are now going to interact this sphere with the reciprocal lattice.

Notes

Summary

1m 35s

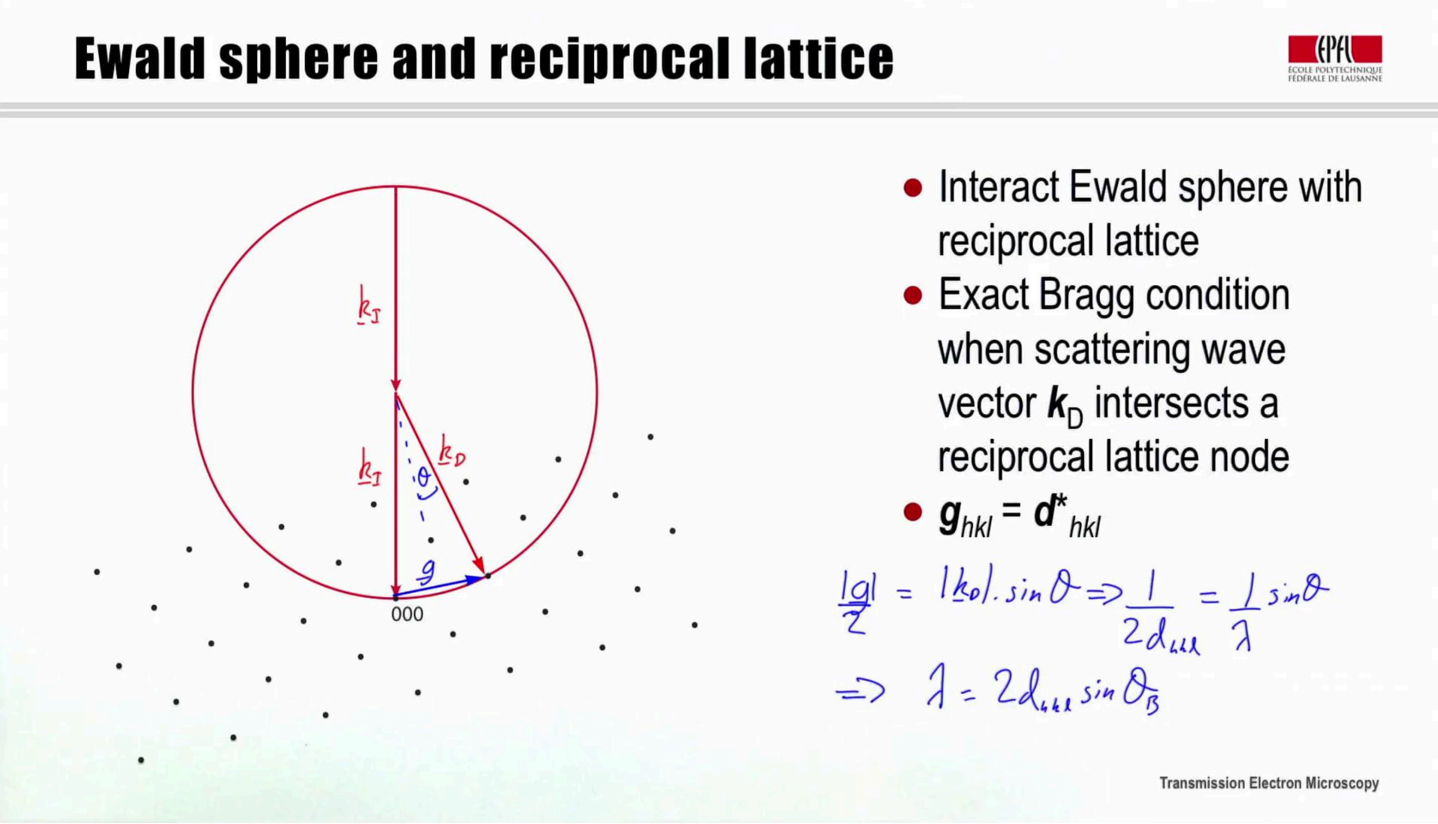


To look at this interaction, on this slide I have drawn both the Ewald sphere and a reciprocal lattice. Looking first at the Ewald sphere, again, here we have the wave vector for the incident electron beam, k_I. If there is no interaction – if there is no scattering – then that wave vector carries straight on, here. We know that, in the back focal or or diffraction plane, that the incident electron beam gives the direct beam in the diffraction pattern: 0 0 0. 0 0 0 also forms the origin of this reciprocal lattice. So, I have also placed this origin at the end of the wave vector for this incident electron beam. Now, if we look at the interaction of the Ewald sphere with the reciprocal lattice, we can see that, here, there is a node in the reciprocal lattice that is intersected exactly by the surface of this Ewald sphere. Now, for this node, we can draw in a wave vector for the diffracted beam: k_D. And, since I am saying that this is the wave vector for the diffracted beam, I can also draw in here the diffraction vector, g, for this particular reciprocal lattice node. Now, we are going to look at the geometry of this scattering for that particular reciprocal lattice node.

Notes

Summary

3m 13s



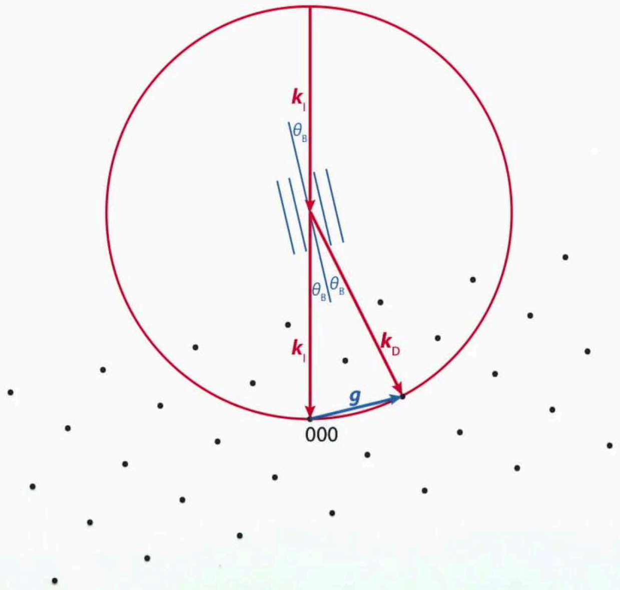
First of all, we are going to look at the angle of scattering, and I will say that the semi-angle of scattering is theta. From this diagram, and by trigonometry, it is clear that the modulus of g, the diffraction vector, divided by two equals the modulus of k_D times sine theta. Now we know that g, the diffraction vector, equals d-star_hkl. Therefore, the modulus of g = the modulus of d-star = one over d. So, you can see that this becomes: 1 over 2 d_hkl = (the length of k_D = 1 over lambda) times sine theta. And this expression should look very familiar to you, because, if we rearrange it, we obtain: lambda = 2 d_hkl sine theta. In other words, we have obtained the Bragg equation, where theta = theta_B, the Bragg angle. Thus, we see that, when the Ewald sphere intersects exactly through a reciprocal lattice node, the plane corresponding to that reciprocal lattice node is at the exact Bragg condition, and so will diffract strongly.

Notes

Summary

4m 42s

Ewald sphere and reciprocal lattice



- Exact Bragg condition when scattering wave vector $\boldsymbol{k}_D$ intersects a reciprocal lattice node
- $\boldsymbol{g}_{hkl} = \boldsymbol{d}^*_{hkl}$

$\lambda \ll d_{hkl}$

$|\underline{k}| \gg d^*_{hkl}$

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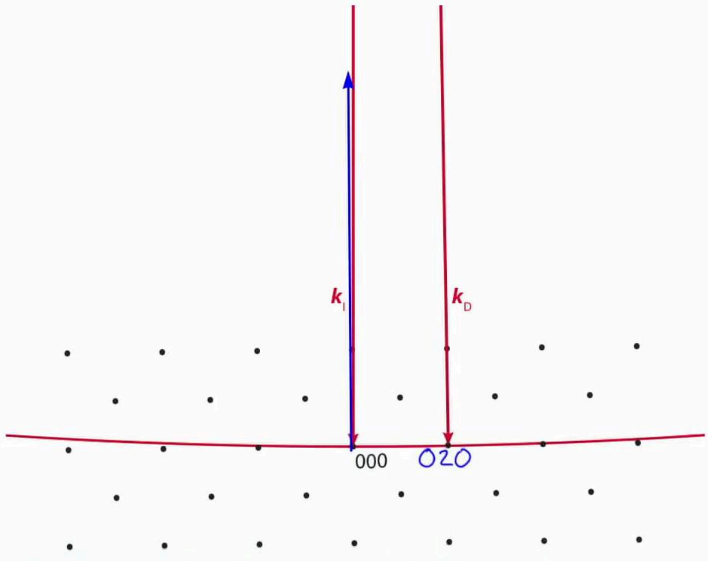
Cleaning up that diagram, we can represent this scattering as follows. So we have the incident wave vector k_I. Here, I have drawn in some Bragg planes at the angle theta_B relative to k_I, scattering at the Bragg angle, leading to diffraction for a plane corresponding to that reciprocal lattice node. Now in this representation, I have had to make an exaggeration to make the representation compact. Specifically, we know that the electron wavelength, lambda, is much smaller than the typical plane spacing d_hkl. Because of that, the length of this wave vector k is going to be much greater than the typical reciprocal lattice spacing, d-star_hkl. So the radius of this sphere for a realistic representation must be much, much greater.

Notes

Summary

6m 15s

Realistic representation of Ewald sphere



- $\lambda \ll d_{hkl}$
  Therefore Ewald sphere almost flat
- Illustration:
  200 keV e^-
  BCC α-Fe
- Crystal and plane still inclined to e^--beam

$\lambda \approx 2.5\,pm$
$d_{020} \approx 0.14\,nm$
$|k| \approx 50\,d^*$

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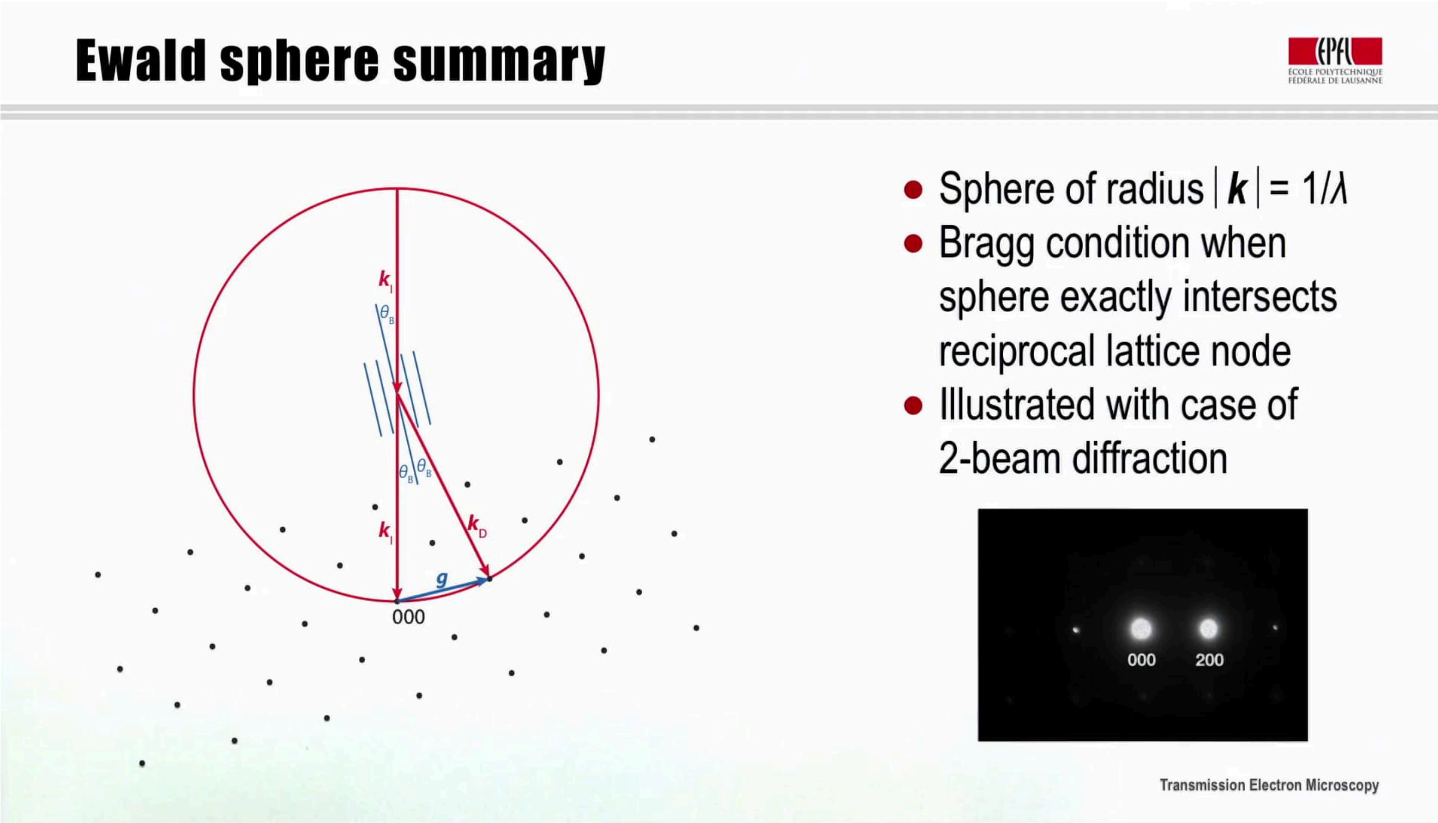
Moving on with that, I make that realistic representation of the Ewald sphere and the reciprocal lattice in this diagram here. Here we have the incident wave vector k_I, the diffracted beam wave vector k_D, and I have drawn them assuming that we have 200 keV electrons. For 200 keV electrons, the wavelength lambda is approximately equal to 2.5 picometers. To complete the illustration, I have taken a reciprocal lattice for the body-centered cubic phase of iron. This particular node here is once again at the Bragg angle and this node is for the (0 2 0) plane. And for BCC iron, d_020 is approximately equal to 0.14 nanometers. The net result is that the length of k, the wave vector, is approximately 50 times greater than the reciprocal lattice spacing, d-star. When we draw that in with this very long radius, we can see that the surface of the Ewald sphere is almost flat. And while this reciprocal lattice is still inclined relative to the incident electron beam, the angle of that inclination is very, very small. As an exercise, you can calculate that angle of inclination, and the Bragg angle of theta_B, and the scattering angle 2 theta_B, for this case of 200 keV electrons and BCC iron, when exciting this 0 2 0 reciprocal lattice node.

Notes

Summary

7m 25s



To summarize, I have introduced the Ewald sphere: a sphere in reciprocal space with a radius of k = one over lambda. And we have seen that when we interact this sphere with the reciprocal lattice, and when the surface of that sphere intersects exactly through the middle of a reciprocal lattice node, the plane corresponding to that node is at the exact Bragg condition, and so will diffract strongly. So far, we have only looked at this in the case of two-beam electron diffraction, where only one of the reciprocal lattice nodes is intersected by the Ewald sphere, and hence we only have strong diffraction on one plane. Giving a diffraction pattern such as this, where, in this case, the (2 0 0) plane is excited strongly, giving an intense diffraction spot. In this case, that plane is inclined at an angle theta_B relative to the incident electron beam. However, in electron diffraction, we can have another scenario, where instead of the incident electron beam being inclined relative to a particular crystal plane, it is in fact parallel to many different crystal planes at the same time, with the e beam aligned on a low index zone axis of the crystalline sample. And in this case, we obtain strong diffraction on many different planes, giving a diffraction pattern with many bright spots: so-called multi-beam electron diffraction. And that is what we will look at in the next lecture.

Notes

Summary

9m 11s