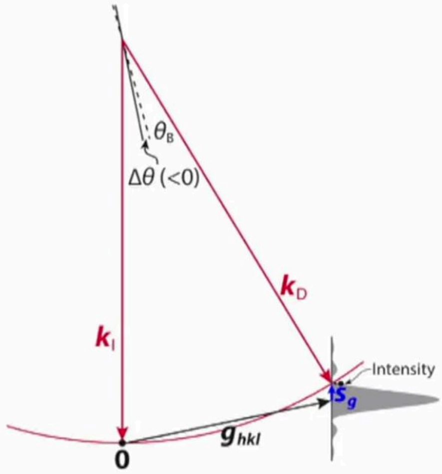
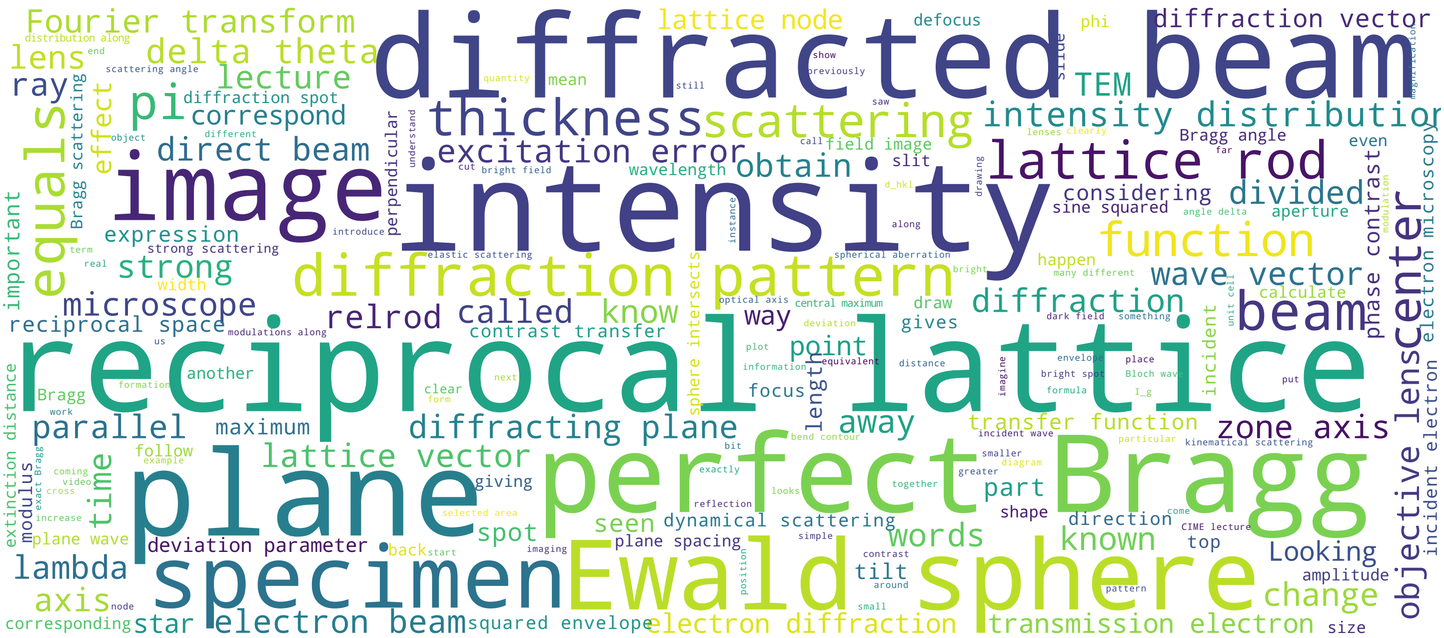
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Deviation from Bragg scattering



Transmission Electron Microscopy

Prof. C. Hébert & Dr D. Alexander



Search MOOC

Video

EPFL

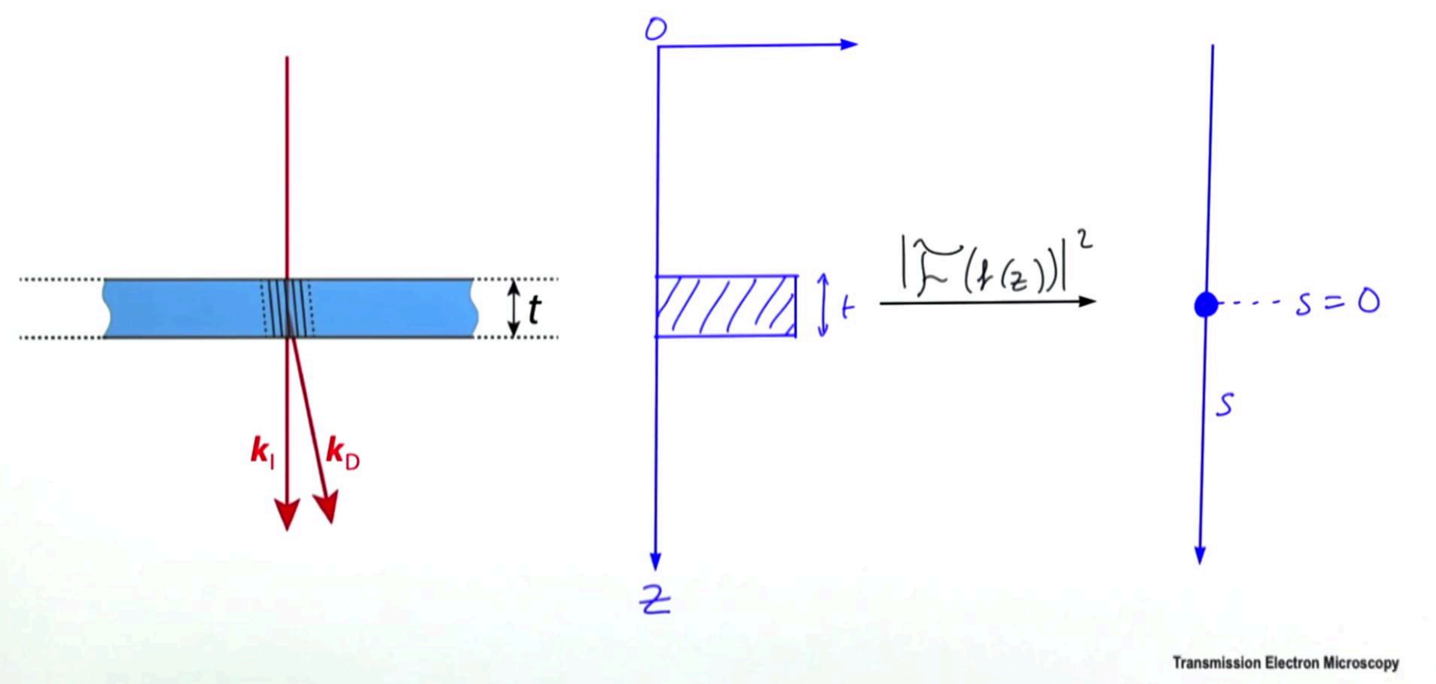
Welcome to CIME's lectures on transmission electron microscopy for materials science. In the last lecture, we saw how the size and shape of the sample, in particular the fact that it is very thin, leads to the reciprocal lattice nodes having an elongated form; the so-called reciprocal lattice rod or relrod form. And it is this elongation that gives the relaxation of the Bragg condition, which in turn allows us to start understanding why, in a zone axis condition, we have such strong scattering from many different crystal planes at the same time. In this lecture, we are going to consider in more detail the intensity along one of these reciprocal lattice rods; but looking not at the zone axis condition, but instead at the two-beam electron diffraction condition. And further, considering what happens to the intensity in a diffracted beam when we deviate slightly from this perfect Bragg scattering condition.

Notes

Summary

0m 05s

Fourier transform of sample thickness

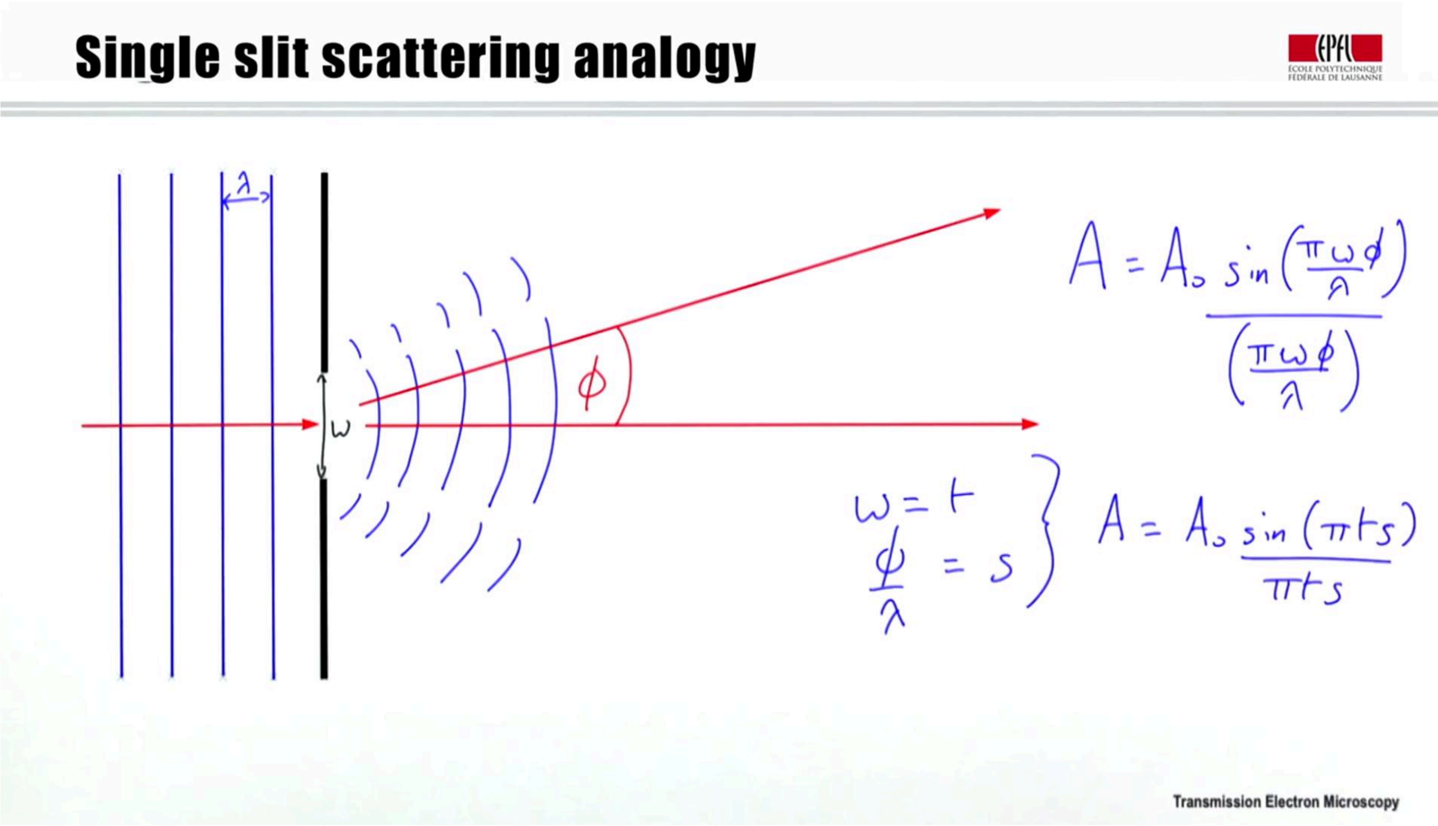


Here, we have a schematic diagram of our sample with strong scattering from this Bragg plane into this diffracted beam k_D, and the sample having a thickness of t. To calculate the intensity along our relrod, we need to determine the Fourier transform of this sample thickness. Effectively, the sample is like a top hat function along this z-axis. We have a function which is either at maximum within the sample, or along the rest of z has a value of zero. We need to calculate the Fourier transform of this function. Once we have identified that, by taking its modulus, squared, we can obtain the intensity distribution along this axis. This, we will plot in reciprocal space along the axis of the relrod. And for reasons that will become clear, we will call the distance along this relrod "s", with a center of the relrod corresponding to s equals zero.

Notes

Summary

1m 04s



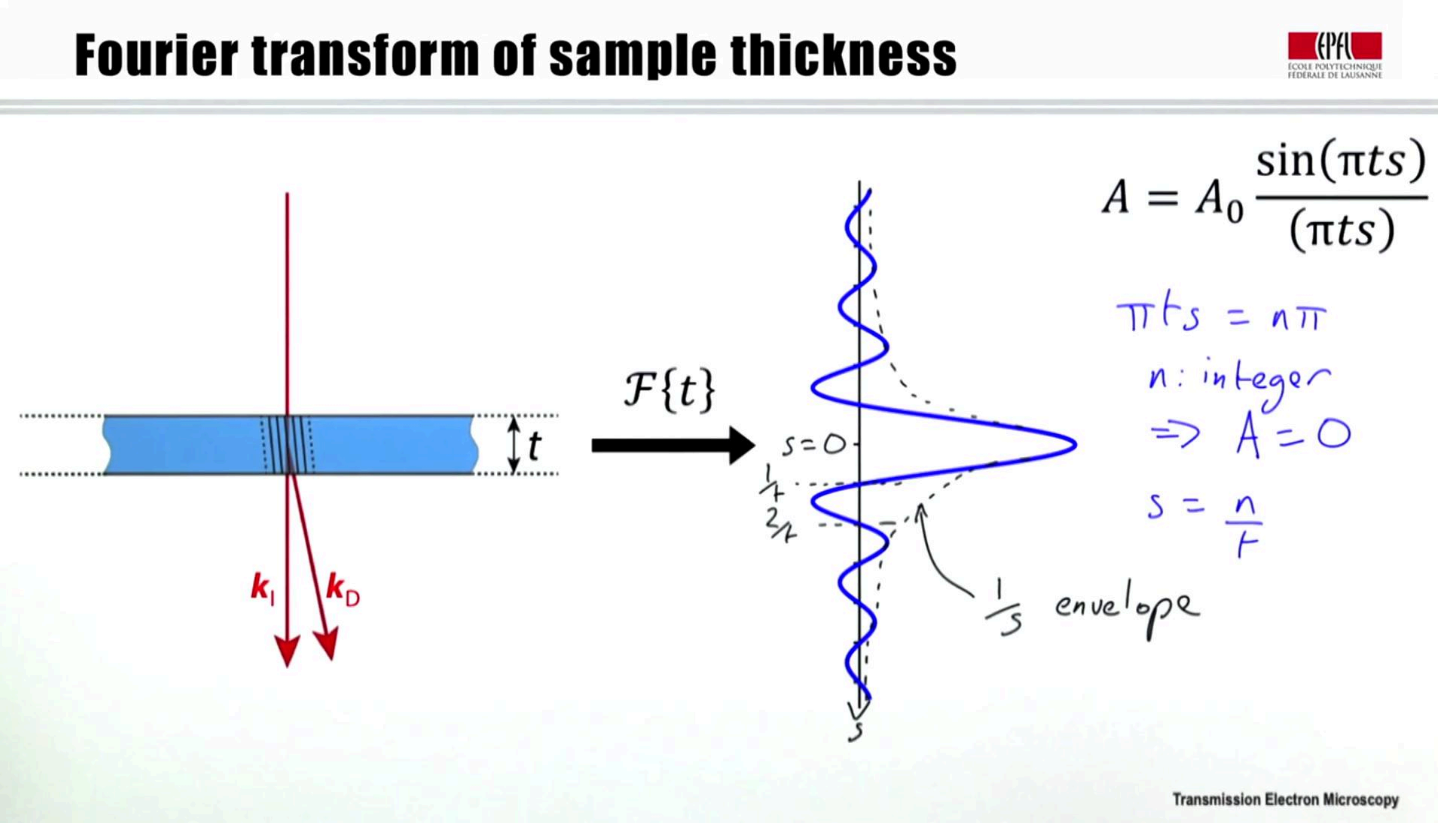
The amplitude and intensity distributions of that top hat function are equivalent to those from the scattering of a plane wave by a single slit with width w. Here, we look at such a plane wave, with a wavelength of lambda, incident on the slit which has this width w. When the wave scatters from that slit, we will obtain some interference pattern, with the waves spreading out, with a central maximum and then other narrower maxima. Looking at the far field, the amplitude of scattering for a scattering angle of phi is given by the formula: A = A_0 sine of (pi w phi over lambda) divided by pi w phi over lambda. In other words, we have a sync function of sine x over x multiplied by A_0, where A_0 is the maximum amplitude observed at scattering angle phi = 0. To translate this formula to the TEM case, we know that w – the width of our slit – is equivalent to the sample thickness t. And further, it can be easily shown that, in reciprocal space, phi over lambda equals s; the distance along our reciprocal lattice rod. Taking these together, we see that: A = A_0 sine of pi t s over pi t s.

Notes

Summary

2m 17s

Fourier transform of sample thickness

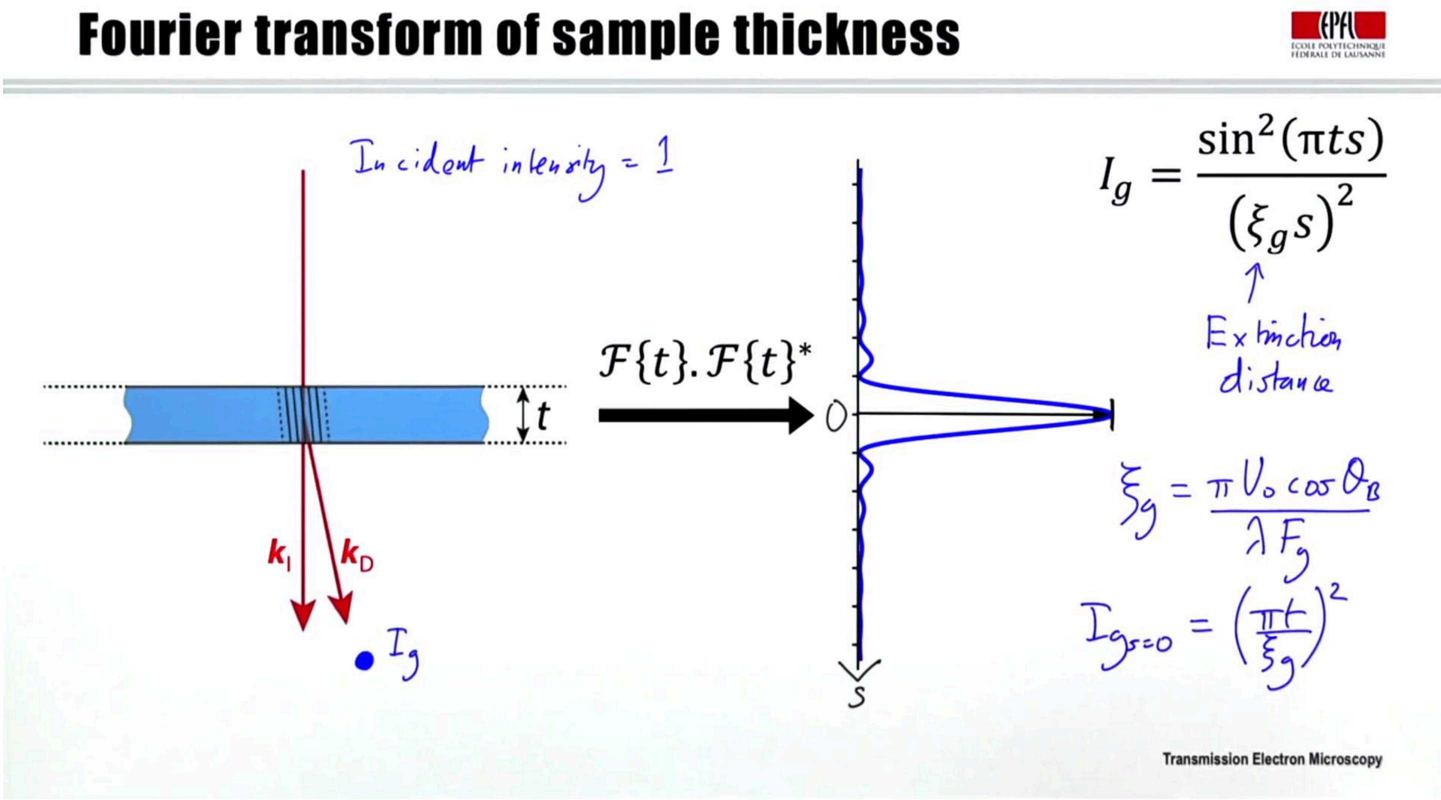


Plotting out this amplitude function along the length of our reciprocal lattice rod, s, we obtain an amplitude distribution that looks like this. With these modulations which are strong in the center, where s equals zero, and decay out either side. Further, considering s away from zero, it is clear that when: pi t s = n pi, where n is an integer, that A = 0. Therefore, we see that for: s = n divided by t, we have zeros along this modulation. The first at one divided by thickness; the second at two divided by thickness t; and so on. Additionally, we see that these sine type modulations sit within a one over s envelope. This is the amplitude function, but in diffraction, we measure intensity. To calculate the intensity distribution, we simply need to take the square of this function – corresponding to this Fourier transform multiplied by its complex conjugate.

Notes

Summary

3m 57s



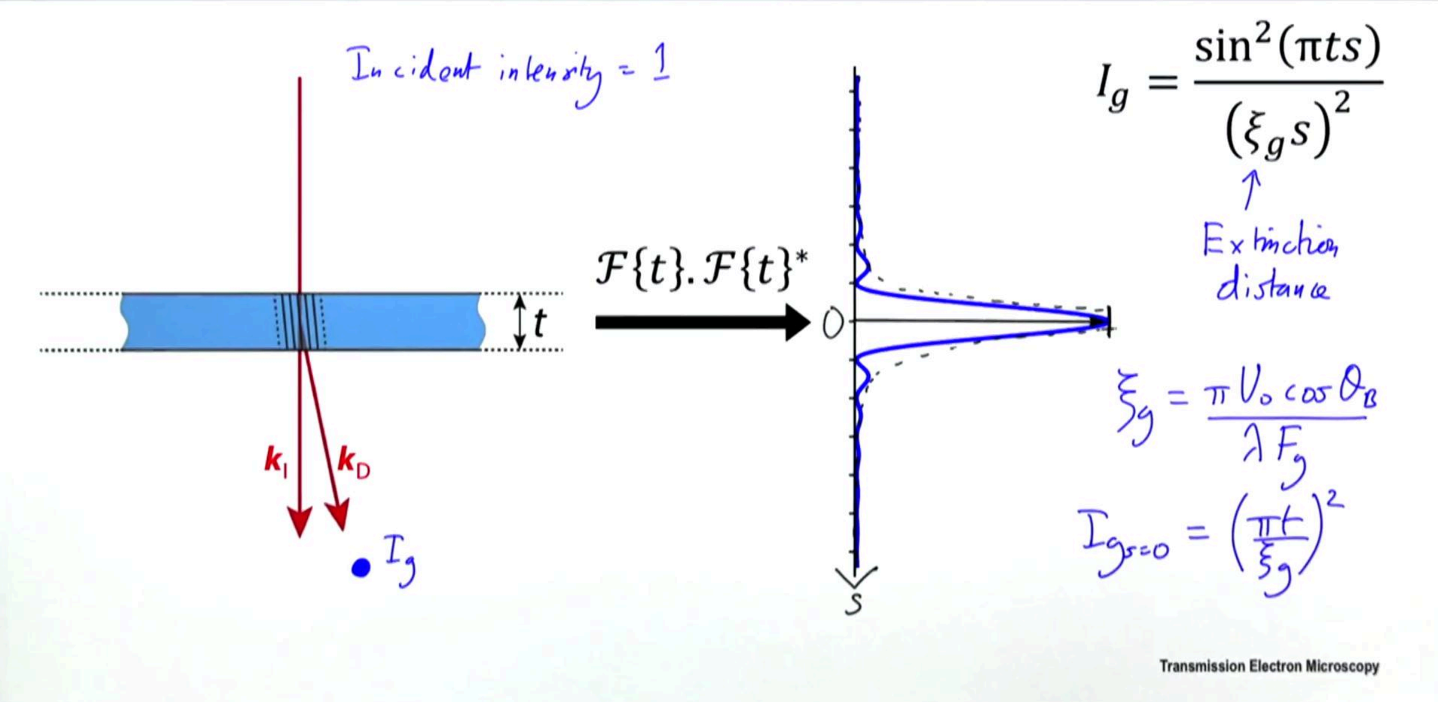
Looking at this intensity function, we now have an intensity proportional to: sine squared of pi t s divided by pi t s squared, or sinc squared pi t s. Along the relrod axis, we again have a central maximum at s equals zero. And again, we have zeros in the modulation at s = 1 over t, 2 over t, and so on. However, this time, these modulations sit within a 1 over s squared envelope. Here, we make that intensity expression yet more specific to the TEM case, by considering that we have an incident intensity on the sample, equal to one. And now, calculating directly the intensity in a diffracted beam, I_g. Where I_g is, again, given by the sine squared of pi t s on the top. However, on the bottom, we have a new term. This xi_g is known as the extinction distance. And while not proved here it is given by the expression xi_g = pi times the volume of the unit cell times cosine theta_B, where theta_B is the Bragg angle, divided by lambda, the wavelength, times F_g, where F_g is the structure factor for that particular reflection. Further, it can be straightforwardly shown that the intensity at the tip of the central maximum – at s equals zero – is given by the expression I_g_s = 0 = pi t divided by xi_g squared.

Notes

Summary

5m 14s

Fourier transform of sample thickness

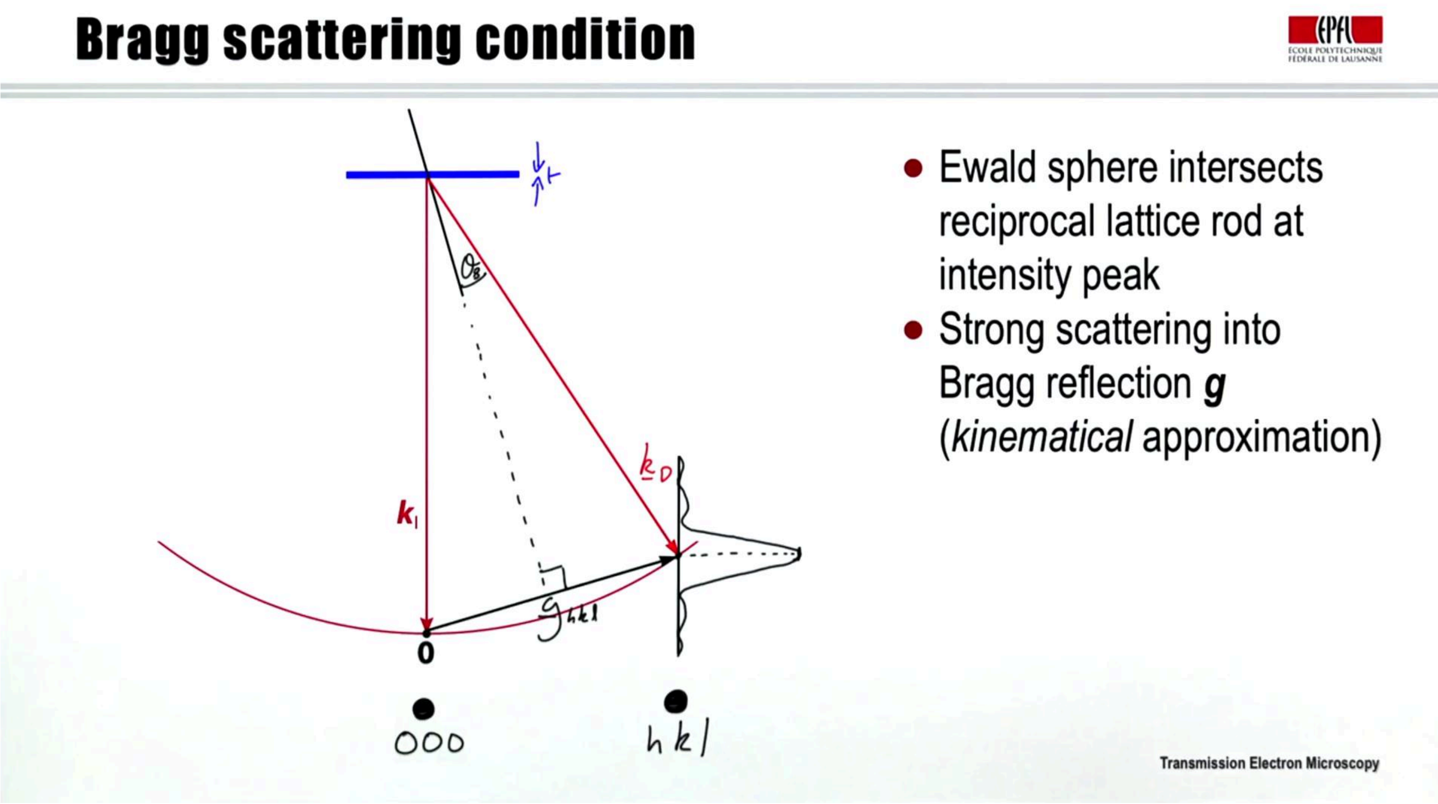


One thing that is very important to mention at this point is that these expressions only apply in the case of what we call "kinematical scattering". Kinematical scattering means single elastic scattering. In other words, the beam will be diffracted at most one time on its transmission or trajectory through the sample. While such kinematical scattering is not an accurate assumption during real electron diffraction, where the probability of scattering is very high, nevertheless, this expression, and this intensity distribution, with this one over s squared envelope, will still give useful insights in the remaining slides, where we will interact this relrod intensity distribution with the Ewald sphere.

Notes

Summary

7m 02s

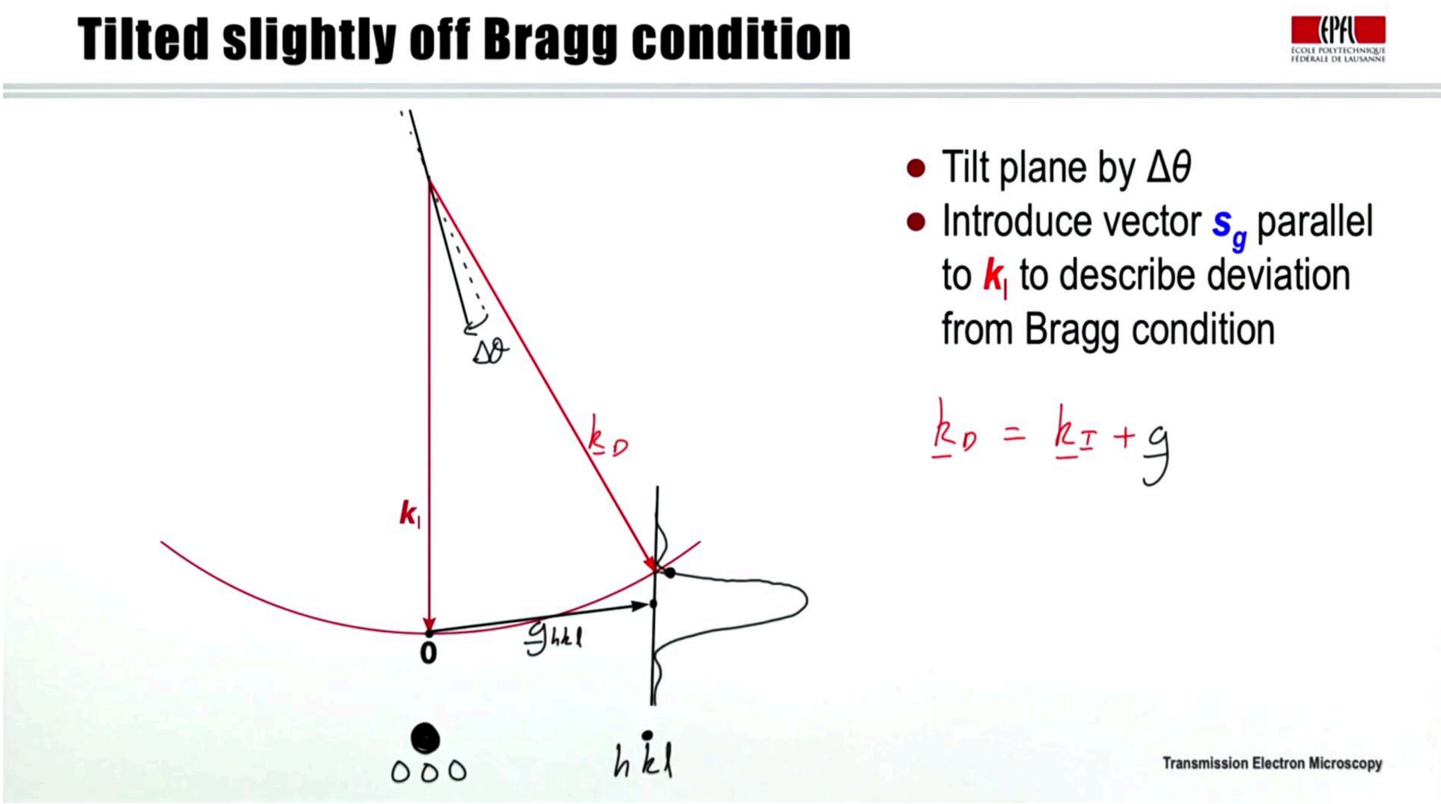


On this slide, we are going to make this interaction, looking at the perfect Bragg scattering condition. So we imagine we have a sample of thickness t, with a plane scattering at a perfect Bragg angle theta_B, giving a diffracted beam as follows. Given that we are at the perfect Bragg condition, the center of the reciprocal lattice node is intersected exactly by the Ewald sphere. Thus, we will have a diffraction vector, g, coming here which is of course perpendicular to our Bragg scattering plane. We know that this reciprocal lattice node is at the center of some reciprocal lattice rod. And now, we are going to plot the intensity distribution along this reciprocal lattice rod. As we saw before, it will have some modulations with a central intense peak. Given that the Ewald sphere intersects in the center of this peak, the diffracted beam will have a strong intensity, given by that maximum. Thus, if we took a diffraction pattern, we will have one bright spot for the 0 0 0 – the direct beam – and another very bright spot for the diffracted beam h k l. On the next slide, we will look at what happens to the intensity in this diffracted beam when we now tilt this diffracting plane slightly away from that perfect Bragg condition.

Notes

Summary

7m 47s



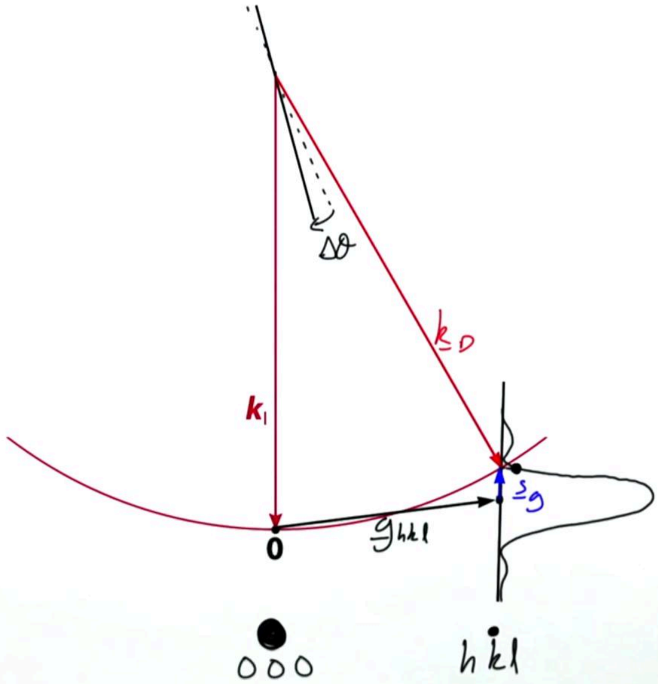
On this slide, if that diffracting plane was previously at this angle, it has now been tilted slightly by an angle delta theta towards the incident electron beam. Since the reciprocal lattice vector is perpendicular to this plane, it also is rotated by an angle, delta theta, compared to previously. The reciprocal lattice rod is going to be centered on this vector, g, as follows. With the Ewald sphere intersecting this relrod here, the diffraction vector k_D plots as follows. Sketching in the intensity modulations along the reciprocal lattice rod, we see that, unlike the perfect Bragg condition, where the intensity in the diffracted beam was given by the maximum in this central peak, the intensity in that diffracted beam is now given by this locus here. Thus, clearly, if we now sketch a diffraction pattern, while the direct beam will be strong, the intensity in that diffracted beam will be much smaller than before. Thus, this deviation away from the perfect Bragg condition has led to a dramatic weakening of intensity in the diffracted beam. In addition, the vectorial expression we had before for perfect Bragg diffraction, where k_D equals k_I, the incident wave vector, plus g, the diffraction vector, no longer applies.

Notes

Summary

9m 14s

Tilted slightly off Bragg condition



- Tilt plane by $\Delta\theta$
- Introduce vector $\mathbf{s}_g$ parallel to $\mathbf{k}_I$ to describe deviation from Bragg condition

$$\underline{k}_D = \underline{k}_I + g + \underline{s}_g$$

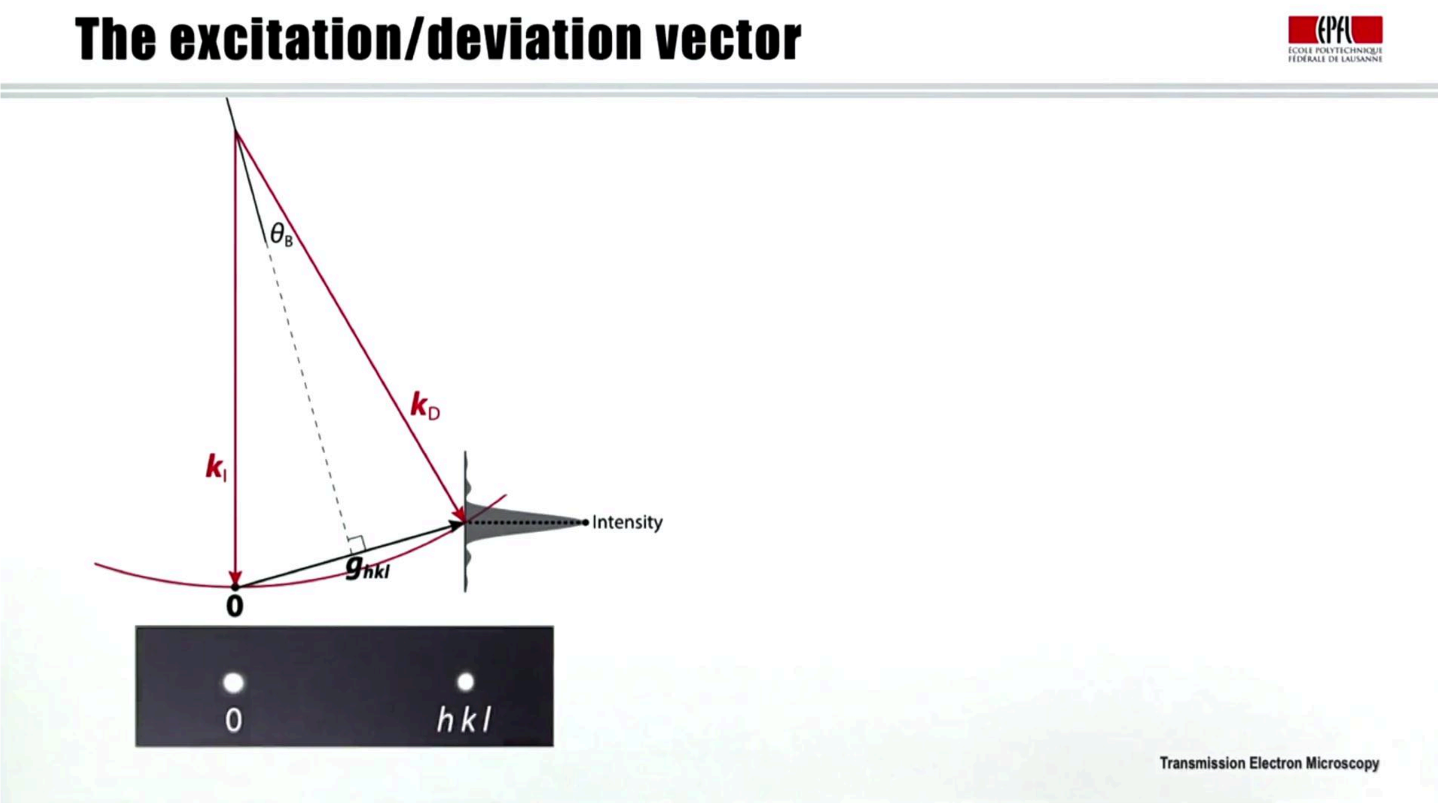
Transmission Electron Microscopy

To solve this, we now introduce another vector, which we will call s_g. By closing the loop, we obtain: k_D = k_I + g + s_g, where essentially, s_g describes the deviation from the perfect Bragg condition.

Notes

Summary

10m 49s



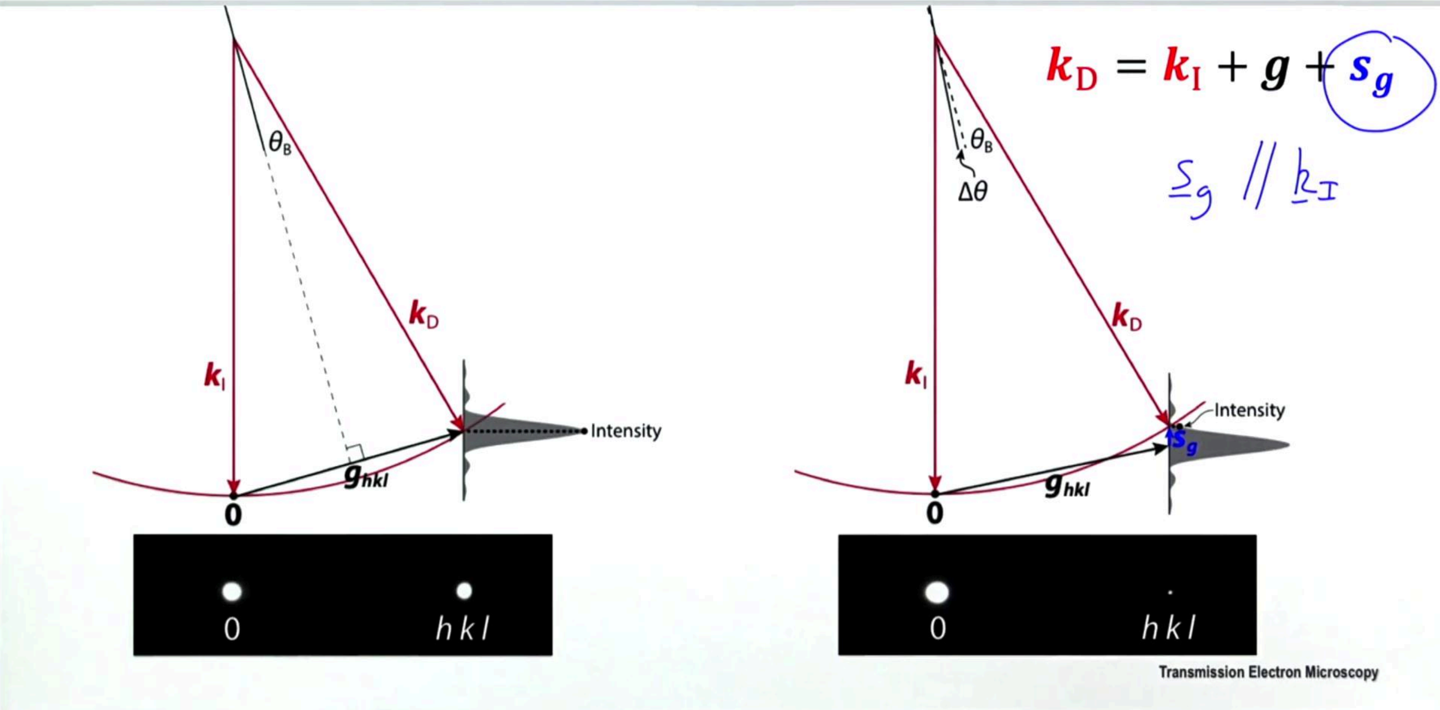
Cleaning these two diagrams up, here we have the schematic illustration for scattering at the perfect Bragg condition, where the Ewald sphere intersects the center of the relrod. Thus, giving an intensity in the diffracted beam which corresponds to the maximum in this sync squared function, as demonstrated by this real experimental diffraction pattern here.

Notes

Summary

11m 11s

The excitation/deviation vector

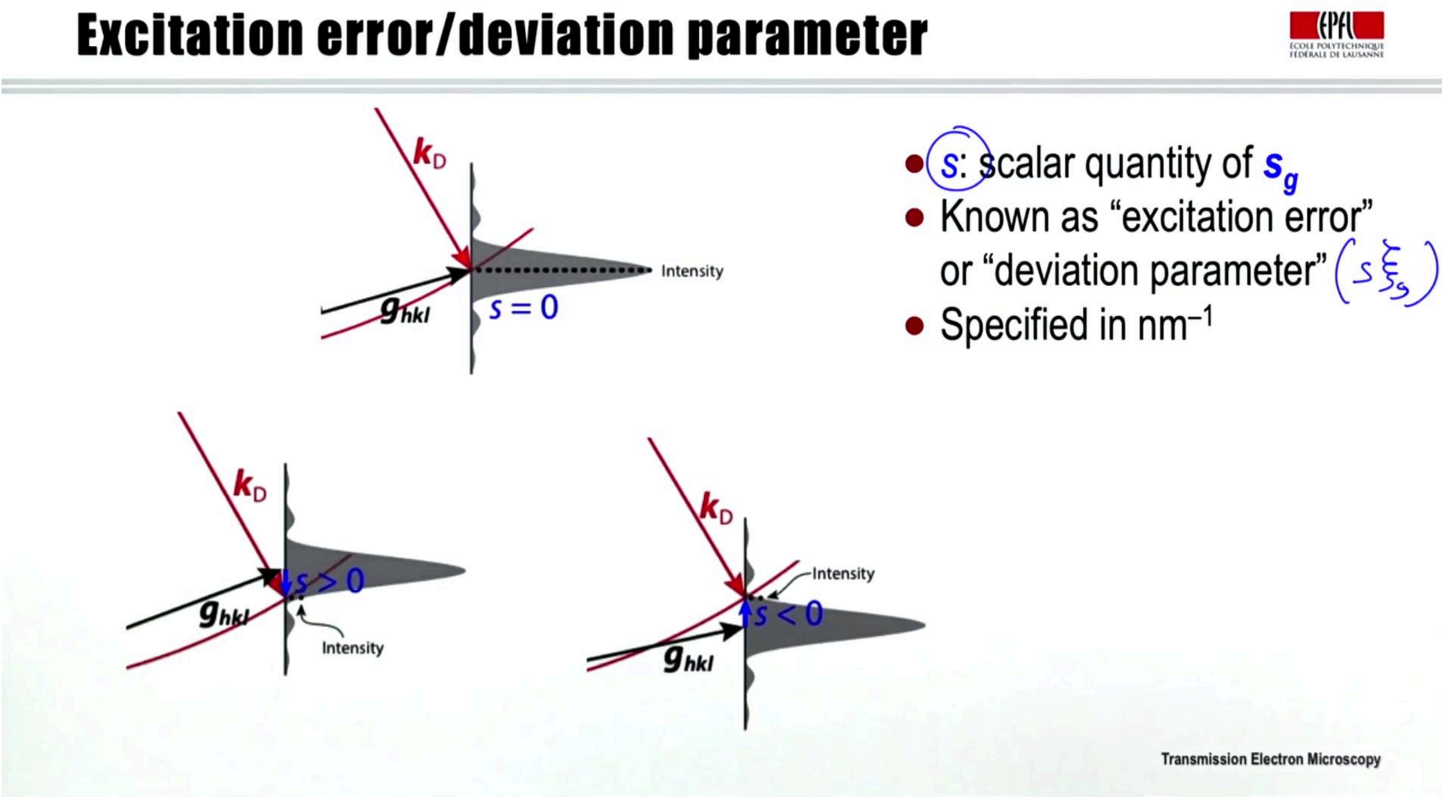


Now tilting away from that perfect Bragg condition by a small amount delta theta, the Ewald sphere intersects away from the center of that peak, resulting in a significant decrease in the intensity of that diffracted beam. Given the one over s squared envelope for this intensity distribution, for a sample with a typical thickness of 50 or 100 nanometers, delta theta just needs to be a fraction of a degree for us to observe a significant reduction in the intensity of this diffracted beam. Finally, to describe this deviation away from the perfect Bragg condition, we introduce this new vector s_g. Where in this case, I define s_g as being parallel to the incident wave vector k_I. Further, s_g is known under two expressions: either the excitation or deviation vector.

Notes

Summary

11m 36s

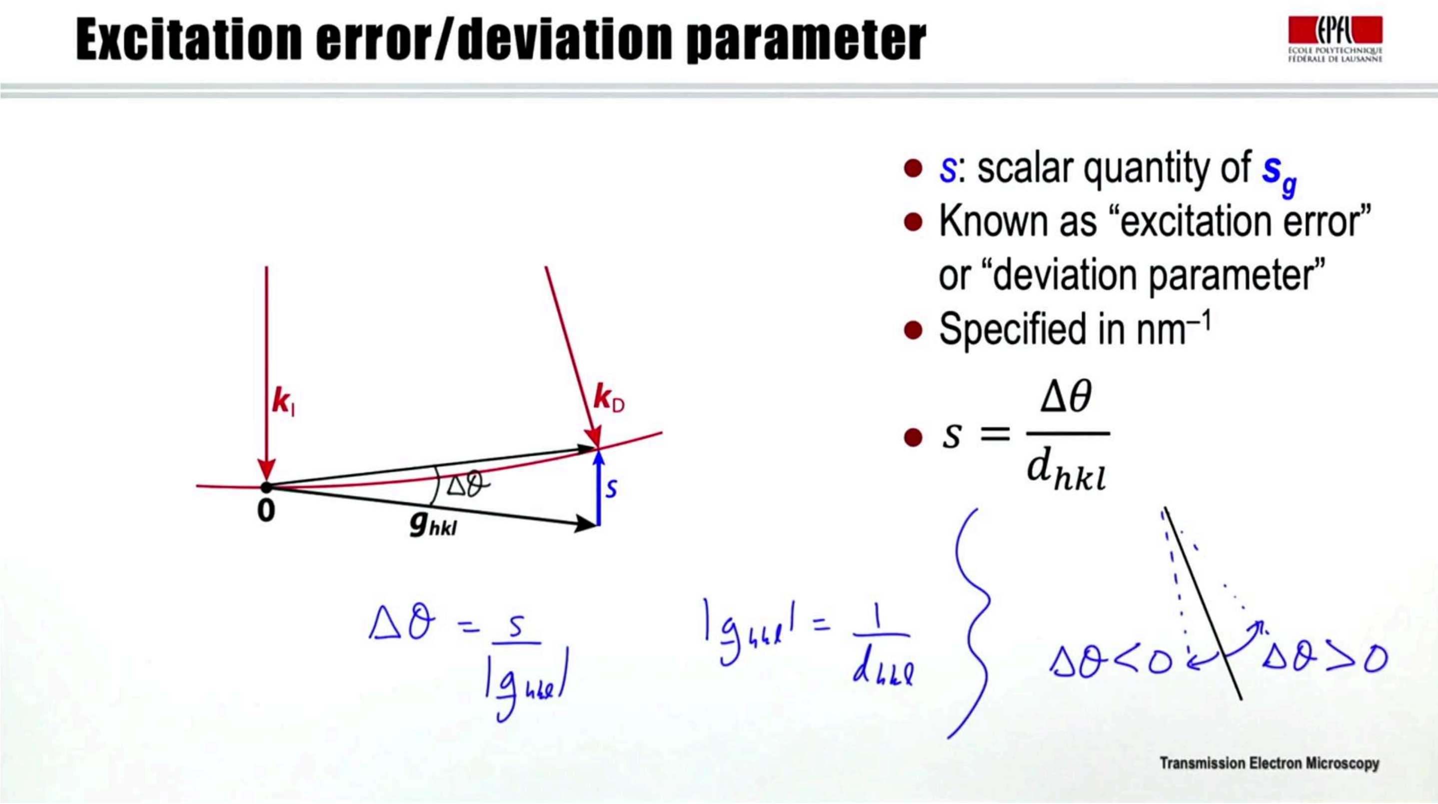


Having defined s_g, I now introduce a scalar quantity: s. So s equals the scalar quantity of s_g. This s is again known under two different expressions. One of them being the excitation error; in other words, how much we are in error of exciting a perfect Bragg condition. Or, alternatively, as the deviation parameter; in other words, how far we are in deviation of the perfect Bragg condition. However, it should be known that, while some people refer to s as being the deviation parameter, in other works, the deviation parameter can refer to a quantity of s times xi_g, the extinction distance. Being in reciprocal space, this excitation error, s, is typically measured or specified in inverse nanometers. Obviously, for the perfect Bragg condition, s = 0. Away from the Bragg condition, if s is within the Ewald sphere, that is corresponding to a tilt of the diffracting plane this way, then s is greater than 0. And if s is outside the Ewald sphere, then it is negative; this time instead corresponding to a tilt of the diffracting plane this way relative to the perfect Bragg condition.

Notes

Summary

12m 33s



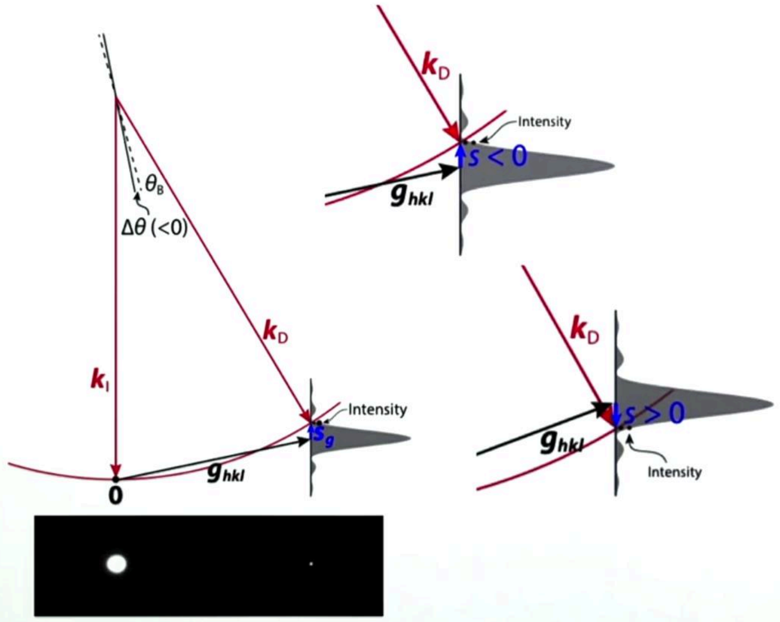
Looking a bit more at that s equals negative scenario, here I have a rather symmetrical illustration, where this would be the g vector for the perfect Bragg condition. Given that the diffracting plane has been tilted away from the perfect Bragg condition by an angle delta theta – which gives an equivalent tilt angle of this reciprocal lattice vector g_hkl – it is clear from this that, in the small angle of approximation: delta theta = s divided by the modulus of g_hkl. Given that the modulus of g_hkl simply equals one over the plane spacing d_hkl, we can see that the excitation error, s, is given by delta theta divided by d_hkl. We know that in this s equals negative case, the diffracting plane was tilted this way away from the perfect Bragg condition. Therefore, for signs to correspond, in this case, delta theta must be negative. Alternatively, tilting the other way from the perfect Bragg condition would give a positive delta theta.

Notes

Summary

13m 53s

Deviation from Bragg scattering summary



- Intensity modulates along relrod, within $1/s^2$ envelope
- s: excitation error/ deviation parameter
- s = 0: exact Bragg, intense diffracted beam
- s > 0 or s < 0: weaker intensity in diffracted beam
- Studied *kinematical* regime (single scattering)

Transmission Electron Microscopy

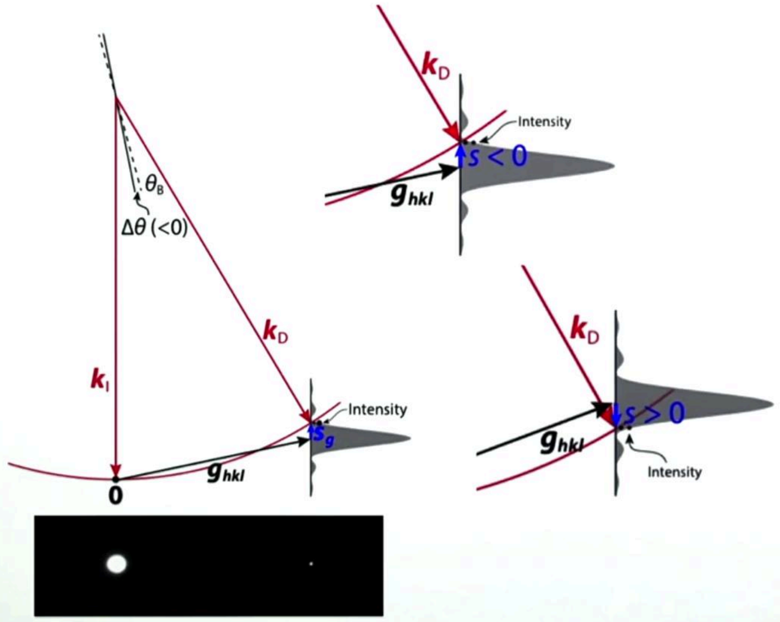
To summarize, in this lecture, we have seen that the intensity distribution along a reciprocal lattice rod modulates within a one over s squared envelope, where s is the excitation error, or deviation parameter. When we are at the exact Bragg condition, s equals zero, and we will have an intense diffracted beam. However, when s is away from zero, the intensity in that diffracted beam can decrease dramatically. Further, we define that: s is greater than zero, when the vector s_g lies within the Ewald sphere, and it is less than zero, when it is outside the Ewald sphere. While all this may seem a bit abstract, knowledge of the excitation error is critical to certain kinds of diffraction contrast imaging. For instance, for imaging dislocations in weak beam or strong beam conditions. Finally, all this was studied in what is called the kinematical regime, meaning single electron scattering. In reality, in a two-beam condition, we typically have what is called dynamical scattering. This is multiple elastic scattering. In the dynamical case, the modulations along the reciprocal lattice rod will be somewhat different. Indeed, you may not even have a maximum in intensity at s equals zero, but at s away from zero.

Notes

Summary

15m 13s

Deviation from Bragg scattering summary



- Intensity modulates along relrod, within $1/s^2$ envelope
- s: excitation error/ deviation parameter
- s = 0: exact Bragg, intense diffracted beam
- s > 0 or s < 0: weaker intensity in diffracted beam
- Studied *kinematical* regime (single scattering)

Transmission Electron Microscopy

However, the general principle that the intensity in the diffracted beam is directly related to the intersection of the Ewald sphere with this intensity distribution remains the same. Thus, this kinematical condition provides a useful introduction to a concept needed for understanding dynamical diffraction.

Notes

Summary

16m 40s