**Computer Lab #2, due Monday October 21st**

**Part 1: Effects of imaging parameters on probe size/shape**

Instructions:

1. Mostly similar to previous labs.

2. In semper, type: *lib hf2000*; then *lib probe* to simulate the image of the probe.

3. Additional parameter is defocus spread. As discussed in the class, the defocus spread

is due to energy spread (E/E), instabilities in high voltage (V/V), instabilities in

objective lenses ((I/I), and drift along z direction, and also depends on chromatic

aberration.

**Part 2: Linear Imaging and Non-Linear Imaging** The term *linear image* is applied to images in which the majority of the intensity is carried by the zeroth-order beam. The advantage of using linear-imaging theory combined with the use of envelope functions to describe chromatic-aberration and beam divergence effects is that, for the system, the Fourier coefficients of the image-plane wave function are separable. At the end, linear imaging reduces the calculation of images including the effects of many images to a single-image calculation.

However, linear-imaging theory cannot be applied to images in which the intensity in the zero-order beam is comparable to the intensity of the other reflections contributing to the images. Similarly, linear-imaging theory cannot be applied to darkfield images because the zeroth-order beam is excluded by the diffraction aperture. In non-linear imaging theory, no assumption is made about the relative intensities of the beams contributing to the image.

In the calculation of HREM images, one does not know, for a general system, under what conditions linear-imaging theory will hold. Hence, calculations should routinely apply nonlinear-imaging theory and only use linear-imaging theory as a special case. Unlike linear-imaging theory, nonlinear-imaging theory is inconvenient in that, the Fourier coefficient of the imaged-plane wave function are not separable.

The previous lab was carried out using linear-imaging theory in simulating the images. This lab will allow you to compare images with the ones from before using nonlinear-imaging theory.

Instructions:

1. In semper, type: *lib hf2000* to set the microscope parameters; then *lib cp2t* (lib cp2t

will calculate two sets of images, left: linear-imaging, right: nonlinear-imaging)

2. Play with the parameters and compare the images (linear-imaging and nonlinearimaging).

Important parameters are: spacings, objective aperture size

3. Use *xv* in a terminal (or *lib paste* in semper) to capture the images – or other software (system dependent).