Tutorial on Linear Image Simulations of Phase-Contrast and Incoherent Imaging by convolutions

Huolin Xin, David Muller, based on Appendix A of Kirkland's book

This tutorial covers the use of **temcon** and **stemcon** to simulate microscope images formed by convolving a set of atomic coordinates with the microscope's point spread function. This can be used as a first check to explore the performance of the instrument, or to check the input files and parameters for the longer, more computationally expensive multislice codes.

Limitations of the codes:

a) They are Matlab scripts that must be run in Matlab. (`incostem.exe` is a stand-alone executable)

b) The codes ignore thickness, and collapse all atoms into a single plane at z=0. i.e. they cannot be used to study depth-sectioning or depth of focus effects without modification

c) Beam spreading in the sample is ignored. You will need to run the multislice code to simulate how the probe evolves in the material

d) The scattering cross is assumed to be proportional to $Z^{1.7}$ for ADF imaging (i.e. high-angle ADF), and $Z^{0.67}$ for phase contrast imaging (i.e. assuming a Thomas-Fermi atom). These are not quantitatively correct. `Incostem` and multislice give more accurate cross-sections.

The files needed for this tutorial are on web at
http://people.ccmr.cornell.edu/~davidm/WEELS/summer06/

Download the compressed folder stemcon.zip and save it to the **StudentFolder** directory, which is located under My Documents. This is the workspace where you will be able to write and save files.

Running the codes:

temcon requires the files temcon.m, tempot.m, and ctemconvolution.m to be in the current Matlab directory or path.

stemcon requires the files stemcon.m, stempot.m, and ctemconvolution.m to be in the current Matlab directory or path.

1. Launch Matlab from the desktop.
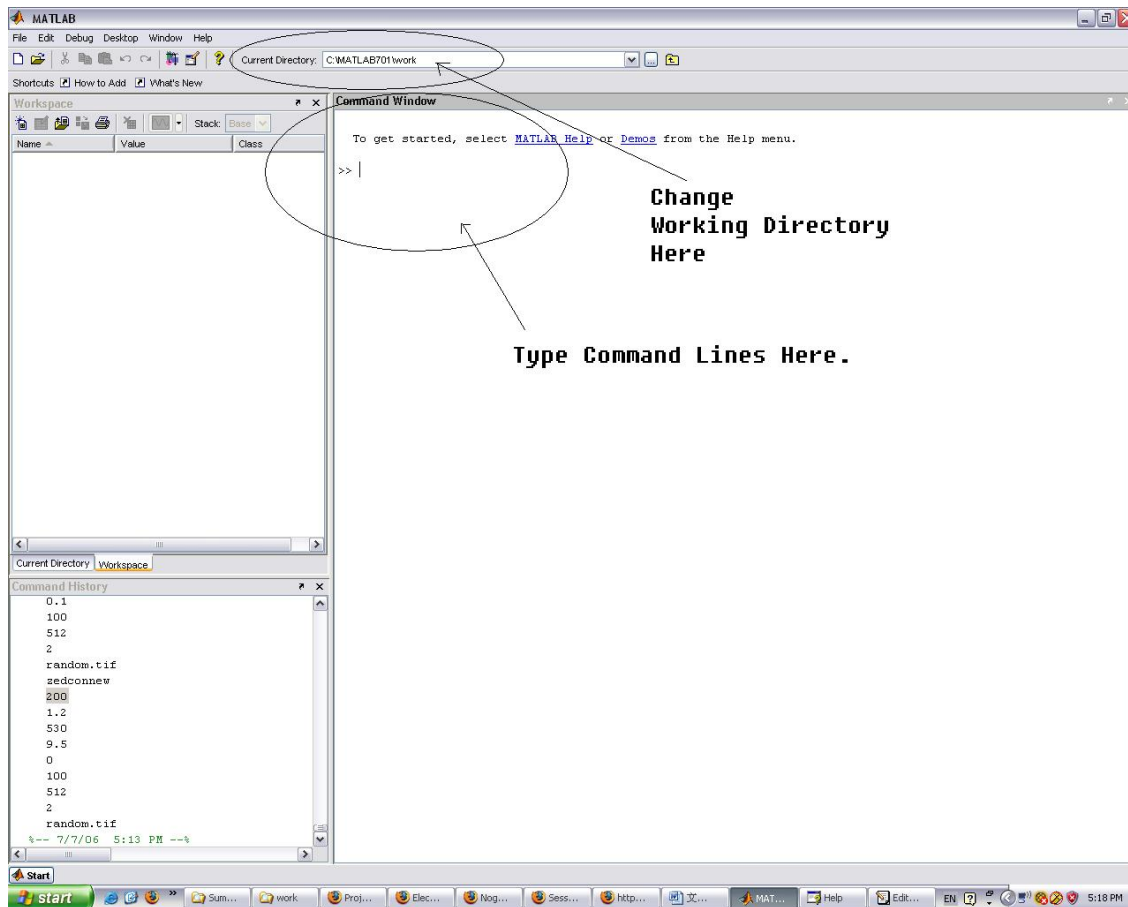2. Change the working directory to   MyDocuments/StudentDirectory

Fig. 1

Our programs will generate images and save them as .jpg files. If you want them to be saved in your directory such that you can re-look at them, go to the 'Current Directory' as indicated above and change it to your directory.

2. You may want to know how to plot a function in Matlab.

Let's generate a sine wave. Type the following lines in the command window.

>> x = 0:0.01:2*pi; ↵

>> y = sin(x); ↵

>> plot(x,y); ↵

(if you leave off the semicolon, Matlab will print the contents of the variable)
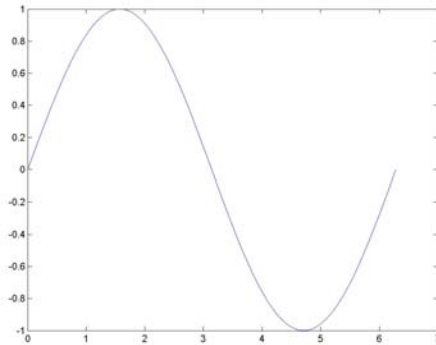
You will find a plot as in Fig. 2.

Fig. 2 Sine wave

3. You also need to know how to display a two dimensional matrix as an image.
First type in a 3-by-3 matrix;
>> a = [1 2 0; 2 5 -1; 4 10 -1] ↵
Then we use imagesc(a) to display this matrix as an image
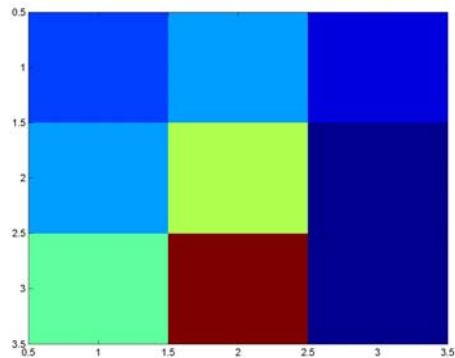**>> imagesc(a);** ↵
You will find the plot below,

Fig. 3

If you want to know the mapping between the values and the colors, you can type
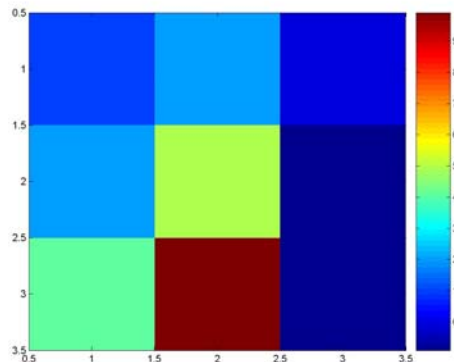**>> colorbar;** ↵

Fig. 4

You can also change the colormap to gray scale;
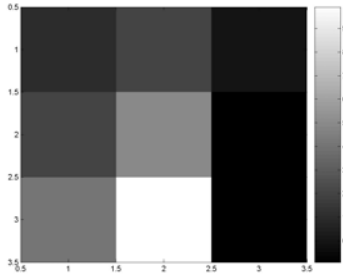**>> colormap(gray);** ↵

Fig. 5

4. Simulation of Point Spread Functions

Appendix A of Kirkland's book (pg 185) has simple Matlab scripts to plot PSF and CTF functions for both phase-contrast and ADF images. Slightly modified versions are included in the stemcon.zip file. These are not as robust as the `drawmtf.html` java script, which we will use later.

To simulate the PSF for your microscope in STEM mode type in the MATLAB command window (after the **>>** prompt)
>> stempsf;
Enter the beam voltage and spherical aberration coefficient of your microscope
The code will suggest the optimal defocus and aperture size. Take it's suggestions.
The code will plot both the point spread function and its radial integral (which is a good way to check for probe tails. Locate on the radial integral the radius which encloses 80% of the signal. This is called R-80%. R-80% and R-90% are often used as measures of resolution for analytical work.

Now run the code again with an aperture that is 20% larger than optimal
How much further did R-80% and R-90% increase?

To simulate the CTF for your microscope in STEM run
>> **stemtf**;
Compare the CTF for the optimal aperture and the one that is 20% larger.
How does the contrast level at the Si (111) spacing (0.313 nm) compare?
How does the information limit compare?

The phase contrast CTF and PSF for conventional TEM or BF-STEM are simulated in **ctemtf** and **ctempsf;** What is the information limit in CTEM when the same parameters are used as for the STEM examples above?

5. Now, we can begin our image simulation with Si [110] plane.

In the command window, exactly type in the lines below.

>> **a = temcon;**

Temcon: Simulate an BF image using the weak phase imaging model

Type electron energy in keV :**200**↵

Type spherical aberration Cs in mm :**1.2**↵

Type defocus df in Angstroms :**500**↵

Type objective aperture semiangle in mrad :**10**↵

Type chromatic aberration defocus spread in Angstroms :**50**↵

Type spread in illumination angles in mrad :**0.1**↵

Type size of slice in Angstroms:**27.15**↵

Type number of pixels in slice:**512**↵

1 - Coordinates file; 2 - image file : **1**↵

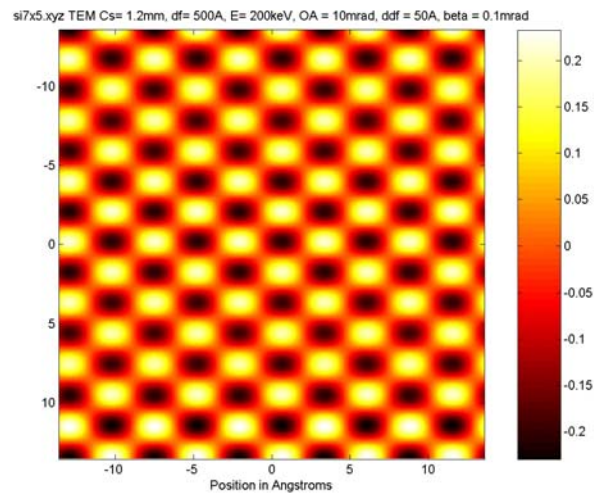Type name of coordinates file(e.g. si7x5.xyz):**si7x5.xyz**↵

Fig. 6

This program(temcon) simulates the TEM bright field image. Those black spots are the projected image of the two adjacent silicon atoms. In this TEM image you cannot tell that one black spot actually comprises of two silicon atoms. Let's see how STEM improves this image.

>> **a = stemcon;**
```
stemcon: Simulate an ADF image using the incoherent imaging model
Type electron energy in keV :200↵
Type spherical aberation Cs in mm :1.2↵
Type defocus df in Angstroms :500↵
Type objective aperture semiangle in mrad :10↵
Type source size in Angstroms :0↵
Type size of slice in Angstroms:27.15↵
Type number of pixels in slice:512↵
1 - Coordinates file; 2 - image file : 1↵
Type name of coordinates file(e.g. si7x5.xyz):si7x5.xyz↵
```
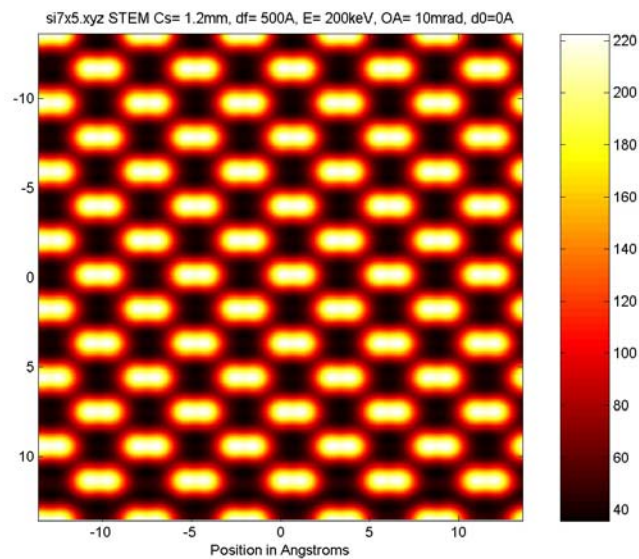

Fig. 7

As show in figure 7, the ADF STEM image is much easier to interpret than the TEM image and the resolution is much higher.

6) Now try running both the codes with `random.tif` as an input file. This is just a square matrix of random numbers – a good approximation of an amorphous material that has no internal order at all. A slice size of 100Å and 512 pixels should work well. Do these images look similar to experimental pictures of a-C thin films?