

# CTF.DOC

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### A. INTRODUCTION

CTF is a program for plotting phase contrast transfer functions on the graphics screen. The program is designed with a moderate amount of flexibility to allow the user several choices as to how to design specific plots.

The basic equations for calculating the phase CTF come from articles by H. P. Erickson and A. Klug ("Measurement and Compensation of defocusing and Aberrations by Fourier Processing of Electron Micrographs" (1971) Phil. Trans. Roy. Soc. Lond. B261:105-118) and D. L. Misell ("Image Analysis, Enhancement and Interpretation" (1978) Pract. Meth.Elec. Microsc. 7:1-305).

The function plotted is  $\sin[\text{CHI}(a)]$ , where

$$\text{CHI}(a) = (2*\text{PI}/\text{lambda}) * (-0.25*\text{Cs}*a^{**4} + 0.5*\text{df}*a^{**2})$$

CHI(a) is the phase shift which the scattered electron wave undergoes at the diffraction plane of the microscope due to the effects of defocus and spherical aberration. The phase shift is a function of the scattering angle, a.

a = scattering angle (radians)  
lambda = electron wavelength (nm or pm)  
Cs = spherical aberration coefficient (mm)  
df = defocus (positive for a weak or underfocused lens)  
(nm)

The plot shows the values of  $\sin[\text{CHI}(a)]$  from -1.0 to 1.0 on the ordinate versus spatial frequency on the abscissa (tic marks are plotted every 0.1/nm units, with larger tic marks at 1.0/nm units).

### B. PROGRAM OPTIONS

TOUCH-KEY options available include:

A Set spherical ABERRATION coefficient value  
B ERASE graphic screen  
C Change COLOR of curve  
D DISPLAY (draw curve)  
F Set DEFOCUS value  
L LIST variable values & other parameters  
P Set PLOT parameters  
R Set RESOLUTION (abscissa) limit  
V Set acceleration VOLTAGE value  
E EXIT program

**OPTION A: Set spherical ABERRATION coefficient value**

Enter a REAL\*4 value (in mm units) for the spherical aberration coefficient for the objective lens of the microscope whose CTF is being plotted (DEFAULT VALUE = 2.0 mm). Most microscope manufacturers list the Cs for the objective lenses they use in their brochures.

**OPTION B: ERASE graphic screen**

This simply erases the ENTIRE graphics screen.

**OPTION C: Change COLOR of curve**

This allows the user the option of changing colors when multiple CTF curves are plotted. The program DEFAULT value for the initial curve color is yellow (RGB = 255,255,0), using color table position #3 (Position #0 is reserved for setting the background color, currently hardwired to a dark blue color; Position #1 is reserved for drawing the axes, tic marks and box outline in white; Position #2 is reserved for the grid lines which are medium grey in color).

Each time the user chooses this option, the program tries to make an "intelligent" guess at new values for RGB, and it uses the next position in the color table. These values are given as DEFAULT prompts, but the user can override them if desired. After entering INTEGER values for RGB the user enters an INTEGER value to choose which color look-up table position to use.

**OPTION D: DISPLAY (draw curve)**

This activates the drawing of the curve using the current parameters set for the various variables which can be listed using option "L".

**OPTION E: EXIT program**

This terminates the CTF program.

**OPTION F: Set DEFOCUS value**

Enter the defocus value as an INTEGER number (in nm units). A negative value corresponds to a strong or overfocused lens, whereas a positive value corresponds to a weak or underfocused lens. A defocus value = 0 corresponds to the condition of "near" focus, where the phase contrast is very minimal. A value of +90 nm corresponds to the optimal defocusing value for high resolution phase contrast microscopy (but not of practical use for negative stain or frozen-hydrated specimen imaging).

**OPTION L: LIST variable values & other parameters**

This lists the current values of all the variables used to compute the CTF curve. In addition, information about the positions of zeroes in the CTF are listed, and, in the case of underfocusing (positive defocus value), the position of the first maximum in the curve is printed. The output at the terminal looks something like:

```
Accelerating voltage           = 10000 volts
Electron wavelength            = 0.003709 nm
Spherical aberration coefficient = 2.0 mm
Defocus (underfocus)         = 300 nm
Horizontal scale factor        = 1.000
Vertical scale factor          = 1.000
GRID lines [not] drawn on plot
*****
* Zeroes in the CTF *
*****
1st zero at infinite nm
2nd zero at 1.032 nm
3rd zero at 0.711 nm
4th zero at 0.563 nm
5th zero at 0.469 nm
First maximum of CTF at 1.492 nm
```

**OPTION P: Set PLOT parameters**

First enter REAL\*4 values for XSCALE and YSCALE which are plot scale factors for the abscissa and ordinate directions. (DEFAULT = 1.0,1.0). When XSCALE or YSCALE are changed, the new values become the default values. Note that, when XSCALE,YSCALE = 1.0,1.0, the overall dimension of the plot area will be about 1000

x 500 pixels. Thus, if for instance XSCALE is set = 2.0, a major part of the curve will not appear on the graphics screen.

Next specify where the center of the plot is to be displayed (DEFAULT XCEN,YCEN = center of the graphics screen: For the 1280 x 1024 pixel LEXIDATA graphics device, this is at the position 640,512). If you change either XCEN or YCEN then the new values become the default values.

Finally, you have the option to draw grid lines (both abscissa and ordinate) on the plot. (DEFAULT = draw the grid lines; 1 = suppress the grid lines). If you opt to draw the grid lines, they will be drawn at a spacing equal to the tic-marks along the abscissa and at values of -0.75,-0.50,-0.25,0.25,0.50 and 0.75 along the ordinate axis. Both sets of grid lines are drawn. There is no current option to plot one or the other.

**OPTION R: Set RESOLUTION (abscissa) limit**

Enter a REAL\*4 value for the highest spatial frequency to plot (in 1/nm units) (DEFAULT = 1.0/nm). For example, if you only want to plot the CTF out to a resolution of 2.0 nm, then type 0.5. If you want to plot the CTF all the way out to 0.25 nm resolution, then type 4.0. Realize, however, that depending on the values of plot scale factors (XSCALEF and YSCALEF, see option "P"), part of the CTF curve may not appear within the boundary of the graphics screen.

**OPTION V: Set acceleration VOLTAGE value**

Enter a REAL\*4 value for the microscope accelerating voltage (in kV units) (DEFAULT = 100.0 kV). With all other conditions being equal, a higher value for the accelerating voltage causes the first maxima of the CTF to shift to higher spatial frequencies.