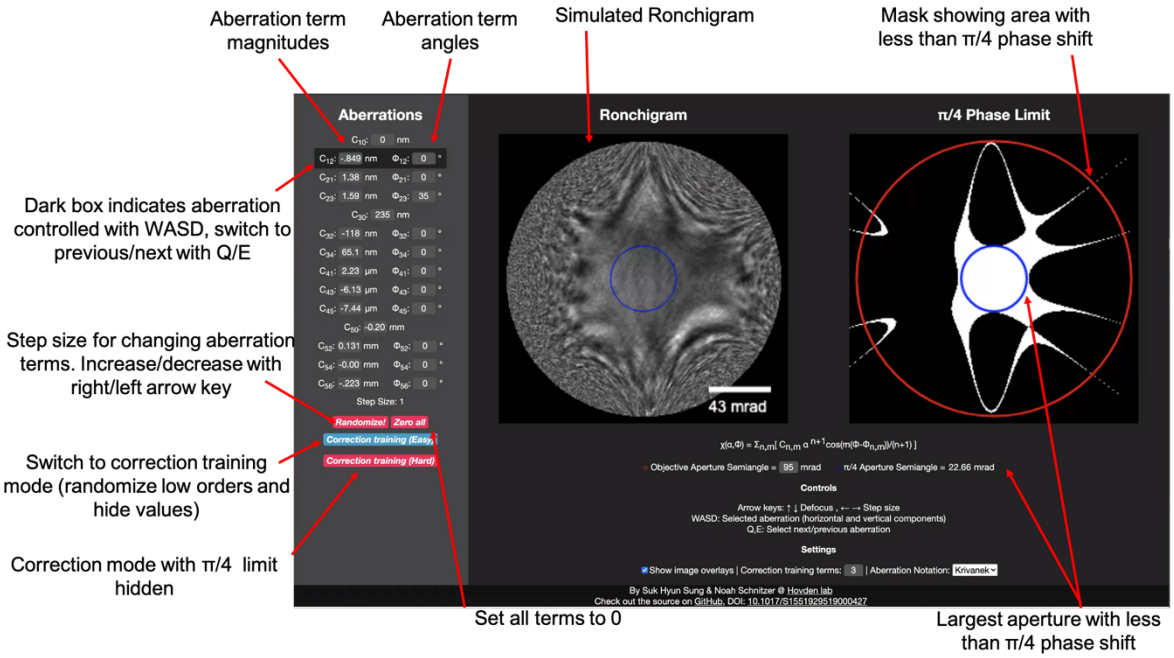
T1: STEM Probe and Imaging

In this 2-part activity, we will explore how aberrations in the microscope affect the electron probe and the image. First, we will simulate how aberrations appear in the electron Ronchigram. In practice, we use the Ronchigram to identify and then correct aberrations in the STEM probe, and in this activity, we will use a web application to simulate that experience off the microscope. Then we will calculate what the probe looks like in real space (the point spread function) and how information is transferred at different frequencies (the contrast transfer function). Finally, we will use a lightweight image simulation to visualize how microscope parameters and aberrations affect the image and can cause artifacts.

1. Assessing aberrations with the Ronchigram

Here we will see how aberrations affect the ronchigram, and how we can use the ronchigram to tune the STEM probe. To begin, open the application in the browser at http://ronchigram.com/vasco.

1.1 Layout and shortcuts



The annotated image above shows the key features of the Ronchigram simulator interface. Keyboard shortcuts allow the aberration function to be quickly changed, it is highly recommended that you use them: WASD change the aberration term with the dark box surrounding it (starts as C_{12}), Q and E change the selected term, the up/down arrows always change defocus, and the left/right arrows change the step size of the aberration

changes. The aberration terms can also be set manually by clicking in the boxes and typing.

If you want to get back to default settings quickly, just reload the page in the browser, or use the shortcut Cmd+r/Ctrl+r in either the browser or executable.

1.2 Ronchigram and aberration basics

The Ronchigram displayed initially is using the aberration function from an actual STEM. The low order aberrations, in particular defocus (C_{10}) and 2-fold astigmatism (C_{12}) are very small but there are significant higher order terms. In the center of the Ronchigram is a fairly large flat region, where the probe wavefunction phase is not fast varying. This flat region can be used to form a spatially confined STEM probe, including areas with large variations increases probe size, but as discussed in lecture there is a tradeoff with the diffraction limited resolution. For this activity we will keep the semiangle at 95 mrad to visualize the effects of the aberrations (as is generally done during tuning), but when imaging a smaller aperture which only uncovers the flat region in the center is used. The blue circle marks one heuristic for a good aperture size for the current aberration function.

- Try increasing defocus (up/down arrows), and look at how the Ronchigram changes. Pay particular attention to what happens to the initially fairly flat region in the center, and how the blue circle changes size as defocus (C_{10}) is increased up to ~15-20 nm (you may want to increase step size using the left/right arrow keys).
- Keeping defocus large, now look at the effect of 2-fold astigmatism (C_{12}). Notice that this term is not radially symmetric, using WASD the W and S keys change the vertical component of the aberration, and the A and D change the horizontal component. With a large amount of 2-fold astigmatism (C_{12}) (~20 nm), observe how the directionality of the streaks in the Ronchigram change when under and over focused (e.g. -20 nm and +20 nm C_{10}). 2-fold astigmatism is a very important aberration to be able to recognize by eye, unlike many higher orders it is generally corrected by hand.
- Bring 2-fold (C_{12}) back to 0, but keep defocus large. Now try increasing Axial Coma (C_{21}) to ~200 nm. Observe how the Ronchigram changes as defocus (C_{10}) is swung through ~-20 to 20 nm: the flat region of the Ronchigram seems to swing across the aperture, the direction of the swing corresponds to the direction of the coma. This is the highest order aberration usually corrected by hand, the strategy for doing so is typically to try to minimize the swing while going through focus.
- Briefly look at the effects of the other aberration terms. C_{23} (threefold astigmatism, occasionally corrected by hand), C_{30} (spherical aberration), and C_{32} (star) all have fairly distinctive effects, but they can be hard to see on the background of the higher orders and will generally not be assessed by eye. If you'd like to look at them individually, you can press the Zero all button to remove all aberrations. Note

that on uncorrected microscopes C_{30} dominates (typically larger than 1mm), giving the Ronchigram a characteristic radial shape if low orders are well corrected.

1.3 Correction Training

- Press the Zero all button, then press the Correction training (Easy) button. By default, this randomizes the first 3 terms of the aberration function and hides all of the magnitudes/angles, all the higher orders are 0.
- Using your understanding of defocus (C_{10}), 2-fold astigmatism (C_{12}), and coma (C_{21}), adjust these terms to make the Ronchigram as flat as possible – try to get the π/4 aperture semiangle (blue circle) to at least 20 mrad (a pop up will come up when you do!) If you're having trouble you can use Cmd/ctrl+r to go back to the initial mode to look at the effect of the aberrations more, or ask for help from the workshop TAs. You can also press the Correction training button to get a new random aberration set.
- Once you're feeling confident with the higher order terms set to zero, try pressing Cmd/ctrl+r, then immediately press aberration correction (Easy). This will randomize the first 3 terms but leave the higher order terms non-zero, making correction trickier. You can also randomize more terms by setting the Correction training terms input higher, and use the correction mode (hard) if time allows.

2. PSF and CTF Plotting, Image simulation

Here we will inspect the probe shape in real space (the PSF) and in reciprocal space (the CTF) to see how much information will be transferred as a function of spatial frequencies. We will change aberrations with spherical symmetry and the convergence angle and see their effect on the probe, as well as simulate images with astigmatism, coma and 3-fold to see how artifacts can occur while imaging due to aberrations.

- For this section, sign in to the VM and copy the whole `Tutorial 1 – STEM Imaging' folder from the 2021-shared-data drive to your home folder, then launch jupyter notebook with the Anaconda Prompt in the task bar (simply type `jupyter notebook` in the prompt) and navigate to the `Tutorial1_STEM_probe_aberrations.ipynb` notebook in your home directory. If you are having trouble with the VM, you can consult the instructions for setup from the T0 section, or ask your breakout room TA.
- As noted inside, when adjusting sliders you should click at the position of interest rather than dragging. **If plots become unresponsive, click the power button in the top right of the plot, then re-run the cell**. If you have a python 3 environment on your computer, you can also download the notebook and required scripts (in the source folder) to run locally, performance may be better.