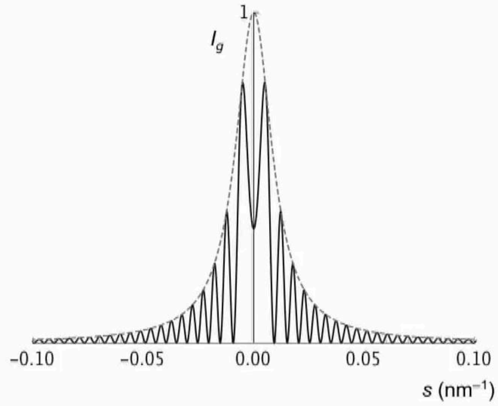
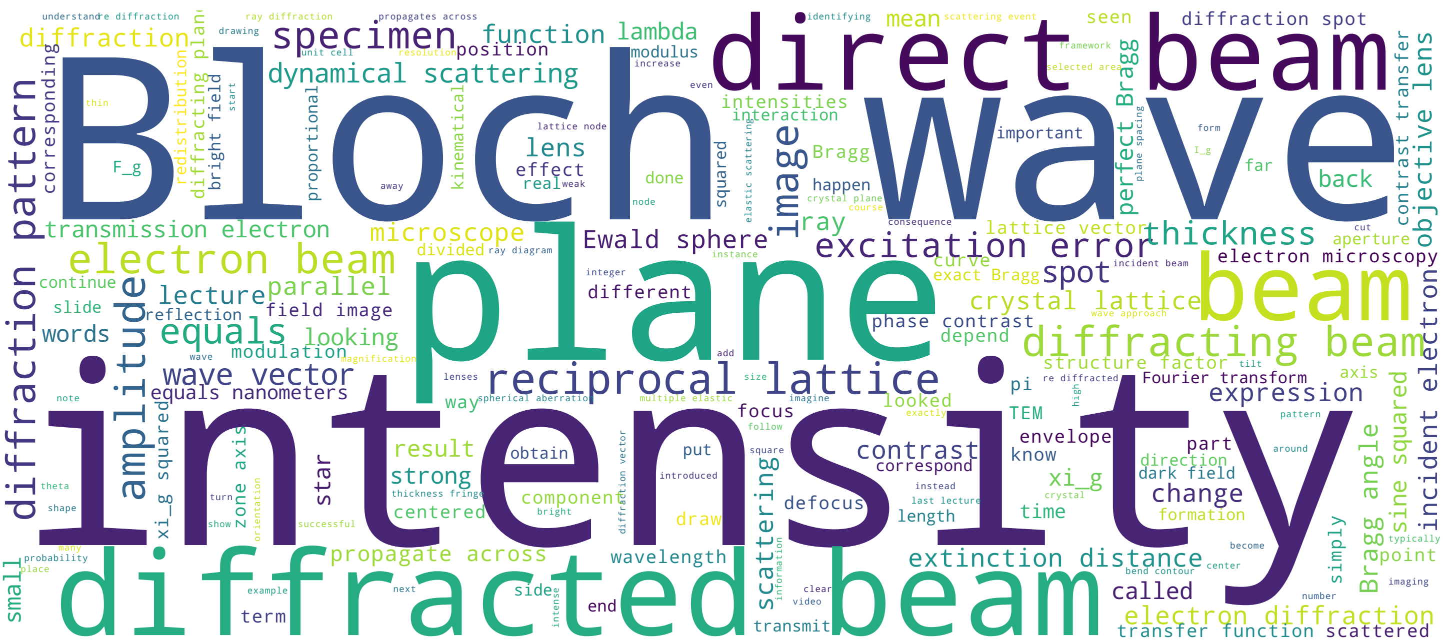


Dynamical scattering

Transmission Electron Microscopy

Prof. C. Hébert & Dr D. Alexander



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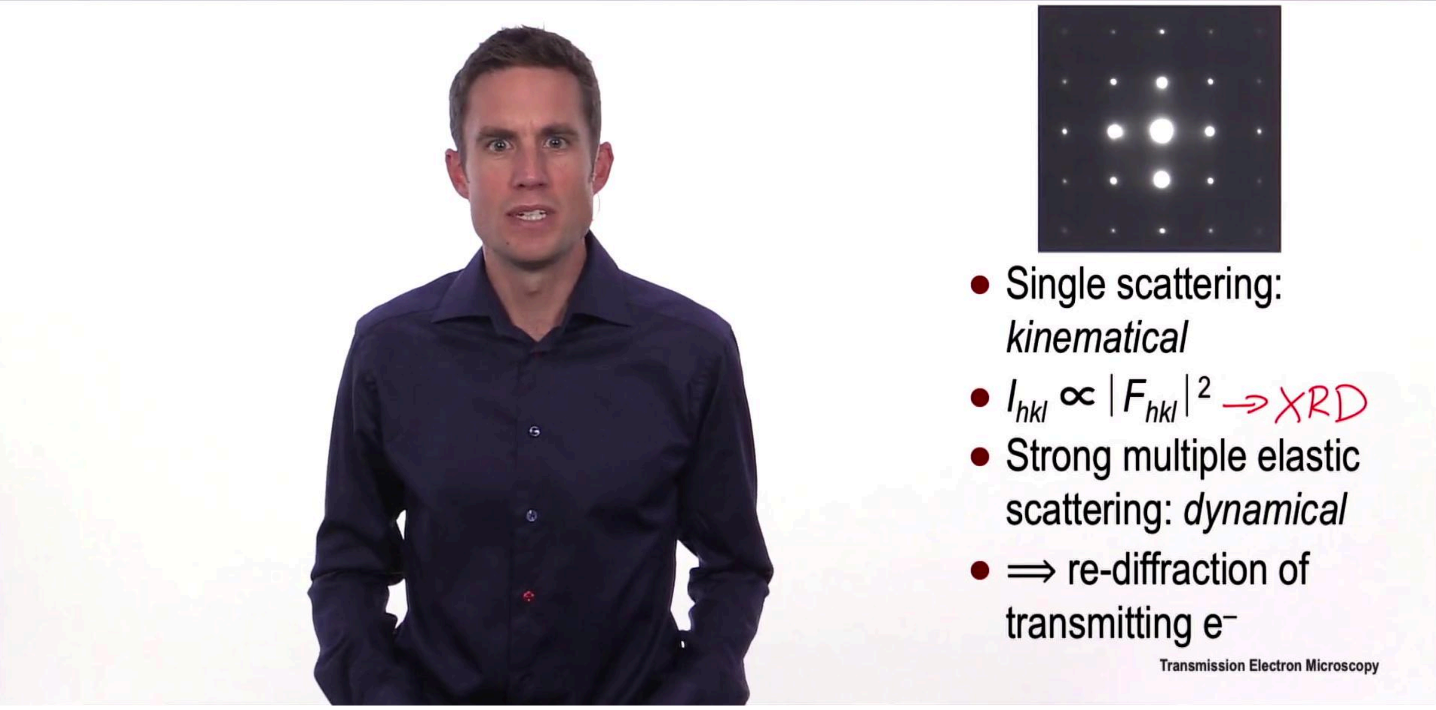
Dynamical scattering



Welcome to CIME's lectures on transmission electron microscopy for materials science, and the first of my lectures on dynamical scattering. So far in this course, we have considered electron diffraction through the framework of the Ewald sphere interacting with the reciprocal lattice. This framework is very successful for identifying which planes diffract under certain conditions of the orientation of the incident electron beam relative to that of the crystal lattice. It is further very successful for identifying the position of each diffraction spot in a diffraction pattern. If electron scattering was kinematical – in other words if we had single scattering such that a beam was diffracted at most one time as it transmits through the sample – additionally the intensity of a diffracted beam would be proportional to F_hkl squared; that is proportional to the square of the structure factor of the corresponding diffracting plane. Indeed in X-ray diffraction, this is typically the case. This is because, in X-ray diffraction, the interaction of an X-ray with the crystal lattice is rather weak. Therefore, the probability of having two consecutive scattering events is very small.

Notes

Summary

0m 05s

Dynamical scattering

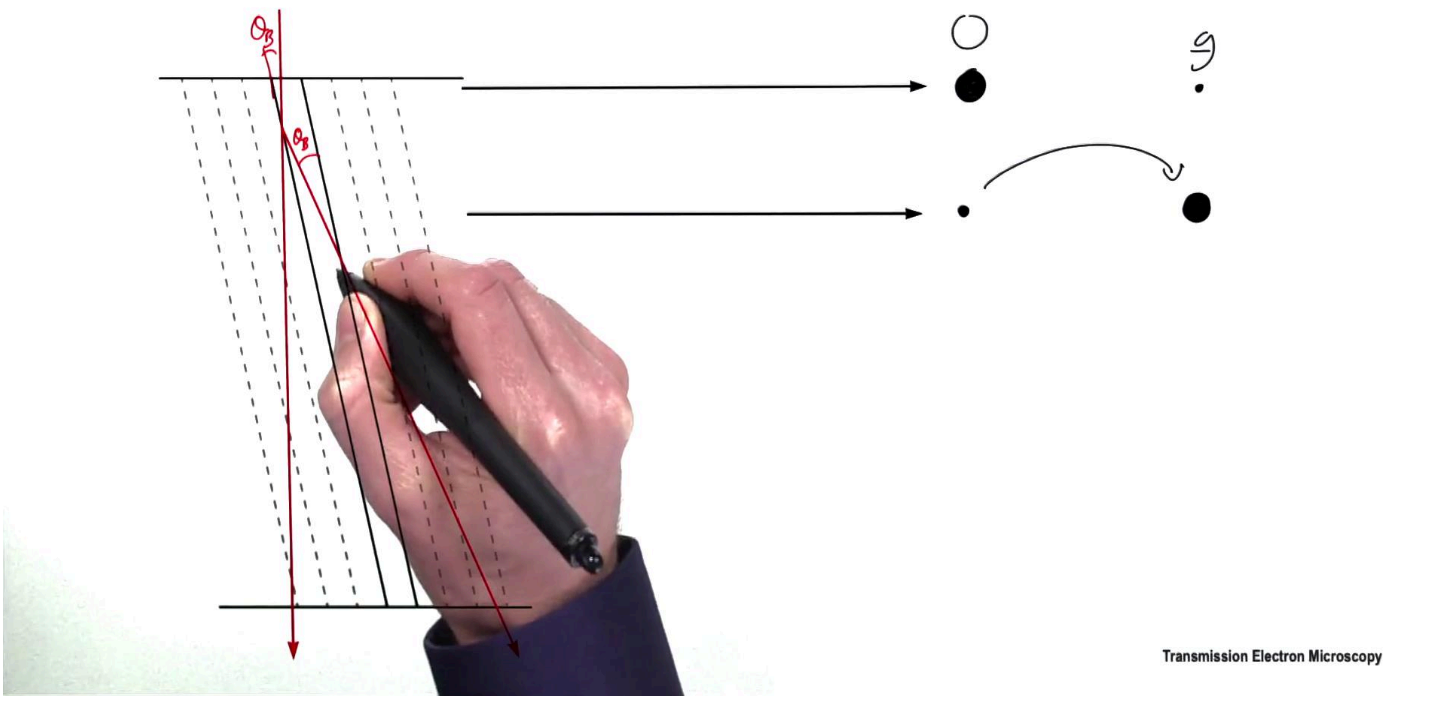
In contrast, in electron diffraction, the interaction of the electron beam with the sample is very strong. This is because the transmitting electrons are charged particles, and they are scattered by the Coulomb field of the atoms in the crystal lattice. Because of this strong interaction, typically we have what is called "dynamical scattering". This means a strong, multiple elastic scattering of the electron beam as it transmits through the sample. Essentially, the electron beam is re-diffracted. In a multi-beam or zone access diffraction pattern, this has an important consequence, because a diffracted beam can be re-diffracted into other beams. As a result the different diffracted beams interact with each other, and so their intensities are interdependent and we lose the kinematical relationship of diffracted beam intensity to the structure factor. Therefore, unlike for X-ray diffraction, the intensities in the electron diffraction pattern are typically not readily interpretable. In this lecture, we are going to look at this dynamical scattering. To simplify matters, we will study it with the idealized case of two-beam electron diffraction, and look at the consequences of dynamical scattering on the intensities of both the diffracted beam and the direct beam.

Notes

Summary

1m 25s

2-beam dynamical scattering



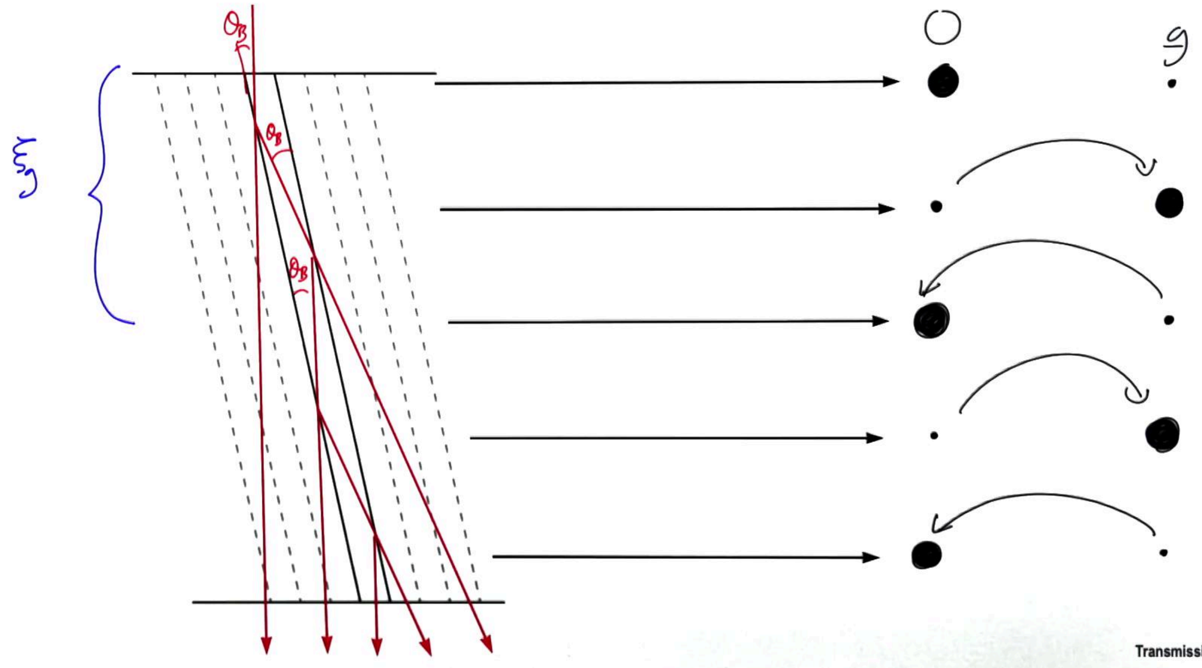
We are first going to look at this dynamical scattering with a simplified ray diagram of a beam being scattered by a plane diffracting at the Bragg angle, as this beam transmits across the sample. Now we know for this two-beam diffraction geometry, in the diffraction pattern we should see two spots: one for the direct beam, the 0 0 0; and the other for g, our diffracting beam. If we put in an incident ray here, which will scatter from this Bragg plane – so this ray is at the Bragg angle theta_B relative to that plane – it is clear if we are high up in the sample – so if we had a very, very thin sample – then the amount of scattering would be very small. Thus if we looked at the diffraction pattern, the 0 0 0 spot would be very intense. And in contrast, the spot for the diffracted beam would be very weak in intensity. As the sample becomes thicker, there will be more and more scattering into the diffracting beam. In the diffraction pattern, this leads to a redistribution of intensity from the direct beam spot to the diffracted beam spot, which in turn now becomes much more intense. However if we look at this ray diagram, we can see that this ray for the diffracted beam is at the perfect Bragg angle to be scattered from this plane here.

Notes

Summary

2m 53s

2-beam dynamical scattering



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When it does this, it will be scattered at the Bragg angle and will end up in a ray parallel to that of the incident beam. Now as the sample gets thicker the probability of this double scattering event will increase. Thus, if we looked at this thickness, we would again see a redistribution of intensity; now from the beam g back into the direct beam zero, and so the direct beam becomes very strong and the diffracting beam becomes very weak. As the beams continue to propagate across the sample, we can see that this beam is again at the perfect Bragg angle, and so can be re-diffracted yet another time, giving another ray which is parallel to the ray for the diffracting beam g. Thus, as the sample becomes thicker, yet again we can have a redistribution of intensity from that direct beam back into the diffracting beam. And this scenario can continue as the electron beam propagates across the sample. Following this simple schematic for diffraction followed by re-diffraction, we can imagine that there will be a certain thickness at which the diffracting beam here will have zero intensity, and all the intensity will be back in the direct beam. Indeed we will see that this thickness corresponds to xi_g, where xi_g is the extinction distance for this particular diffracting plane.

Notes

Summary

4m 31s

2-beam dynamical scattering amplitude

$i = \sqrt{-1}$

specimen thickness : t
excitation error : s

For incident amplitude = 1:

Amplitude of direct beam : $$\emptyset_0 = \exp(i\pi t s)\left[\cos\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right) - \frac{i\xi_g s}{\sqrt{1+\xi_g^2 s^2}}\sin\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right)\right]$$

Amplitude of diffracting beam : $$\emptyset_g = \exp(i\pi t s)\left[\frac{i}{\sqrt{1+\xi_g^2 s^2}}\sin\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right)\right]$$

Extinction distance : $$\xi_g = \frac{\pi V_0 \cos\theta_B}{\lambda |F_g|}$$

λ : Wavelength of e^-

V_0 : volume of unit cell
θ_B : Bragg angle
F_g : Structure factor for plane (hkl)

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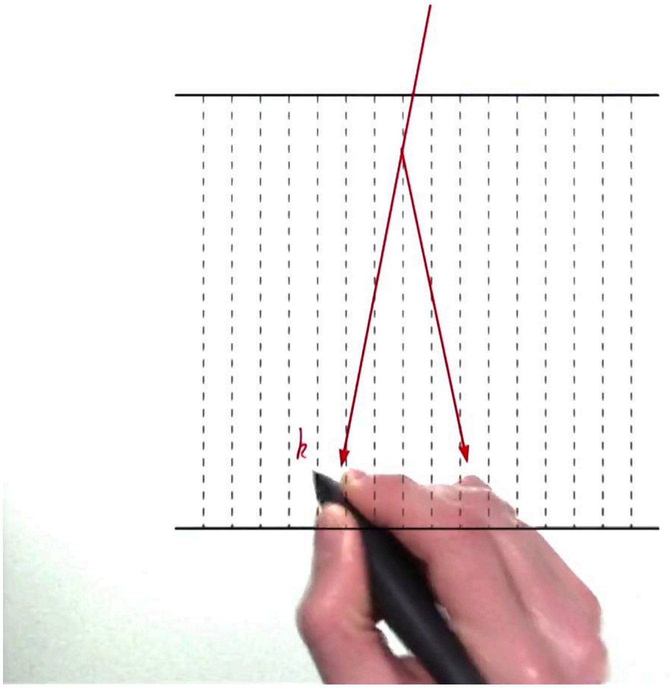
Considering an amplitude of the incident electron beam on the sample equal to 1, in this case of two-beam scattering under dynamical conditions, it has been derived that the amplitudes of the resulting direct beam and diffracting beam leaving the sample are given by these expressions here. Where first we have the amplitude of the direct beam, and then we have the amplitude of the diffracting beam. In these expressions, i is simply the imaginary number t is the specimen thickness, and s is the excitation error that was introduced in the last lecture on deviation from the Bragg condition. Finally we have this parameter xi_g, where xi_g is the extinction distance for the reflection. Where V_0 is the volume of the unit cell, theta_B is the Bragg angle, lambda is the wavelength of the electron, and F_g is the structure factor for the diffracting plane. I note that in the idealized case where there is no absorption of the electron beam in the sample, then F_g is a real number. However if you want to treat absorption this can be modelled by introducing an imaginary component into F_g and also into F_0, the structure factor for the 0 0 0. These expressions given here have been derived by a number of different ways. In the literature, perhaps the most popular of those ways is the Bloch wave theory as first proposed by Bethe.

Notes

Summary

6m 18s

Bloch wave theory of dynamical diffraction



- Solution of Schrödinger equation in crystal potential gives Bloch waves
- Plane waves with amplitude modulated by periodic lattice potential
- For *m* beams: *m* Bloch waves each having *m* plane wave components
- 2-beam: 2 Bloch waves

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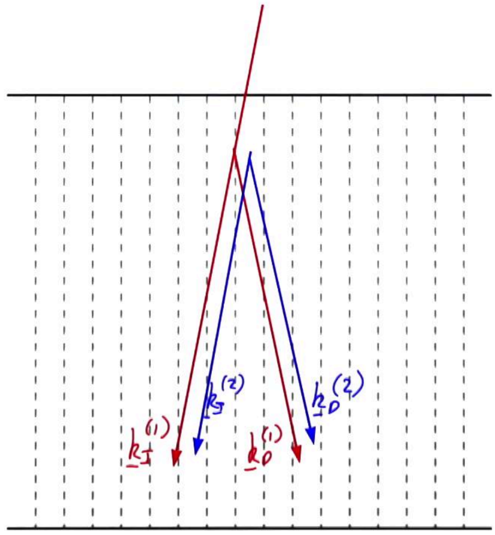
This Bloch wave approach involves finding the solution of the Schrödinger equation for an electron wave moving in the periodic potential of the crystal lattice. The solution results in wave functions known as Bloch waves. These Bloch waves are plane waves which propagate across the sample parallel to the diffracting crystal plane and they have amplitudes which are modulated by the periodic lattice potential. Unlike the so-called Howie-Whelan equations, the Bloch wave approach is fully scalable to many beams. So for m diffracting beams there are m Bloch waves. Each of these Bloch waves has m components, one for each of the resulting diffracting beams. Thus, in the two-beam case, there are two Bloch waves. Now if we consider an incident electron beam at the Bragg angle relative to this crystal plane, so far we have only considered one diffraction wave vector. However in the Bloch wave approach we now consider that there are two Bloch waves which propagate across the sample and each Bloch wave has a wave vector component corresponding to the direct beam and the diffracted beam. Thus here for instance we have the wave vector components from Bloch wave one.

Notes

Summary

8m 09s

Bloch wave theory of dynamical diffraction



- Solution of Schrödinger equation in crystal potential gives Bloch waves
- Plane waves with amplitude modulated by periodic lattice potential
- For *m* beams: *m* Bloch waves each having *m* plane wave components
- 2-beam: 2 Bloch waves

Transmission Electron Microscopy

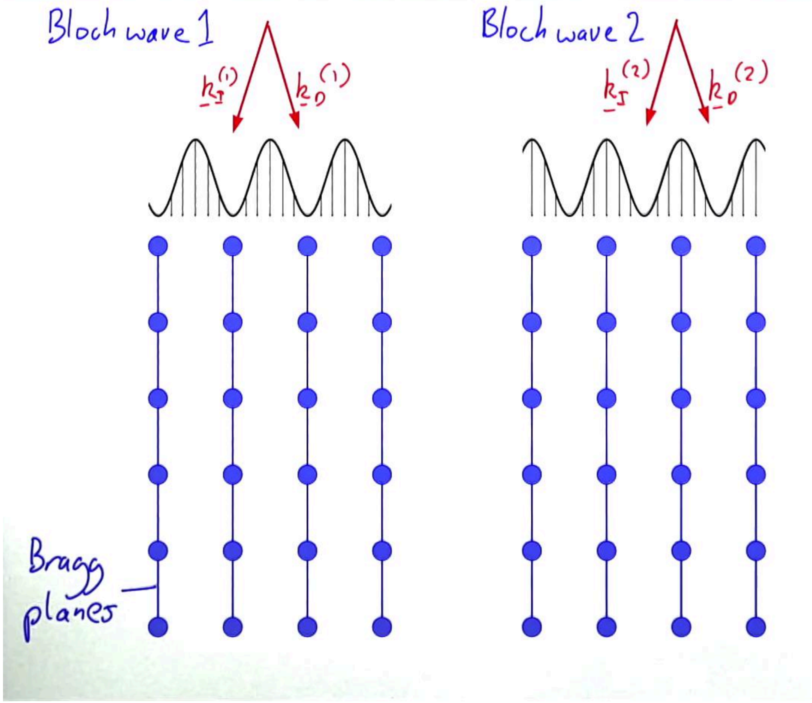
So here is the component from Bloch wave one for the direct beam and here for the diffracting beam. And then we also draw on corresponding wave vectors for the second Bloch wave, which again have components for the direct beam and for the diffracting beam. So after the Bloch waves have propagated across the sample, the components for the direct beam would add up to give the direct beam amplitude, and the components for the diffracting beam would add up to give the amplitude of the diffracting beam.

Notes

Summary

9m 33s

Bloch wave theory of dynamical diffraction



- Solution of Schrödinger equation in crystal potential gives Bloch waves
- Plane waves with amplitude modulated by periodic lattice potential
- For *m* beams: *m* Bloch waves each having *m* plane wave components
- 2-beam: 2 Bloch waves

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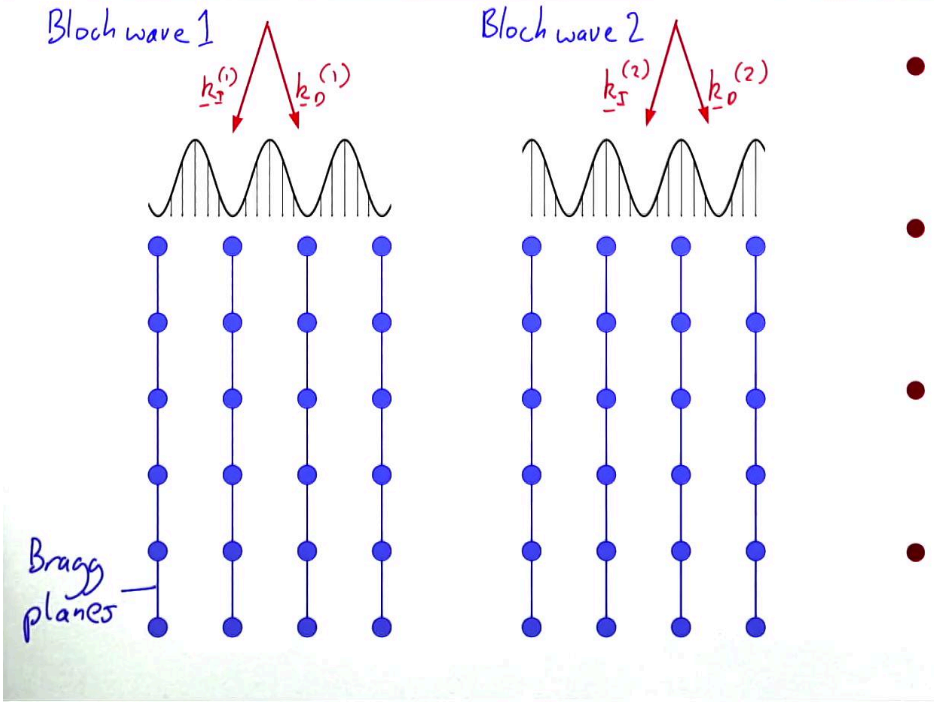
Following Hashimoto, these Bloch waves can be schematically illustrated as follows. So here is Bloch wave one and here is Bloch wave two. In this illustration, we are looking at a simple cubic lattice with these being the Bragg reflecting planes. As explained in the last slide, each of these Bloch waves has components corresponding to the direct and diffracted beams. With this curve representing the amplitude of Bloch wave one, we can see that its amplitude is centered in between the atomic planes. In contrast the amplitude of Bloch wave two is centered on the atomic planes. As a result of being centered on the atomic nuclei, this Bloch wave two experiences a stronger negative potential as it propagates through the crystal lattice. This stronger potential accelerates this Bloch wave two more compared to Bloch wave one, decreasing its wavelength, or equally increasing its wave vector relative to Bloch wave one. As a result, a phase difference develops between Bloch wave one and Bloch wave two as they propagate across the crystal lattice. A result of this phase difference is that there is a beating between the two Bloch waves as they propagate across the crystal lattice.

Notes

Summary

10m 14s

Bloch wave theory of dynamical diffraction



- Solution of Schrödinger equation in crystal potential gives Bloch waves
- Plane waves with amplitude modulated by periodic lattice potential
- For *m* beams: *m* Bloch waves each having *m* plane wave components
- 2-beam: 2 Bloch waves

Transmission Electron Microscopy

And it is this beating that gives result to the thickness dependence in the sine term of the amplitude of the resulting diffracting beam. In the case where we assume that there is no absorption, when the excitation area s equals zero – in other words we are at the exact Bragg condition – then the amplitudes of the two Bloch waves are identical. However if we leave this perfect Bragg condition by tilting slightly away from it, creating either a positive or negative excitation error, then the amplitudes of the two Bloch waves cease to be equal. And this gives rise to the amplitudes of the resulting direct and diffracting beams being also in function of the excitation error s. Finally, considering absorption, the Bloch wave two being centered on the atomic nuclei is absorbed more strongly than the Bloch wave one. And this gives rise to so-called “anomalous absorption effects” in the intensities of the diffracting and direct beams. It also connects to channeling effects which you might come across in chemical analysis.

Notes

Summary

11m 43s

2-beam dynamical scattering intensity

Direct beam amplitude:

$$\emptyset_0 = \exp(i\pi t s)\left[\cos\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right) - \frac{i\xi_g s}{\sqrt{1+\xi_g^2 s^2}}\sin\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right)\right]$$

Diffracted beam amplitude:

Phase term

$$\emptyset_g = \exp(i\pi t s)\left[\frac{i}{\sqrt{1+\xi_g^2 s^2}}\sin\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right)\right]$$

Intensity of diffracted beam: $I_g = |\phi_g|^2 = \frac{1}{(1+\xi_g^2 s^2)}\sin^2\left(\pi t\sqrt{\frac{1}{\xi_g^2}+s^2}\right)$

Intensity of direct beam: $I_0 = |\phi_0|^2 = 1 - I_g$

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Returning to these expressions for the amplitudes of the direct beam and the diffracted beam, we can easily determine the intensity of the diffracted beam by calculating the square of the modulus of phi_g. Since this term here is a phase term, it just contributes a factor of one to the intensity, and then the intensity of the diffracted beam is simply going to be: 1 over 1 + xi_g squared s squared times sine squared of pi t root 1 over xi_g squared + s squared. So we have some sine squared modulation, in function of both thickness and the excitation error s. If you also calculate the intensity of the direct beam, which can simply be done by multiplying this term here by its complex conjugate, you find that its intensity equals: 1 minus I_g. In other words we have conservation of intensity. With the incident amplitude of one, the incidence intensity is one, and this intensity is conserved into the two beams, such that they are complementary to each other.

Notes

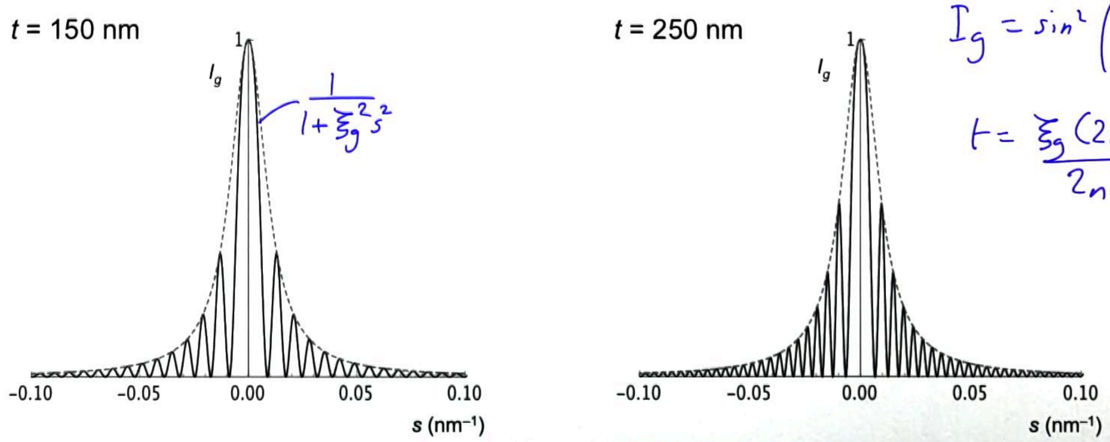
Summary

12m 53s

Intensity as function of excitation error s

- Plot I_g vs s for different t
- Model using: ξ_g = 100 nm

$$I_g = \frac{1}{(1+\xi_g^2 s^2)} \sin^2\left(\pi t \sqrt{\frac{1}{\xi_g^2} + s^2}\right)$$



$$I_g = \sin^2\left(\frac{\pi t}{\xi_g}\right)$$

$$t = \frac{\xi_g (2n+1)}{2n}$$

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Having in the last lecture looked at the kinematical case of the intensity of a diffracted beam as a function of the excitation error s, we are now going to use this expression to look at that intensity in the dynamical case. So here this intensity has been modeled using an extinction distance of 100 nanometers for various specimen thicknesses t. Looking first at this curve, for t equals 150 nanometers, we can see that there are oscillations in intensity inside an envelope, where now this envelope corresponds to: 1 over 1 plus xi_g squared s squared. In other words, this envelope does not depend on thickness; it only depends on the excitation error and the extinction distance. What does depend on thickness is the frequency of these modulations. We can see as we go to a thicker sample, the modulations go to smaller excitation errors s, similarly to the kinematical case. When s equals zero, we can see that the intensity in the diffracted beam is simply given by: I_g equals sine squared of pi t over xi_g. In these plots here I have specifically chosen thicknesses, where the thickness t = xi_g times 2n plus 1 divided by 2n where n is an integer.

Notes

Summary

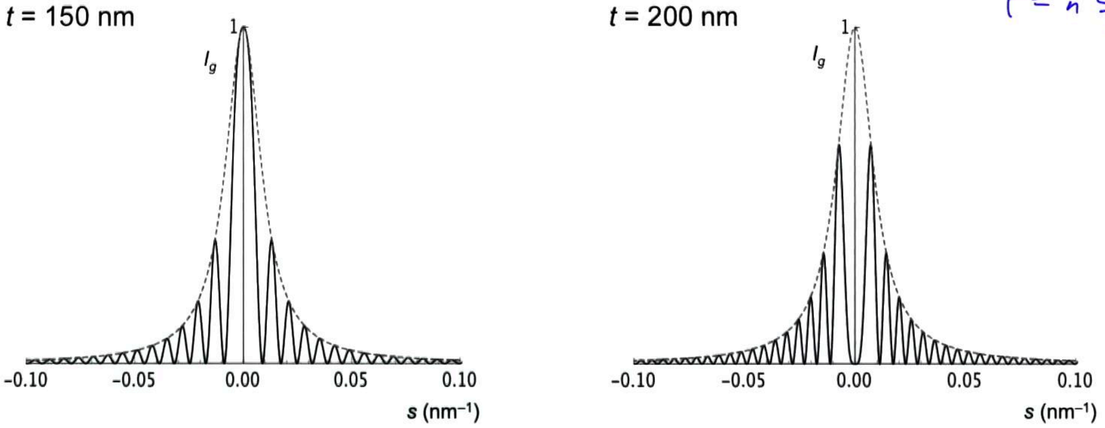
14m 22s

Intensity as function of excitation error s

- Plot I_g vs s for different t
- Model using: $\xi_g = 100$ nm

$$I_g = \frac{1}{(1+\xi_g^2 s^2)} \sin^2\left(\pi t \sqrt{\frac{1}{\xi_g^2} + s^2}\right)$$

$t = n\,\xi_g$



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Because in this case, when s equals zero, the intensity in the diffracted beam equals one; as we see here and here. However we can ask ourselves: what happens when we deviate from this nice condition? That is what I have done on this slide. Here, I have kept the t equals 150 nanometers curve, whereas here, I plotted the curve with t equals 220 nanometers. Now we can see there is a marked effect on the intensity at s equals zero. The intensity is no longer at a maximum. Indeed there is a dip in intensity for s equals zero. Now what will happen if we reduce t further, to t equals 200 nanometers, when t will become an integer multiple of the extinction distance? We look at that on this slide. Now we have t equals n times xi_g, where n is an integer. In this case, when s equals zero, here we now take the sine squared of pi times n, which will be zero. Therefore the intensity in the diffracting beam is zero. Indeed, looking at this t equals 200 nanometers curve, we can see that, at s equals zero, there is no intensity in the diffracted beam. So all the intensity would now be in the direct beam, with zero in the diffracted beam for this thickness at the exact Bragg condition.

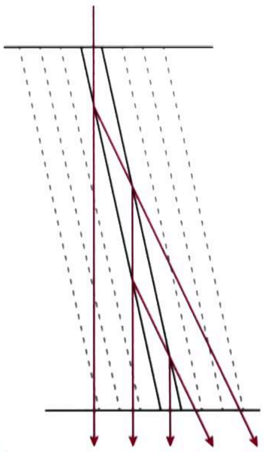
Notes

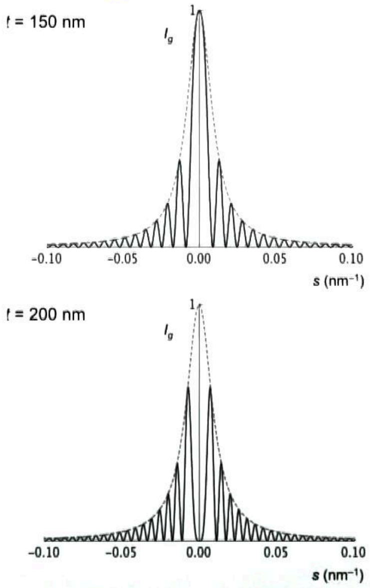
Summary

16m 00s

Dynamical scattering summary

"Rocking curves":





- Dynamical scattering: multiple elastic scattering of e⁻-beam transmitting through sample
- Strong interactions in TEM: hence typically dynamical
- In 2-beam condition I_0 & I_g given by simple function of:
  – specimen thickness t
  – excitation error s
  – extinction distance ξ_g

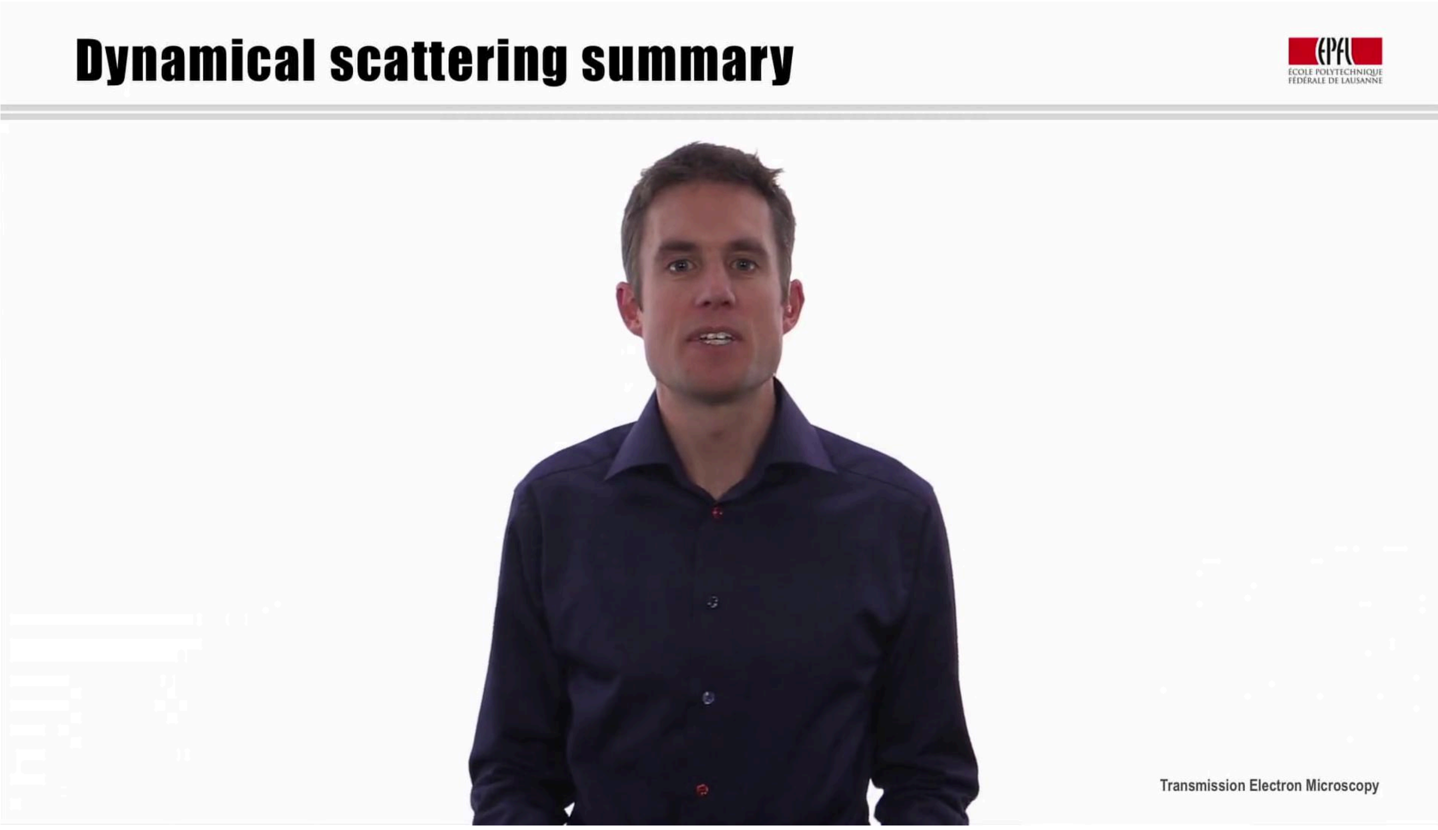
Transmission Electron Microscopy

To summarize on this lecture, I have introduced dynamical scattering as being the multiple elastic scattering of the electron beam as it transmits through the sample. In transmission electron microscopy, this is the typical case because the interactions of the electron beam with the sample are very strong. In the two-beam condition, this can be interpreted in a rather simple way as a diffraction and then re-diffraction of an electron beam as it propagates across the sample. And depending on the number of diffraction events, there is a modulation in the intensity of the diffracted and direct beams as a result of this. Further we have looked at the full expressions for the intensity of the direct and diffracted beams, which are a simple function of the specimen thickness t, the excitation error s and the extinction distance xi_g. And then we have looked at the consequence of these expressions on these curves of intensity versus excitation error. I note that, in the literature, these curves are often referred to as "rocking curves". This expression comes from a technique known as rocking beam electron diffraction where the incident electron beam is tilted or rocked from side to side. And as it changes in angle relative to the sample, you are able to measure the intensity of a beam at different excitation errors s.

Notes

Summary

17m 25s



Having introduced dynamical scattering in this lecture, in the next lecture we are going to look at another dynamical effect in imaging mode, in the formation of thickness fringes in bright field and dark field images.

Notes

Summary

18m 55s