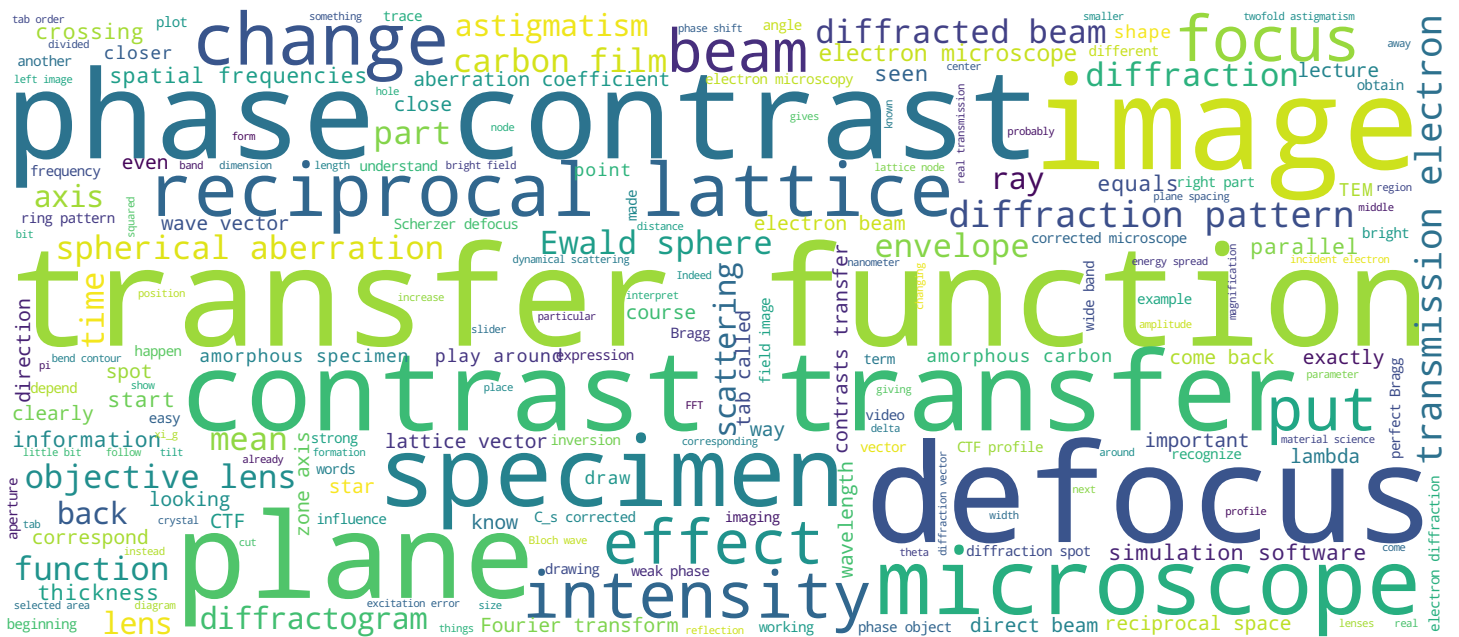


## Phase contrast: the phase contrast transfer function

## Transmission Electron Microscopy

Prof. C. Hébert &amp; Dr. D. Alexander

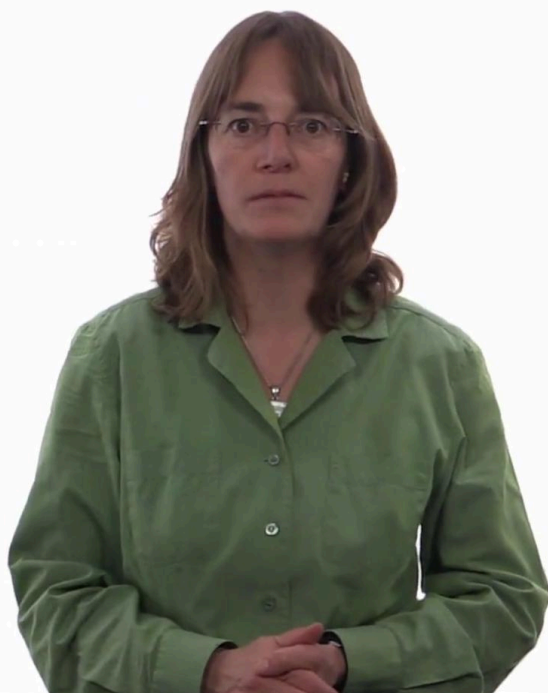


## Search MOOC



## Video





Transmission Electron Microscopy

Welcome to CIME's lectures on Transmission Electron Microscopy for material science. In this video, we will have a closer look at the phase contrast transfer function and we will first look at it with a simulation software and then see its effects in a real transmission electron microscope on amorphous carbon. So from the last video, you remember that we arrived to the phase contrast transfer function when we are imaging a weak phase object with the objective lens.

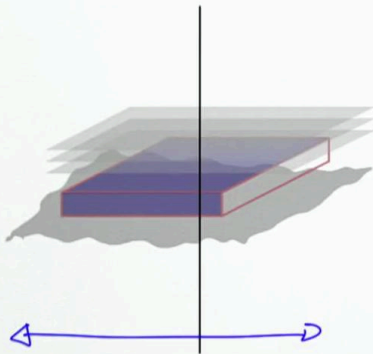
Notes

Summary



0m 05s

# Phase Contrast Transfer Function



$$T(\vec{u}) = \overset{\text{envelope}}{A(\vec{u})} \overset{\text{phase shift}}{E(\vec{u})} 2 \sin \chi(\vec{u})$$

- If we only have defocus and spherical aberration:

$$\chi(\vec{u}) = \pi \Delta f \lambda u^2 + \frac{1}{2} \pi C_s \lambda^3 u^4$$

Transmission Electron Microscopy

This function is made of two parts: an envelope part and a second part which corresponds to a phase shift applied by the objective lens, which depends on the scattering vector, the reciprocal space vector  $u$ . Even if we only have defocus and spherical aberration, this phase shift is already a complicated function of  $u$ , including the defocus, the spherical aberration coefficient and the wavelengths of the electrons. Now in reality we have other aberrations like astigmatism. To each of them corresponds in an analytical formula that can be included in the phase contrast transfer function. So getting an intuitive interpretation of that function is not easy. We will use the simulation software called JEMS to plot this function as a function of  $u$  and also the phase contrasts transfer function, including the envelopes. You have all the instruction to download and install JEMS student edition on the MOOC. And I strongly suggest that you do so to practice and follow what we will see now.

Notes

Summary



0m 41s

jems

File

Crystal

Drawing

Imaging

Indexing

Measuring

Parameters

Window

jems::4.1520U2014

Help

Atom(s) in the unit cell

#	Atom	Wyckoff	x	y	z	D-W	Occ.	Ab
0	Si	h	0.1742	0.7678	0.250	0.000	1.000	0.03
1	Si	h	0.8258	0.2322	0.750	0.000	1.000	0.03
2	Si	h	0.2322	0.4064	0.250	0.000	1.000	0.03
3	Si	h	0.7678	0.5936	0.750	0.000	1.000	0.03
4	Si	h	0.5936	0.8258	0.250	0.000	1.000	0.03
5	Si	h	0.4064	0.1742	0.750	0.000	1.000	0.03
6	N	c	0.333333	0.666666	0.250	0.000	1.000	0.02
7	N	c	0.666667	0.333334	0.750	0.000	1.000	0.02
8	N	h	0.329	0.039	0.250	0.000	1.000	0.02
9	N	h	0.671	0.961	0.750	0.000	1.000	0.02
10	N	h	0.961	0.290	0.250	0.000	1.000	0.02
11	N	h	0.039	0.710	0.750	0.000	1.000	0.02
12	N	h	0.710	0.671	0.250	0.000	1.000	0.02
13	N	h	0.290	0.329	0.750	0.000	1.000	0.02

3-D view

Si3N4P63m : [0, 0, 1]=[0, 0, 0, 1]

Status

java VM:Free memory = 1120387688, available memory = 1130496000, percent used = 1

10:07:31 PM

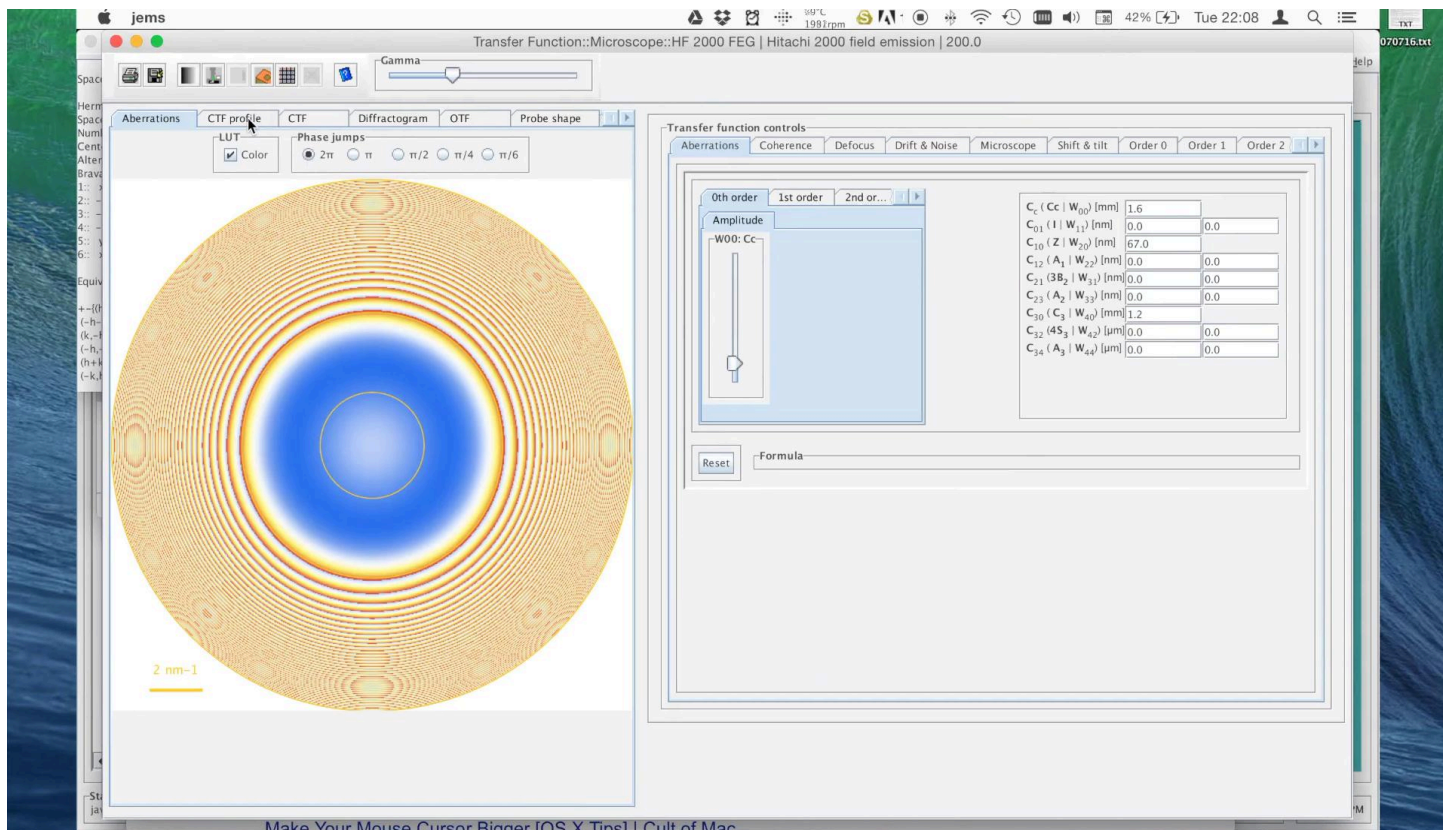
After starting JEMS student edition, you go to the tab called “drawing” and you choose “transfer function”. You have a new screen appearing.

Notes

Summary



2m 08s



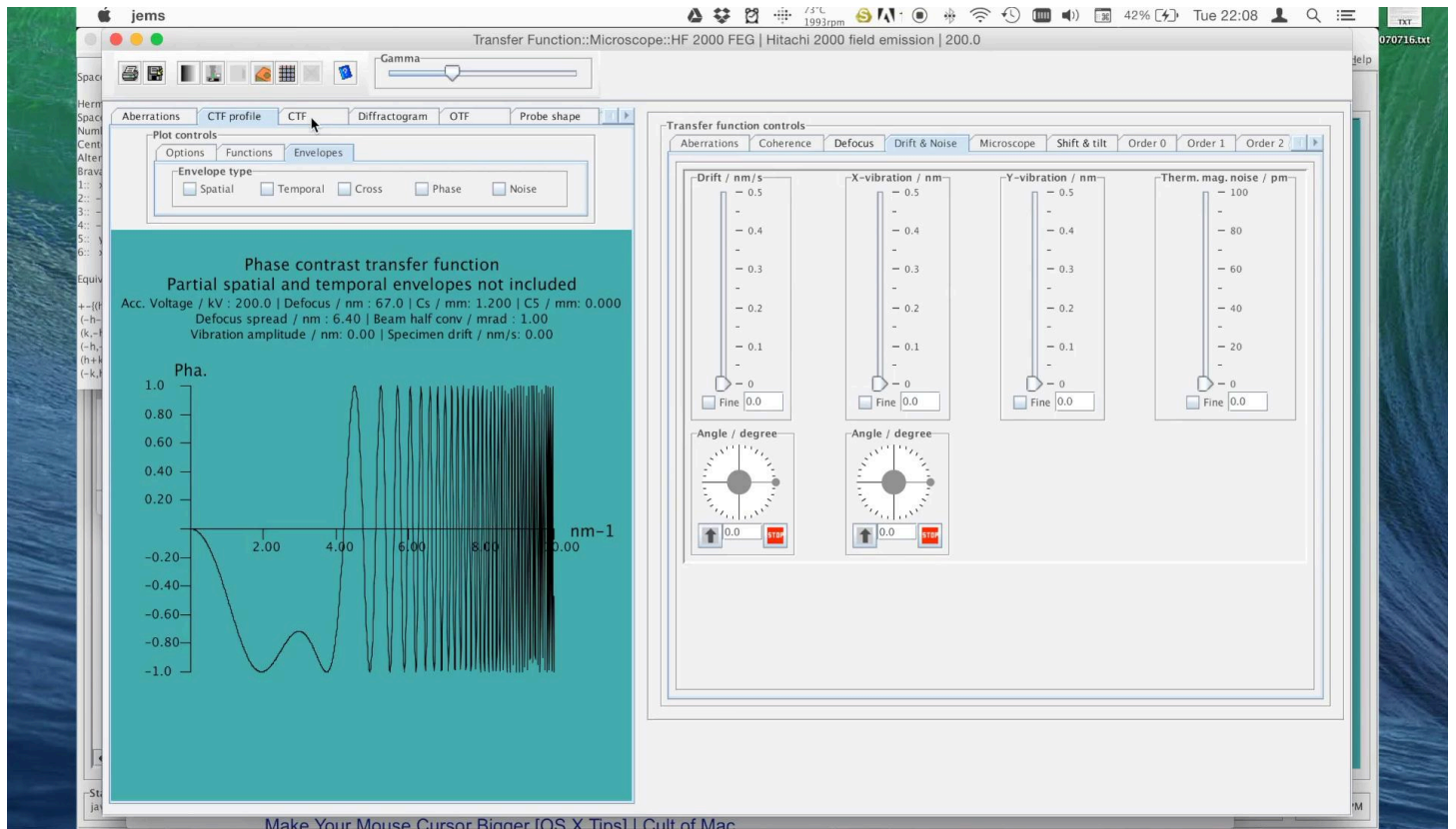
And the first thing we will do will be to select the kind of microscope we will be working with. For the beginning, we take a generic microscope. Let's take the HF2000. This is a Hitachi model but it has 200 kilovolts, 1.6 millimetre for the chromatic aberration coefficient, 1.2 millimetre for the spherical aberration coefficient and here, an energy spread of 0.6. We will put it to 0.8. With this we have a standard field emission gun transmission electron microscope for material science without  $C_s$  correction. Of course, if you know the microscope you are working with, you are free to change those parameters to adapt them to your exact situation.

Notes

Summary







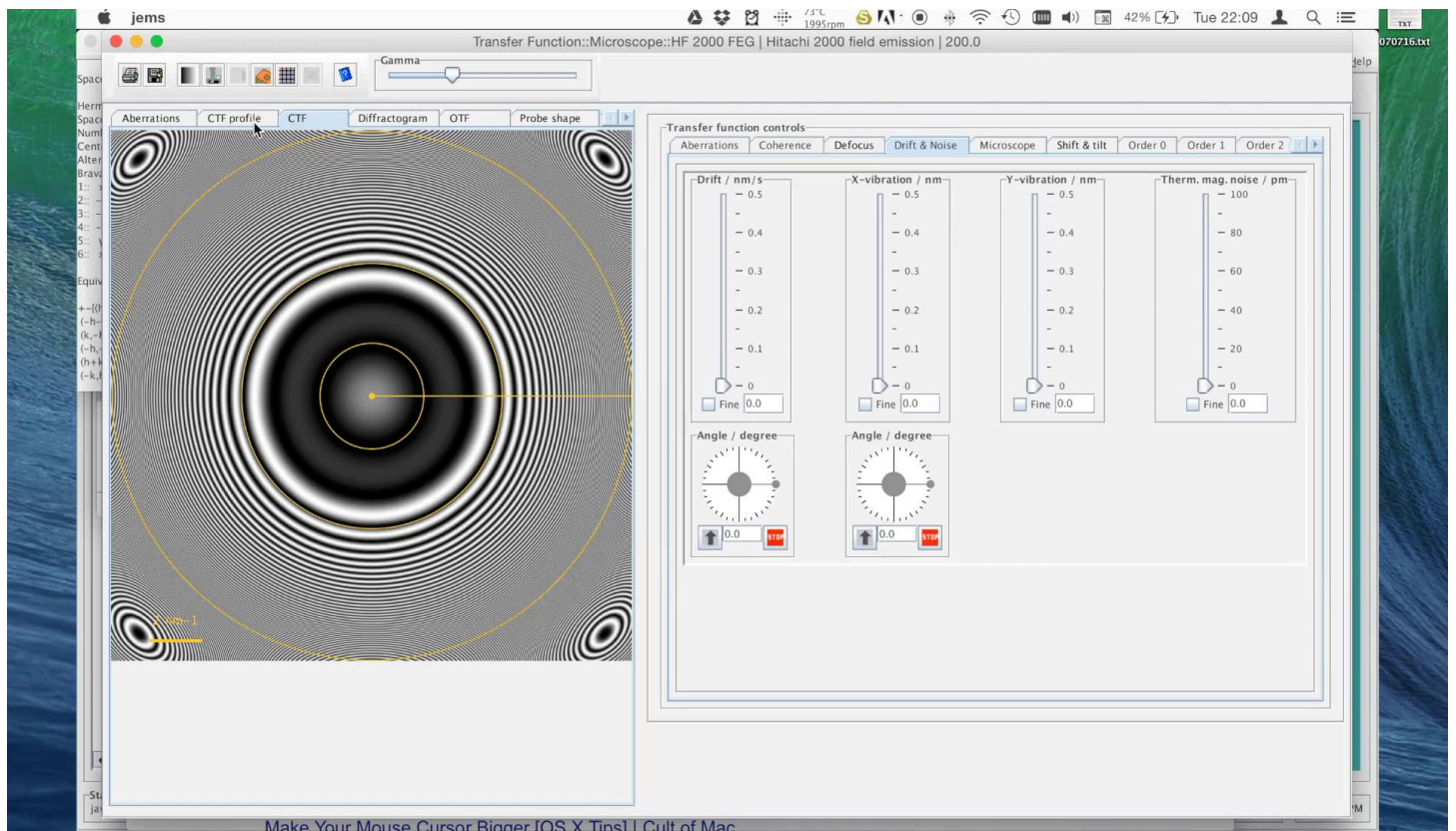
In the tab “CTF profile”, we see a plot of the phase contrast transfer function as a function of reciprocal unit length - so nanometer minus one, it is in reciprocal space - and of course, this is only a trace in one particular direction in the reciprocal space which has normally two dimensions. It includes all the terms at the beginning but we will start by removing the influence of the envelopes. So we go to the tab called “envelope”, and we remove all those envelopes. Also, there is a remaining influence from the tab “drift and noise” which we put to zero as well. With this, the phase contrast transfer function is as we expect, oscillating strongly and between one and minus one, it is because it is the same function of this complicated function of  $u$ , including  $C_s$ , defocus and wavelengths of the electrons.

Notes

Summary



3m 28s

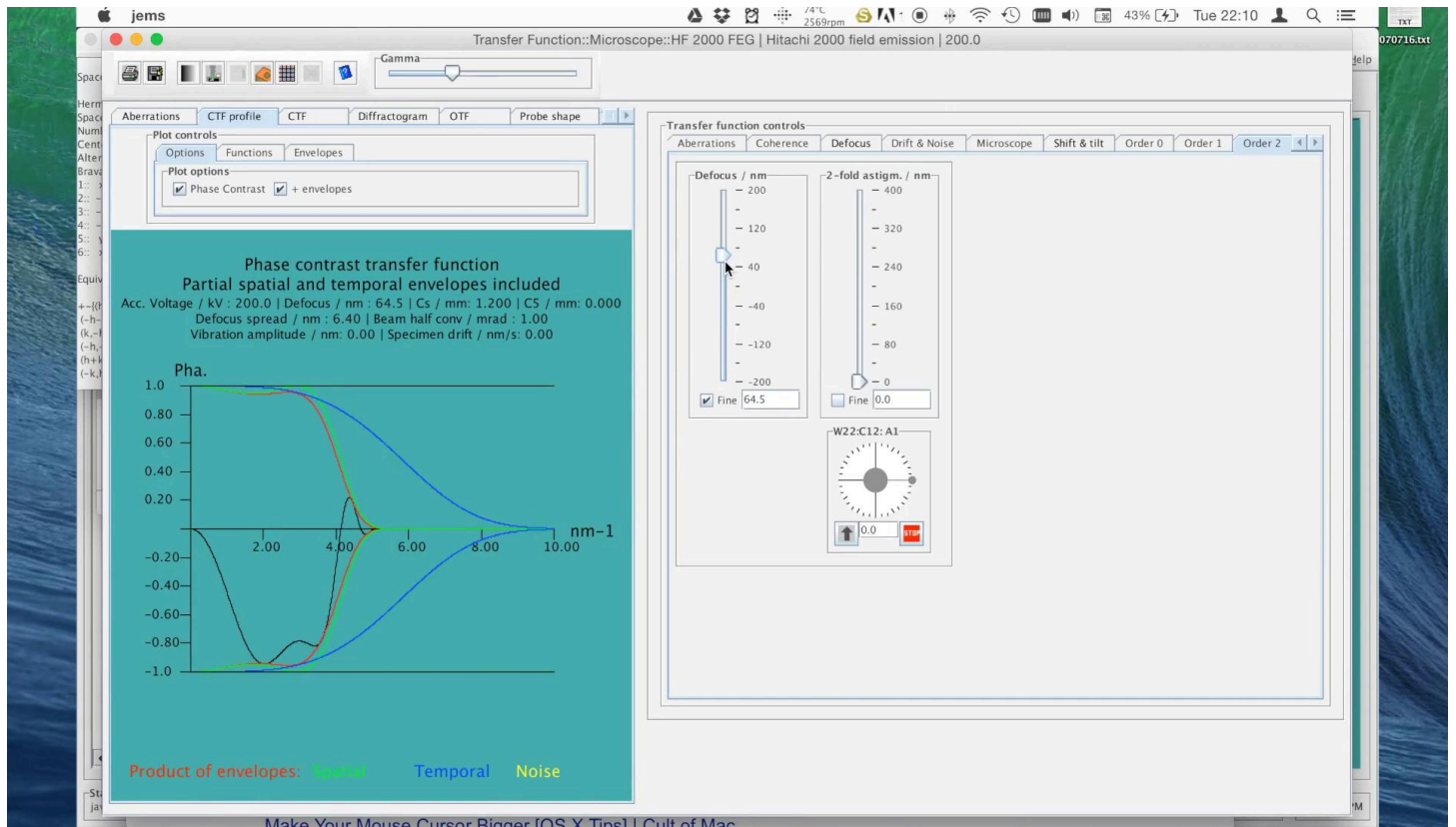


In the tab called “CTF”, besides the CTF profile, you can have a look at the 2-D drawing of the contrast transfer function, also in reciprocal space, but here we have the view of the reciprocal vector and not just the trace in one direction.

- Notes

## Summary





The CTF profile will be sufficient for now as we are working with aberration which have a cylindrical symmetry. So the CTF are circular and we have all the information in a clear way from the profile. On the right part of the screen, in the tab "order two", I have access to the defocus of the microscope. Let's do it with the "fine" so we don't change it too much and see what happens if we change the defocus with this slider. You see how the oscillations change as we change  $\Delta f$  which will influence the phase contrast transfer function. But whatever we do, at high spatial frequency we have these strong oscillations. Let's put back the envelopes, spatial and temporal, and go to "option" and plot them. Sow now we see not only the effects on the envelope but the trace of those. You can change the parameters that influence the envelopes in the tab called "coherence", especially the energy spread of the microscope. OK. No we can come back to this "order two" and change the defocus while we have the effect on the envelopes.

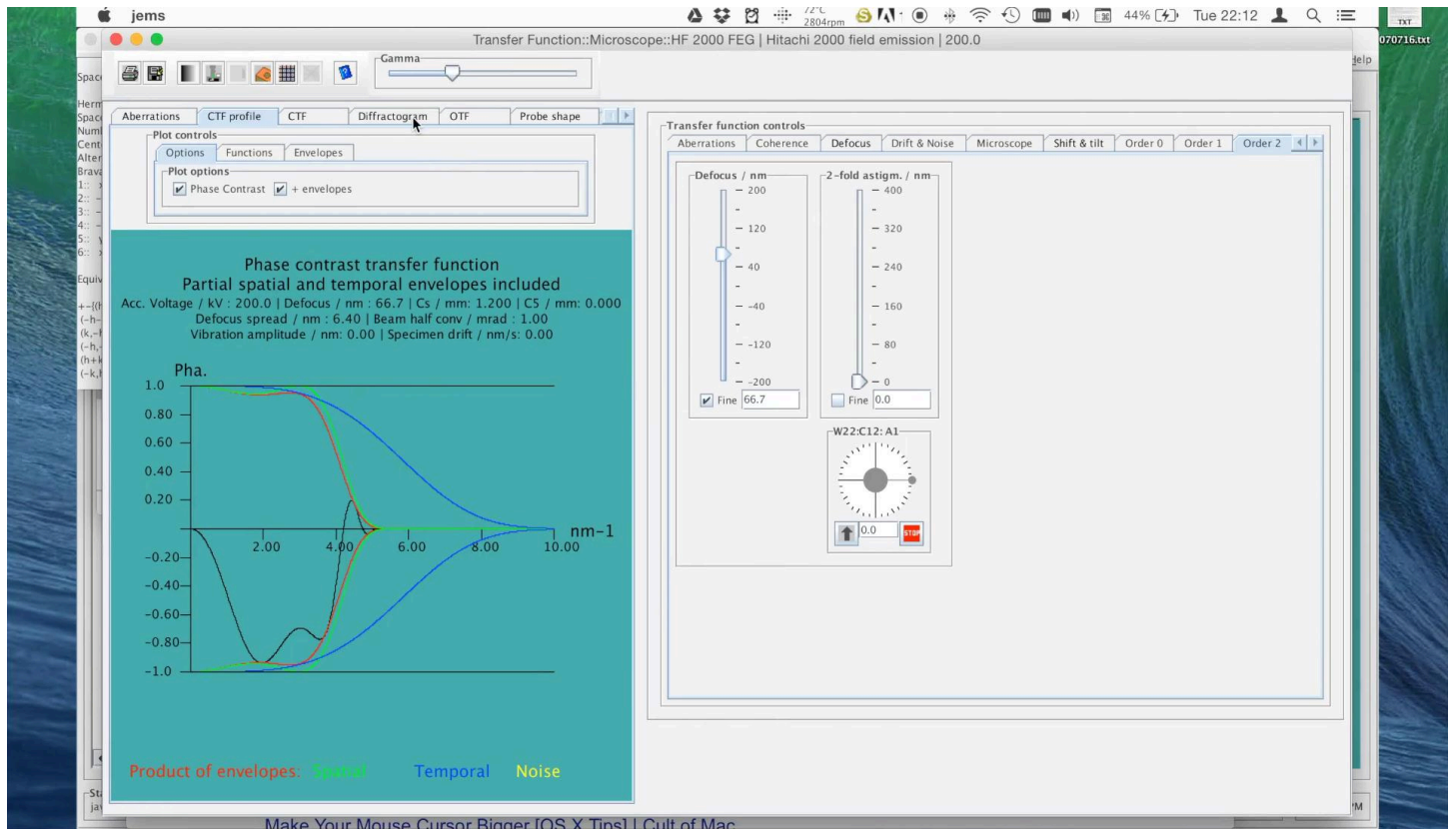
Notes

Summary



5m 14s



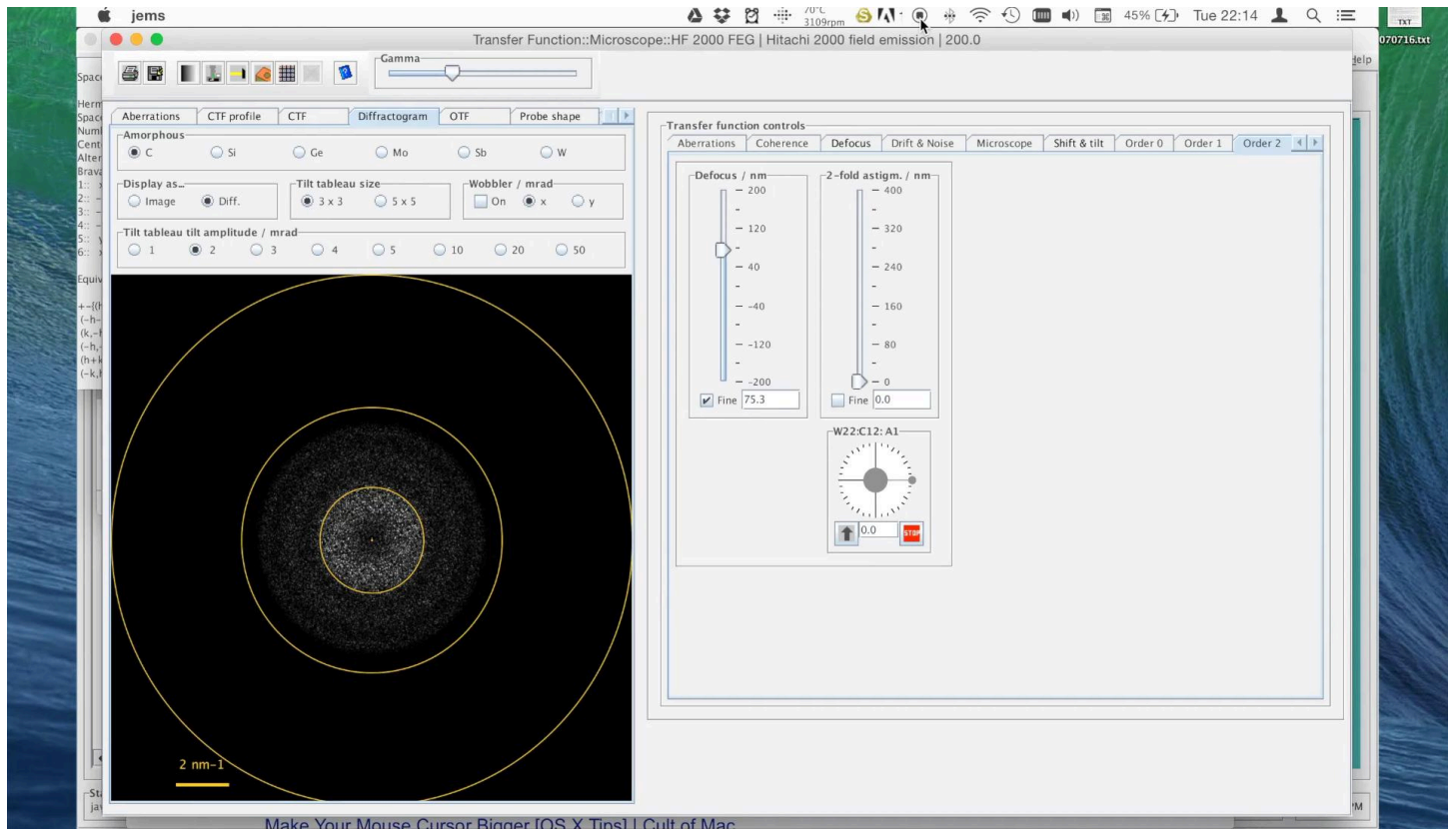


Still we see strong changes in the phase contrasts transfer function and we see that we are able for example to put it in a way where we have a relatively wide band where the phase contrasts transfer function is close to minus one at more or less constant, while in other range of the defocus we have a crossing of the zero axis in the middle of the accessible spatial frequencies. A zero crossing means that we have no phase contrast transfer at these particular spatial frequencies. In other words, we have no information transferred. So we will be missing part of the information in the image. Also, around the crossing, we have an inversion of the sign of the phase contrast transfer function. This means that we will have an inversion of contrast for the different spatial frequencies, before and after the crossing. Obviously, an image acquired under those conditions will not be very easy to interpret. Playing around with the defocus, we find only one value of delta f which gives us this wide band of transferred frequencies. Now in the tab called "diffractogram", I have the possibility to simulate the image of an amorphous specimen, for example carbon or its diffractogram, which is the fast Fourier transform of the image.

Notes

Summary



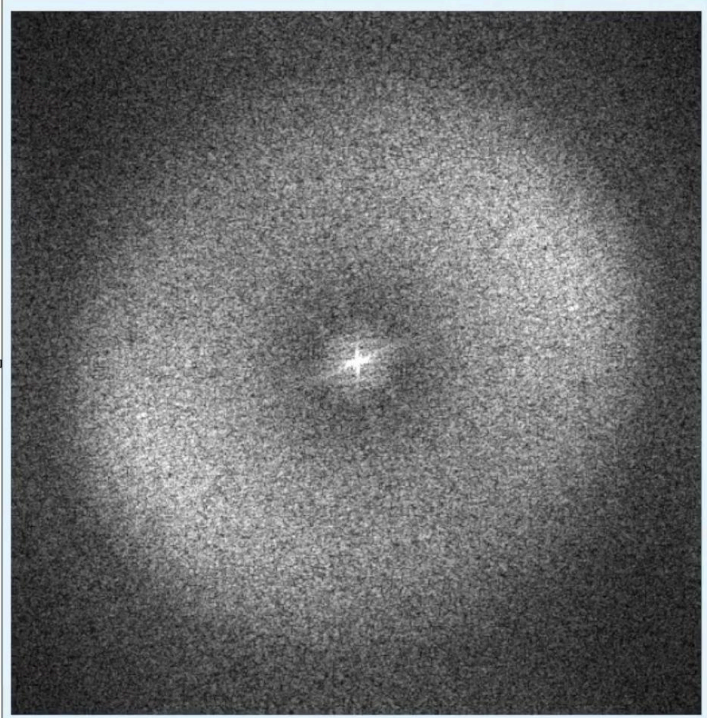
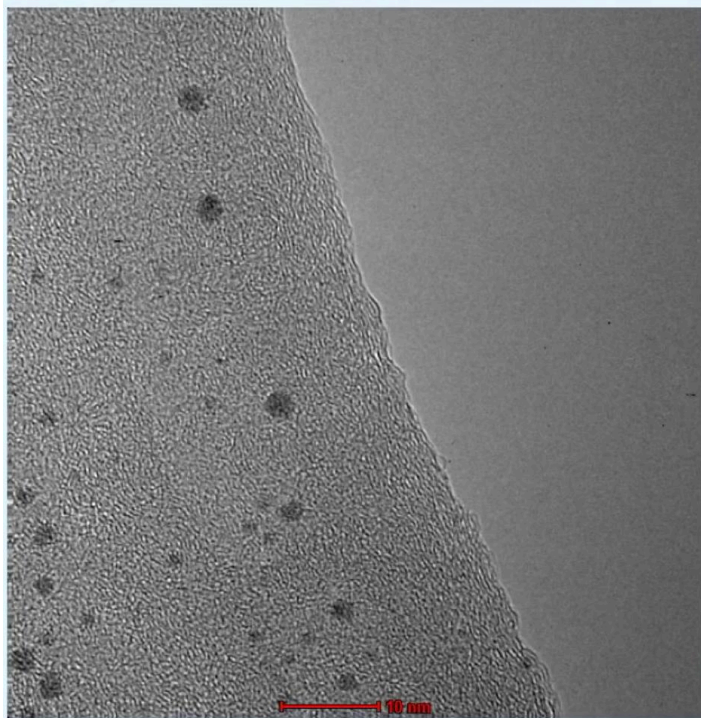


This diffractogram is closely related to the phase contrast transfer function. Dark rings correspond to regions where no info is transferred, hence crossing of the zero axis in the phase contrasts transfer function. The dark circles that you see appearing at some defocus and some value of  $u$  means that, at those particular frequencies, I have no information transfer. Using an amorphous specimen to look at the contrast transfer function is a good idea because amorphous specimen will have a wide band of spatial frequencies over the whole specimen region. Now we will go to the real transmission electron microscope to see how things look like with an amorphous carbon film when we take an image and build the fast Fourier transform of this image.

Notes

Summary





Here, my specimen is an amorphous carbon film with a few very small particles. And on the right part of the image there is a hole, so no specimen. In the right pannel, you see the fast Fourier transform, also called diffractogram, of the left image. Now I will start to change the focus, going to under focus and then back to over focus. You see two things: on the right part in the diffractogram, you see this ring pattern like we had in the contrasts transfer function. On the left part on the image, you see clearly the defocused carbon film. Now I'm back towards focus. When I'm in focus, I have the minimum contrast and now my contrast is increasing again. I see again the rings. It is important to keep in mind that those black rings are spatial frequencies which are not transmitted by the optical system. So in that region I have no transfer of information.

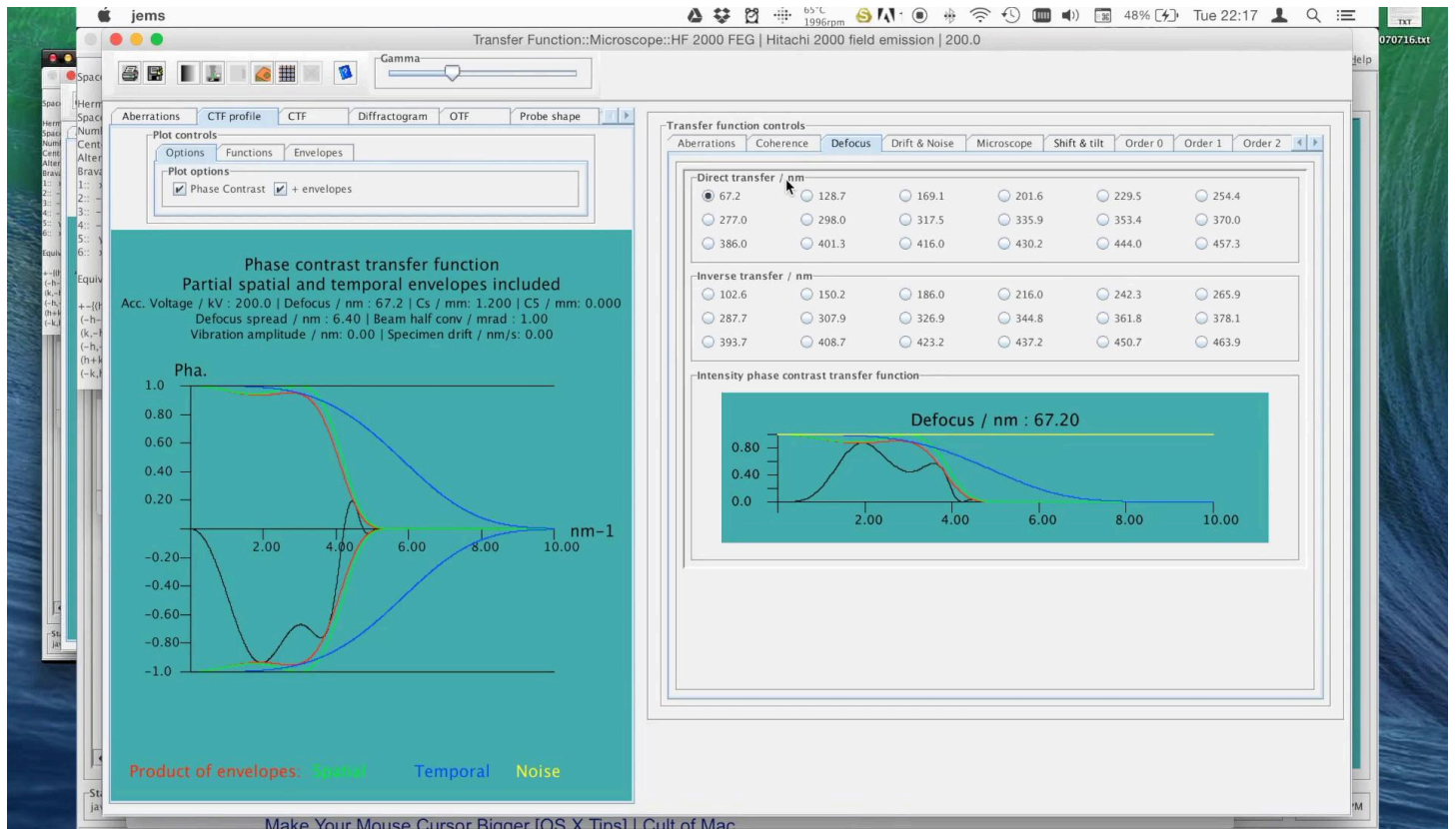
Notes

Summary



9m 29s





So back to the simulation software, we will now have a closer look at the particular defocus for which I had a good transfer of information. We come back to the CTF profile and we play around with the focus to see if we can find an optimal value of  $\Delta f$ . Clearly I have a tradeoff between the width of this band and the small indentation in the middle of it. If we look at the tab “defocus”, we have the preselected value of the defocus, and actually, the first one gives me a good compromise. No surprise. This is Scherzer's defocus. And we will now try to see close up what it really means in the transmission electron microscope.

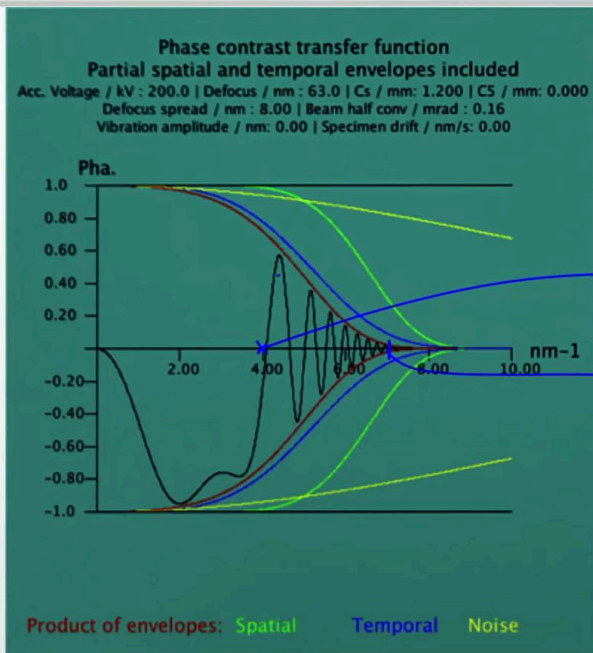
Notes

Summary





# Point resolution and information limit



Scherzer's defocus:

$$D_{\text{Scherzer}} = 0.66 \lambda^{3/4} C_s^{1/4}$$

point resolution of the microscope

Transmission Electron Microscopy

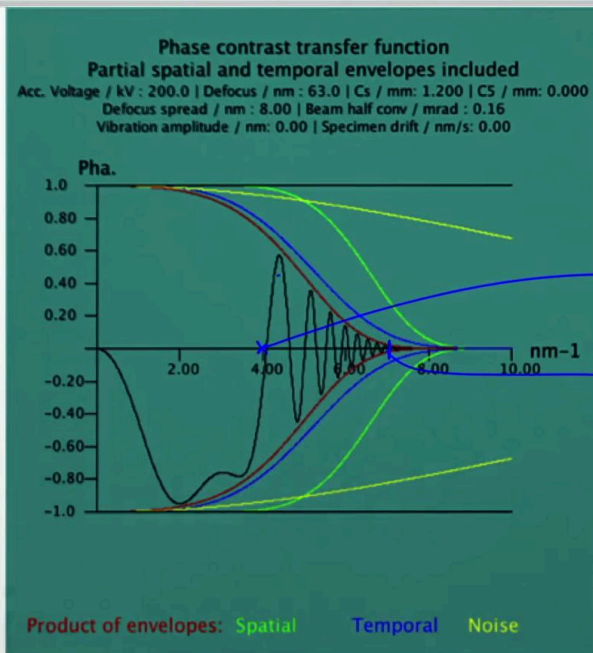
Let's have a closer look at the situation. When I choose this value for the defocus, I have then the first crossing of the phase contrast transfer function with the zero axis. At this frequency, I have no contrast transferred. And after this frequency, the phase contrast transfer function is oscillating. This means that we will have several crossing with the zero axis where no contrast is transferred as well as parts where the contrast is positive and parts where it is negative. This will produce images which are difficult to interpret. We refer to this crossing as being the point resolution of the microscope. I can obtain it for the particular value of defocus called Scherzer's defocus which depends on the wave length and the spherical aberration coefficient and which will give a good compromise in terms of width and value of the phase contrast transfer function in this first band. But even after this first crossing, you will see that I am able to transfer some frequency and by tweaking the defocus I could be able to map all this frequency domain up to a certain point. When the envelopes are cutting completely the phase contrast transfer function, then I cannot get anything more out of my microscope.

Notes

Summary



# Point resolution and information limit



Scherzer's defocus:

$$D_{\text{Scherzer}} = 0.66 \lambda^{3/4} C_s^{1/4}$$

point resolution of the microscope

information limit.

Transmission Electron Microscopy

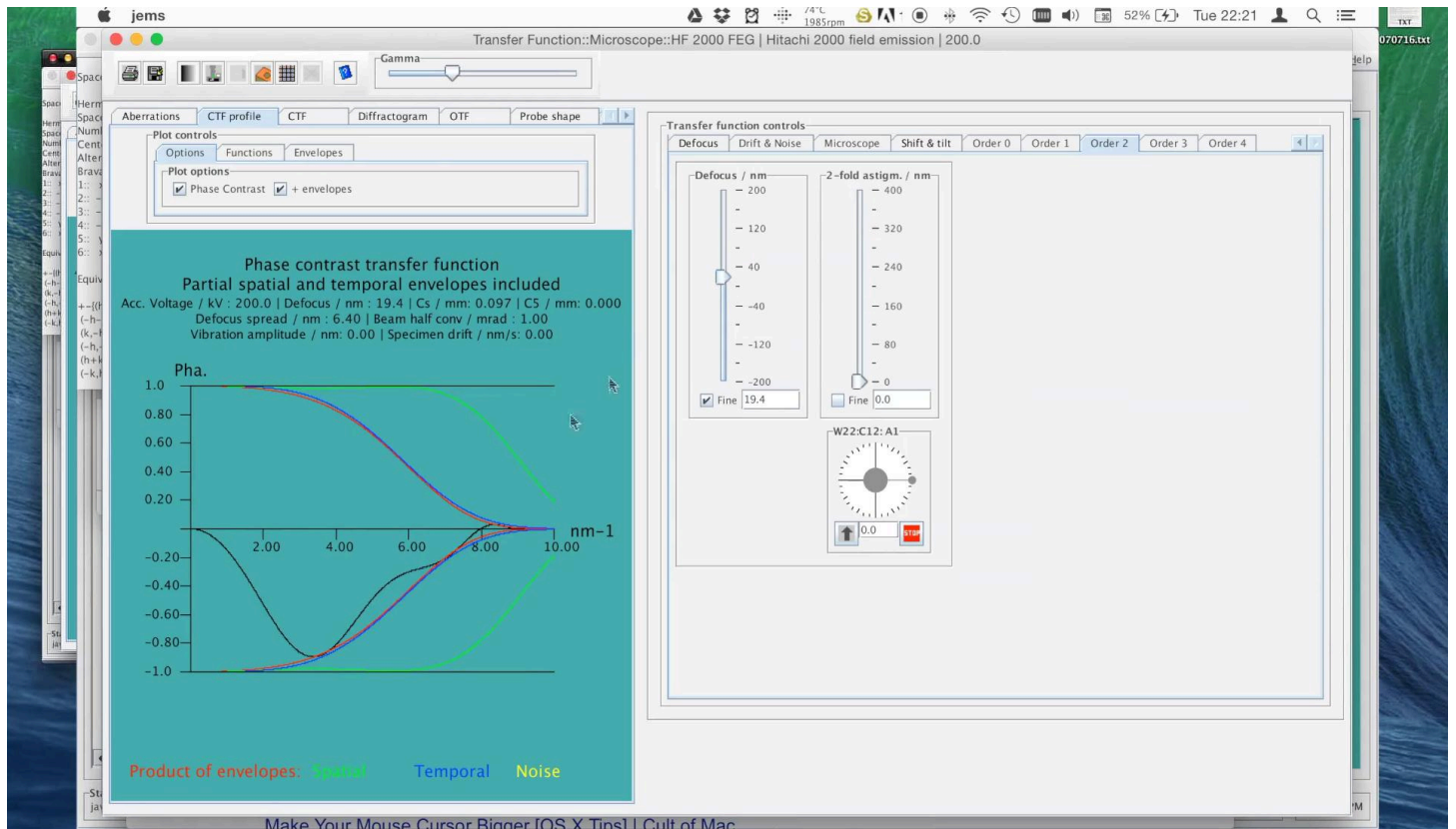
This is called the "information limit". But what is happening if I have a C<sub>s</sub> corrected microscope? For a C<sub>s</sub> corrected microscope, the spherical aberration coefficient can be corrected and be equal to zero. Would that mean that the Scherzer's defocus would also be zero? Let's have a look at what the simulation software tells us.

Notes

Summary



13m 54s



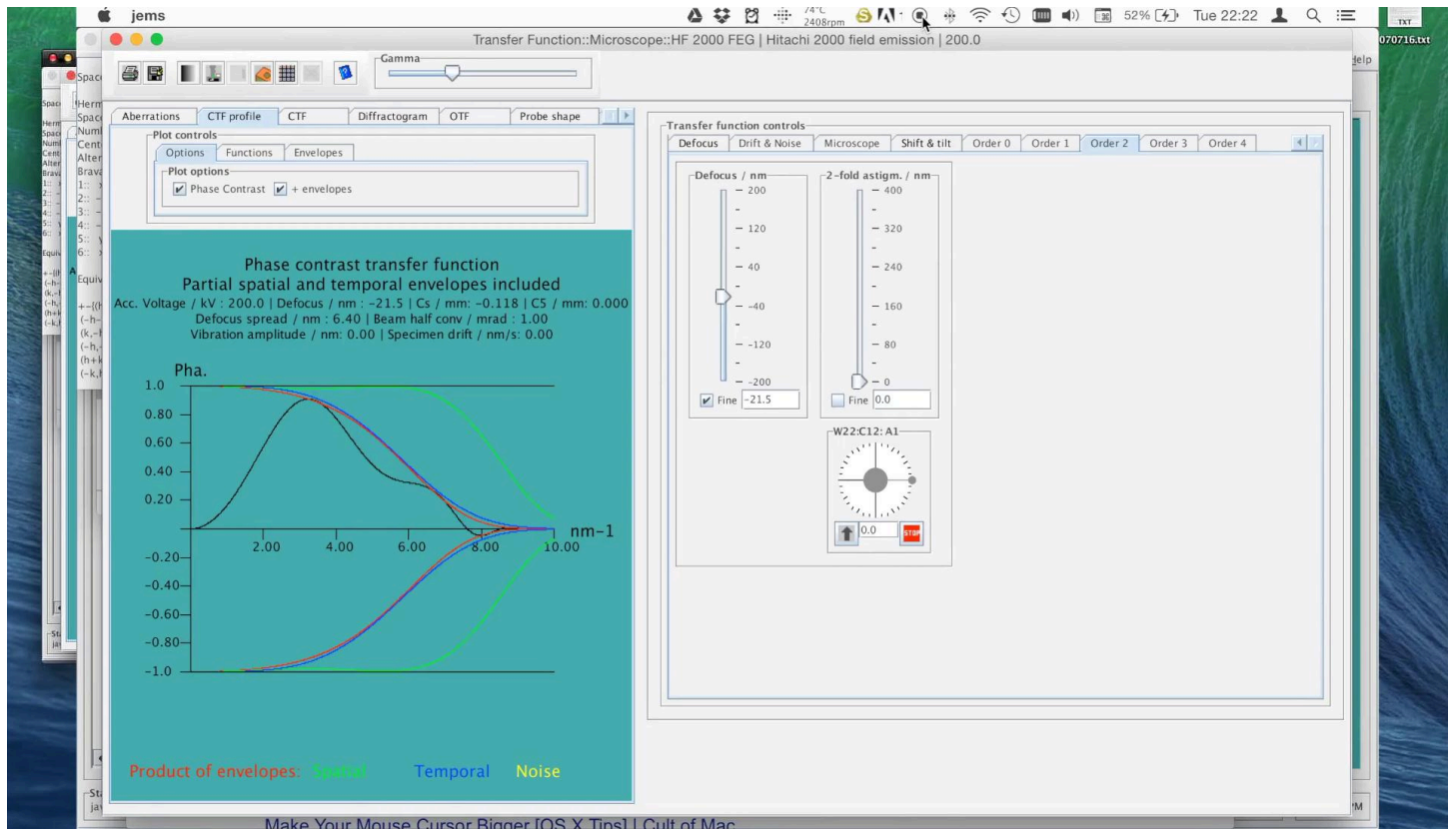
So now I come back to the same situation and microscope as before, but I will change it to have a corrected  $C_s$ , so a spherical aberration which is put to zero. I find this in the tab "order 4", and I can take the slider and put the  $C_s$ , actually to the value I want but I will be choosing exactly zero. Whoops! What happens there? I don't see my phase contrast transfer function anymore. The Scherzer's defocus is zero, and I am now at Scherzer, zero defocus, but what happened? Let's look at the tab where I have the defocus and play a bit with the defocus. Indeed, if I add some defocus I see my phase contrast transfer function coming back. That is a well known effect. If you have a perfect correction of the spherical aberration, no defocus and a weak phase object, we will have zero contrast. Very good resolution but no contrast so no image of the specimen. Of course, if you have a specimen that goes beyond the weak phase object approximation, you will probably see something but it will not be easy to interpret. The work around is to put a little bit of  $C_s$ , but much smaller than what you usually have in a microscope, so in some micrometer range. And then, playing around with the defocus, I can again find the condition where I have this Scherzer's defocus or white band.

Notes

Summary

14m 20s





And the good thing is there that the point resolution is very close to the information limit of the microscope. But what I can do too is put a negative C<sub>s</sub>, because that is allowed by the C<sub>s</sub> corrector. And then you see an inversion of the contrast and especially if you adjust the defocus to have the proper wide band of phase contrast transfer function, then you have a positive contrast and this will give you very nice images, especially if you are imaging small particles or very thin layers.

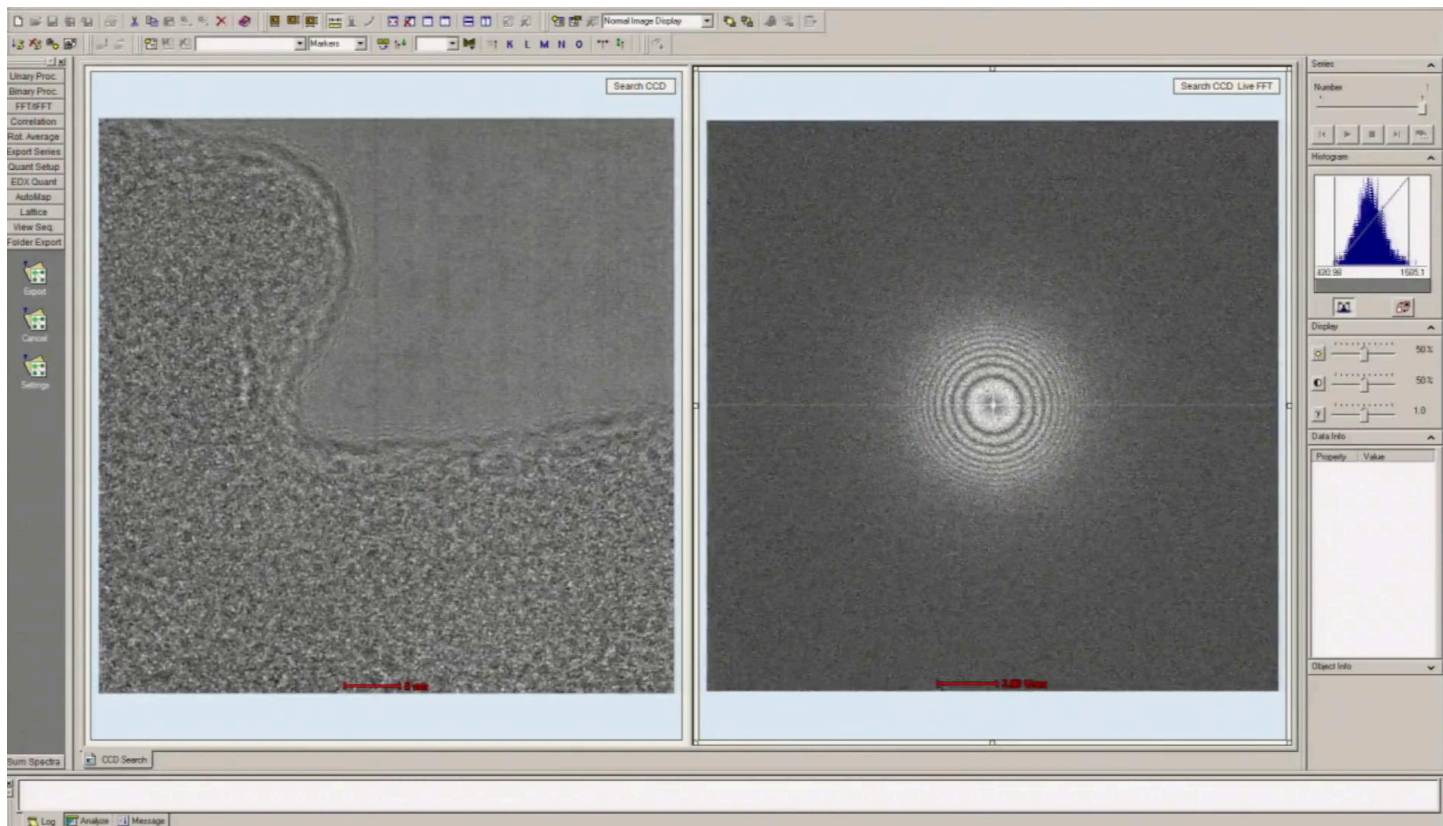
Notes

Summary



16m 23s



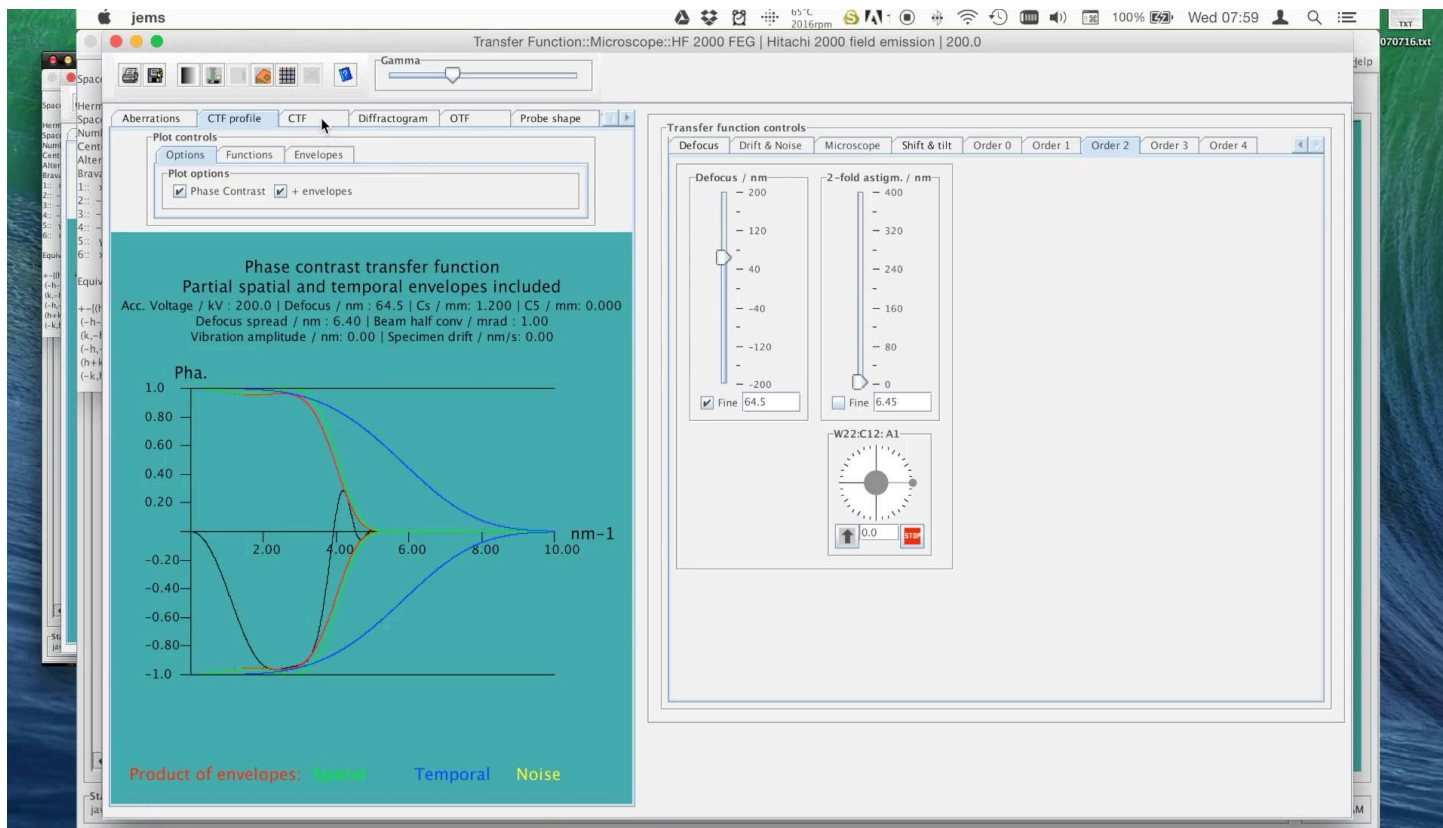


Now we will have a quick look at what a thin amorphous carbon film looks like in a C<sub>s</sub> corrected microscope. At the beginning, I have a defocus of zero and actually so few contrast that you probably cannot recognize where the film is and where the hole is. On the right part, you see the FFT of the left image. Increasing the defocus, you see progressively the contrast appearing and exactly the same ring pattern as before on the non C<sub>s</sub> corrected microscope. Here we are not so much limited by the envelope but made more available spatial frequencies given by the carbon film. And now I will come back to zero defocus and see how the ring pattern and the image are changing. After that, the next step would be to look at the effect of astigmatism.

Notes

Summary





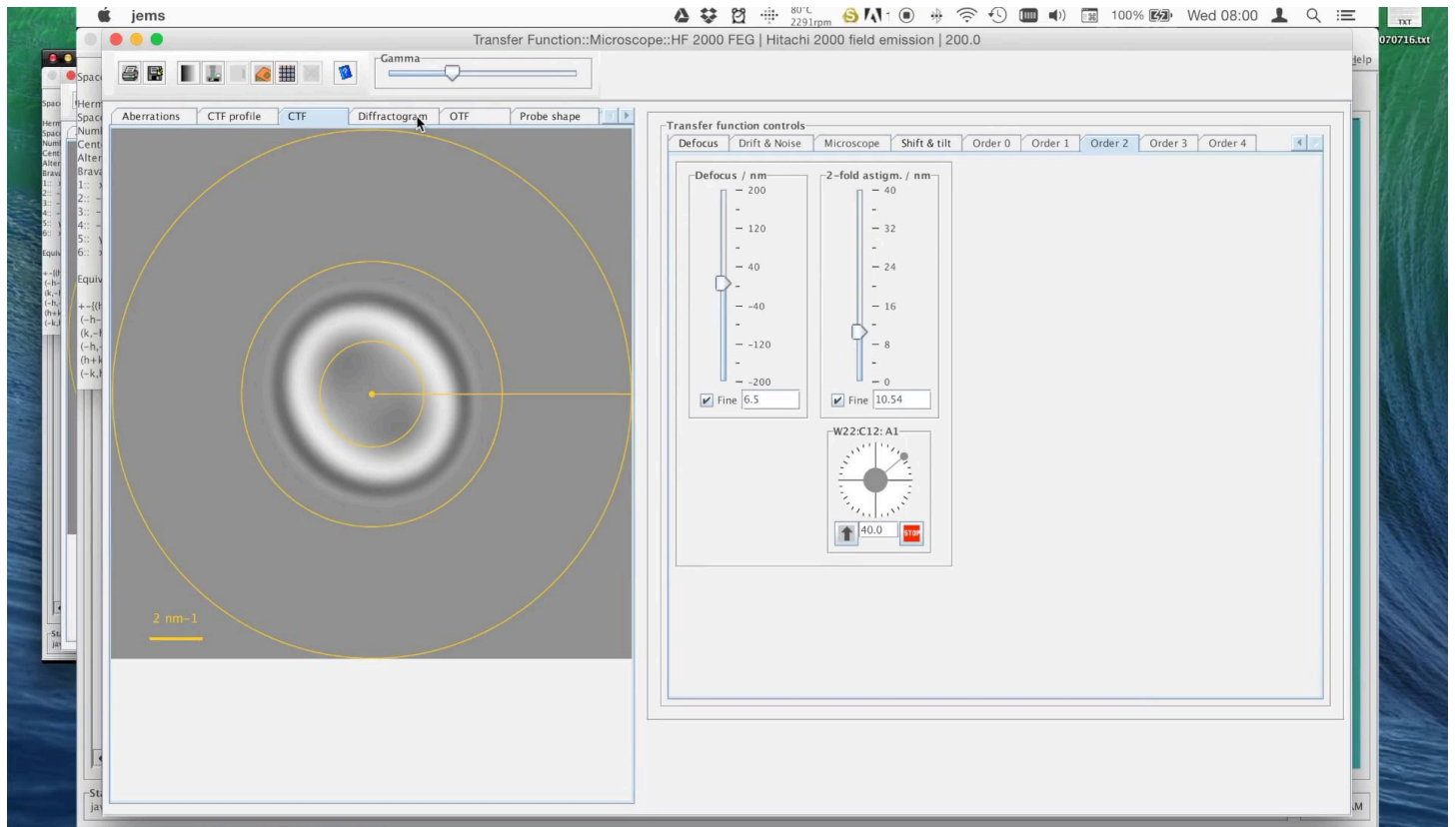
So now we are back to the simulation software to look at the effect of astigmatism. First of all I want to take the same microscope as before and we will put the spherical aberration back to 1.2 millimetre. With this, the CTF has the usual circular symmetry. Back to the tab which contains the defocus but also twofold astigmatism. We can for example change the twofold astigmatism or first put the defocused to a value which is close to the Scherzer's defocus we have seen before. If I now play around with the twofold astigmatism, actually I don't see much difference with what happened before.

Notes

Summary



18m 21s

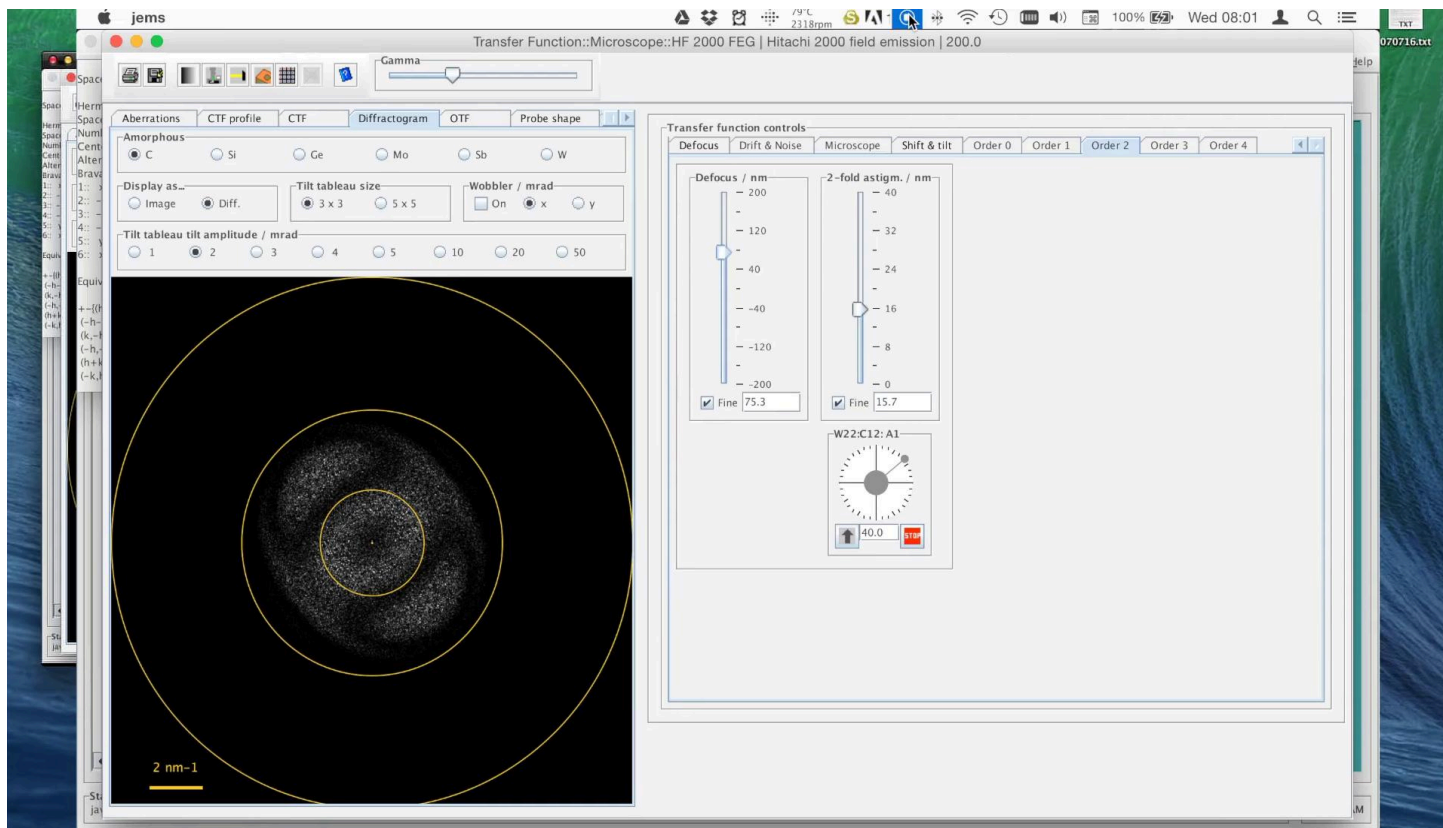


We should not forget that we are looking at an aberration which has different effects in two perpendicular directions. So we really need to look at the CTF and not at the profile to understand what is going on. Here, you see the strong asymmetry in the CTF in two dimension and with this slider, we are able to turn it on the screen. Once I have put a lot of astigmatism, I can play around with the defocus and see how the pattern changes in a relatively complicated way, also including crosses, oval patterns, ring patterns and so on. I suggest that you play around yourself with the JEMS software to see a little bit what effect you can get. Watching the shape of the CTF, which you can see in the FFT of the image of an amorphous sample, will obviously be a big help to correct the astigmatism of your microscope.

Notes

Summary





Looking at the diffractogram, we recognize a similar shape than the one we had in the CTF. And indeed, that would be easy to recognize on your microscope. So now, we will jump to the real microscope and see if we can see exactly the same shape as we head here.

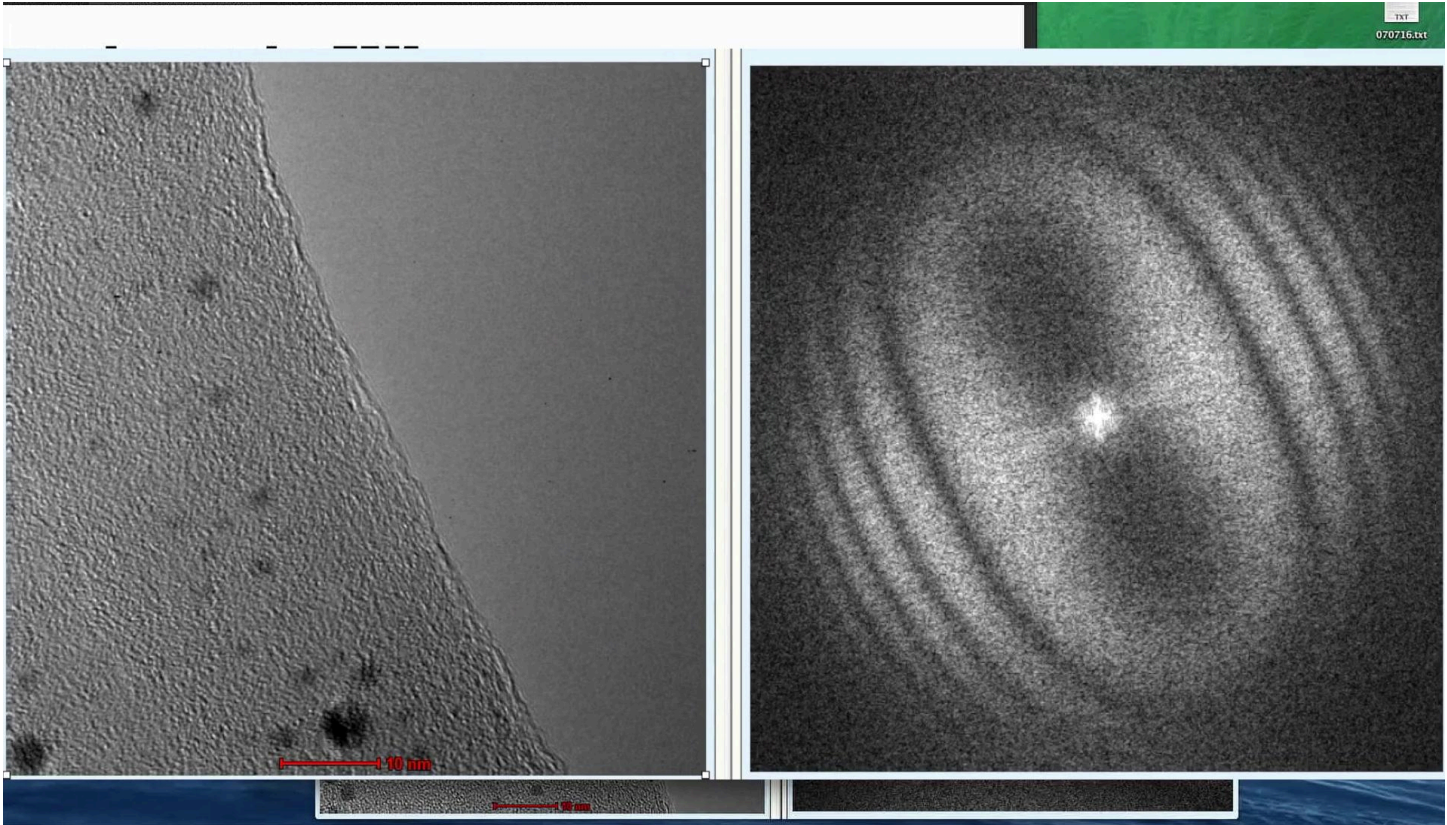
Notes

Summary



20m 42s





Back to the same specimen as before, just having a slight defocus to see one black ring. My microscope was correctly adjusted and now I will start to mess up with the astigmatism correction. You see how the diffractogram loses its symmetry - it is becoming oval. Now I change the focus and you see the same changes in the diffractogram as we had in the CTF using JEMS. Back to the same under-focus as before, now I will increase the astigmatism even further. So that will make the diffractogram more oval. And if you look on the left image, you start to see an elongated structure in the carbon film. And when you go through the focus and then to over-focus, you see how the direction of the structure changes in the film. This is a typical effect of astigmatism in a carbon film. And clearly the diffractogram will be a big help to correct astigmatism and have a well aligned microscope OK.

Notes

Summary

21m 14s



# Conclusion



Transmission Electron Microscopy

with this video you have seen the effect of the phase contrast transfer function on a thin amorphous specimen, and how it is possible to draw it with a simulation software and to image it with a carbon film in the transmission electron microscope.

Notes

Summary



22m 45s