



Saving Palace CLUTs in *GraphicConverter*

GraphicConverter uses color table files much like Photoshop's. The procedure for creating a Palace CLUT is about the same.

*Photoshop users take note — GraphicConverter color table files are **not** in the same file format as Photoshop's. If you use both programs, you will need to save a color table file for each program.*

First open most any Palace room GIF ("pgate.gif" is preferred, since it's guaranteed to have the complete map). The room pictures *should* all have the same color map, and your avs should use that same set of colors.

Once you've opened the GIF, select "Save As..." under the GraphicConverter "File" menu. A dialog will pop up, showing you the image. Change the Format from "GIF" to "Color Table" (the name will change to "pgate.PAL") and hit the "Save..." button (I saved mine as "Palace.PAL"). Once the color map is saved, you can just close the GIF — you won't be needing it any more.

One extra note of caution — if you've been using GraphicConverter's "split" option (part of the "Save As..." dialog box), make sure you've turned it off before hitting the "Save" button, or you'll get lots of little (and identical) color table files..... you only need one!

Using the Color Map

For any picture you want to use with the Palace, as a room background or a prop, you'll need to make sure it uses that color map. Unless the picture started as a Palace image (like the room GIF, or something pasted *from* the Place prop editor), we'll need to convert it. There are essentially three kinds of pictures we will convert:

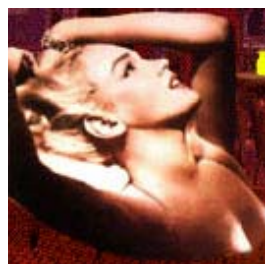
- RGB (24-bit or 32-bit) full-color images (such as color JPEGs)
- Grayscale (8-bit) images (such as B&W Photos, JPEG or GIF)
- "Alien" indexed-color images (such as GIFs you might find on the net)

For both grayscale and indexed-color images, you must convert to RGB color via the "Picture->Colors->Change to 16.7 Mill. Colors (32-bit)" menu *first*, before converting to indexed color using the Palace color map. GraphicConverter will always assume that grayscale GIFs should be mapped to exactly 256 grayscales; and it has no good way to directly convert from one color table to another. A short time in RGB mode is the necessary in-between step.

Remember: *Save Your RGB Image.* You may need it later, for changes or fixes.

To force GraphicConverter to use your stored Palace color map, you select "Colors->Options..." under "Picture." A dialog will pop up. Press "Use Custom Color Table" and the "Open..." button. In the "Dither" check box, press whatever you like — "dither off" will generally give you the smallest file size, while "dither on" will give the nicest tonal gradations. Now press "OK."

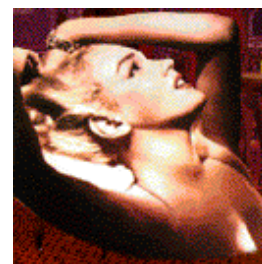
Once the color table is ready, we can convert RGB images the Palace map. Select "Colors->Change to 256 Colors (8 bit)" under "Picture." Now look at your image: it's living in the Palace world.



RGB Original



No Dithering



Dithered

Not sure about that "Dither" option? Just hit "Undo" and convert it again in several different ways. Or duplicate the image and convert each copy a different way, to compare side-by-side. Above are three samples, superimposed over a bit of Harry's Bar.



[Feedback/Suggestions/Guess Book](#)

Updated 4 Nov 96

EMFFT.DOC

(last update Mar 5, 1992)

A. INTRODUCTION

EMFFT is used to examine and/or manipulate FFT data. Filtered FFT data may be output to a disk file with the normal FFT format or it may be back-transformed ("B") to produce a filtered IMAGE stored on disk (normal IMAGE file format). Note that use of two or more options may produce additive or multiplicative effects on an FFT.

NOTE ON TERMINOLOGY: the term TSU (transform sample unit) denotes a unit of reciprocal space measure. Each TSU corresponds to a single step in the transform. For example, for a IDIM1 by IDIM2 transform in which IDIM1=IDIM2, each TSU will represent $1.0/(IDIM1 \times \text{pixel size})$. Thus, if IDIM1=512 and the pixel size = 0.51nm, then each TSU is (1.0/261 nm). Because the right, left, top, or bottom limits of a 512x512 transform are at 256 TSU, the resolution limit at these extremes is $256 \times (1.0/261 \text{ nm}) = (1.0/.981 \text{ nm})$, or 2.0 pixel resolution, consistent with the Whittaker-Shannon sampling restrictions.

B. PROGRAM OPTIONS

EMFFT provides several options which are selected from a TOUCH-KEY MENU as shown below.

TOUCH-KEY OPTIONS:

```
-----  
A  Multiply two FFTs (CCF)           M  FFT --> MAP format  
B  BACK-transform the FFT           S  Get STATISTICS  
C  Compute CIRCULAR average  
D  DISPLAY on graphics device       O  OPEN new FFT file  
F  FILTER the FFT                   R  READ and transform  
                                     IMAGE data  
G  Extract structure factors        W  WRITE current FFT to  
                                     disk  
K  *FIX values in FFT              E  EXIT program  
L  LATTICE refinement               ?  INFO on EMFFT program  
  
PF1  Spawn to VMS DCL commands  
PF2  
PF3  Turns main MENU option list ON/OFF  
PF4  Graphics routines  
*    Option not yet available
```

The first option the user must choose is either "O", to OPEN a new FFT file and read in the array of structure factor data, or "R", to READ in an IMAGE file which is then Fourier transformed. Whenever option "W" is chosen to WRITE a FFT array to a disk file, the user must again choose either "O" or "R", or else EXIT the program ("E"). You may string several operations together before saving the result in a disk file. Realize that operations are performed sequentially, thus the only way to fully recover an "untouched" FFT is to reuse option "O" or "R".

OPTION A: Multiply two FFTS

This allows one to multiply the current FFT data with another FFT. The filename for the second FFT is entered by the user. Note that it is possible, using this option, to produce either an auto-correlation or cross-correlation FFT which can be back-transformed using option "F" to produce the corresponding auto- or cross-correlation image as is accomplished using the program EMCOR.

OPTION B: BACK transform the current FFT

This option will take the current FFT, including any filter masks that have been applied, and back transforms it to produce a "filtered" IMAGE. If an FFT that has had no mask applied is back transformed, then an unfiltered IMAGE identical to an original boxed IMAGE will be the result. The only input required by this option is a filename for storing the resulting IMAGE and an optional HEADER. To do anything with the back-transformed IMAGE you must exit EMFFT ("E" or touch PF1 and run, for example, EMIMG).

OPTION C: Compute CIRCULAR average

This option will produce a circular average of the FFT amplitudes (DEFAULT) or intensities that can be displayed on the graphics screen and/or dumped to an ASCII file (FFT_1D.TMP). This option is similar to the "C" option of EMIMG.

First decide what interpolation factor to use (type a negative number to exit the routine). If you plan to use the FFT_1D.TMP data file to produce a plot on one of the personal computers with, for example, a program like LOTUS FREELANCE, etc., then just use an interpolation of 1.0. Choose whether you want to display amplitudes <CR> or intensities (1), whether or not you want to see a display on the graphics device (DEFAULT=N), and whether or not you want to create the FFT_1D.TMP file (DEFAULT=N).

If you display the circular average on the graphics screen, you will then be able to use the data tablet puck to pick points and get a readout of the radial distance (in TSU) from the origin. Hit the GREEN button to exit this routine and either start over with a new interpolation factor, or exit the "C" option by setting the interpolation value to a negative number.

OPTION D: DISPLAY the current FFT

"D" is used to display the FFT amplitudes or intensities, scaled in a variety of ways. The scaled FFT values are displayed with a black & white Color Look-Up Table, CLUT, using the lowest 6-bit planes of the graphics memory. Several display options are available as specified in the following touch-key menu.

FFT_DSP TOUCH-KEY MENU	Values
-----	-----
A AMPS/INTENSITY toggle	amps/INTENSITIES
C CLEAR display	
D DISPLAY the FFT	
M MAGNIFICATION (FFT size)	512 X 512
L/R Portion of FFT displayed	LEFT/RIGHT
T/B Portion of FFT displayed	TOP/BOTTOM
P POSITION center of display	320 256
S SCALING method	LINEAR/log/non-linear
% Threshold FRACTIONS	0.000 0.005
E EXIT	

SUB-OPTION A: AMPS/INTENSITY toggle

This toggles between a choice of whether amplitude or intensity FFT data are used.

SUB-OPTION C: CLEAR the display screen

"C" erases the entire graphics display screen.

SUB-OPTION D: DISPLAY the current FFT

"D" will display the FFT with the current settings given in the right half of the touch-key menu.

SUB-OPTIONS L/R/T/B: Select portions of the FFT for display

These keys select/deselect portions of the FFT for display. The initial DEFAULT is to have LEFT/RIGHT/TOP/BOTTOM all selected so the entire FFT is displayed. Certain options are disallowed (e.g. TOP and BOTTOM or LEFT and RIGHT cannot both be deselected simultaneously).

SUB-OPTION M: Toggle FFT display MAGNIFICATION

"M" is used to toggle through different size displays (if allowed). The initial DEFAULT is to display the FFT at maximum size allowed by the graphics device (1024x1024 for the LEXIDATA in B-141 and 640x512 for the LEXIDATA in B-403). The display can be no SMALLER than the actual dimensions of the FFT (IDIM1, IDIM2).

SUB-OPTION P: Select center POSITION for display

Choose "P" to select a new center position (2I FORMAT) for the FFT display. The initial DEFAULT (either 640,512 or 320,256) depends on which graphics display device is being used. Anytime you input a new center position, that becomes the new DEFAULT. Note that this routine permits FFTs to be displayed with a portion outside the graphics screen boundary.

WARNING: EMFFT options such as "L" assume that the FFT is Displayed EXACTLY centered in the graphics screen, otherwise they will not work properly.

SUB-OPTION S: Toggle SCALING method

"S" is a toggle switch that selects how the FFT data are scaled. Linear scaling is the initial DEFAULT mode, but the data can also be displayed on logarithmic or non-linear scales. DEFAULT thresholds (see sub-option "%" below) are automatically selected each time you switch to a different mode of scaling. These DEFAULTS can be overridden with the "%" option. Non-linear scaling produces an asymptotic CLUT which depends on two parameters, K and S, set using the "%" option.

SUB-OPTION %: Select threshold FRACTIONS

The "%" key is used to select threshold FFT values (FRACT_MIN and FRACT_MAX, given in fractional units of the maximum, scaled FFT value) so that values below FRACT_MIN*FMIN are displayed with the lowest CLUT intensity (usually 0) and values above FRACT_MAX*FMAX are displayed with the highest CLUT intensity (usually 63). DEFAULT threshold values are used whenever the linear or logarithmic scale modes are selected but a different scheme is used if non-linear scaling is selected (see below). The DEFAULTS for linear and logarithmic scaling modes are set as follows:

Scale Mode	FRACT_MIN	FRACT_MAX
Linear	FAVG/FMAX	(FAVG+FSTD)/FMAX
Log	LOG10(FMAX)*FAVG/FMAX	LOG10(FMAX)*(FAVG+FSTD)/FMAX

where FAVG, FMAX, and FSTD are the average, maximum, and standard deviations of the FFT amplitudes or intensities (depending on the current choice selected by "A").

If "%" is chosen when non-linear scaling is chosen, two parameters, K and S, are specified. K fixes the midpoint of the CLUT (range = 1.0-255.0) and S effectively sets the slope (contrast) of the CLUT. The initial DEFAULT values for K and S are set as follows:

$$K = 255.0 * (FAVG + FSTD) / FMAX$$

$$S = 0.25$$

The value for S is set initially to 0.25 although this may need to be changed. Higher values give a steeper curve (higher contrast) whereas lower values give a flatter curve (lower contrast). Beware that very small or large values of S can and probably will lead to overflow or underflow problems and will crash the program. The value of K will almost certainly have to be adjusted from the DEFAULT setting. If the screen appears totally white, K is too small (and S may be too small). If the screen is totally black, K is probably too large. Obviously, to get non-linear scaling to work properly requires much operator intervention and experience. The linear and logarithmic scaling modes should suffice for most "normal" circumstances.

Once K and S are set, the CLUT value for a given FFT intensity or amplitude is remapped as follows:

$$CLUT_VALUE = 255.0 * (1.0 / ((10.0 ** (S * (K - VALUE - 1.0))) + 1.0))$$

where VALUE = (F*(LUTHI-LUTLO)/FMAX) + 5.5 and LUTLO and LUTHI are normally set equal to 6 and 63 for the compressed black and white FFT CLUT.

OPTION F: FILTER the FFT

"F" is used to generate filter masks to multiply the FFT data by. There are currently two separate sub-options in the following touch-key menu:

EMFFT_FILTER TOUCH-KEY OPTIONS

-
- A Apply low and/or hi-pass filter
 - B Apply 2D reciprocal lattice mask
 - C Apply 2D layerline mask
 - E EXIT routine

SUB-OPTION A: Apply low and/or high-pass filter (Resolution cutoff)

Enter values for RES_MIN, RES_MAX, CUT_MIN, and CUT_MAX (4F FORMAT) to identify the inner and outer radii in the Fourier transform (in TSU) for the HI-PASS (RES_MIN) and LOW-PASS (RES_MAX) filters. CUT_MIN and CUT_MAX specify hard (0.0) or soft (>0.0) edges.

For example, for HI-PASS filtering, the FFT is zeroed out to RES_MIN-CUT_MIN, and rises exponentially up to full weight (1.0) at RES_MIN. A LO-PASS filter has full weight out to RES_MAX and drops exponentially to 1/exp at RES_MAX+CUT_MAX (if CUT_MAX=0.0, the FFT is zeroed beyond RES_MAX). To produce a simple low-pass filter (i.e. with no high-pass filtering), set RES_MIN=0.0. For simple high-pass filtering, set RES_MIN=RES_MAX>0.0. Use CUTMIN or CUT_MAX = 0.0 to apply a sharp cutoffs with no Gaussian falloff.

SUB-OPTION B: Apply 2D reciprocal lattice mask

This is used to produce a mask with circular "holes" at the positions of an ideal, 2D reciprocal lattice. The vector coordinates of the two principal lattice dimensions (a* and b* given in TSU) may be entered by hand (4F FORMAT) or read in directly from the FFTLAT.DAT file produced after refinement of the reciprocal lattice by use of EMFFT option "L".

Specify the radius for all circular holes (in TSU). You may create holes with "soft" or "hard" edges. For holes with "hard" edges, points inside the hole are given full weight and points outside are set equal to zero. In "soft" holes, points inside the hole are scaled with a Gaussian weighting function with the weight determined by the relative distance of the point from the center of the hole: points at the hole edge are down weighted by 1/exp of their original value. "Soft" holes are generally made using a slightly larger radius than is appropriate for "hard" holes.

SUB-OPTION C: Apply a 2D layerline mask

This produces a mask consisting of a series of parallel slits (rectangular holes). Specify values for ANGLE,SPACE and FALLOFF (3F FORMAT). ANGLE (in degrees) specifies the orientation of the slits with respect to the horizontal (X) direction of the FFT (a positive value is measured as a counterclockwise rotation from the X-axis). SPACE is the distance between slits in TSU. FALLOFF determines the "softness" of the slit edges: sample points a distance FALLOFF from the center line of the slit are downweighted by $1/\exp$. There is currently no provision to construct "hard" edge holes as is allowed in sub-option "B". Also, the parameters ANGLE, SPACE, and FALLOFF must be entered by hand.

OPTION G: Extract structure factor

This allows one to extract structure factors from the FFT of the image of a 2D crystalline specimen. This is usually run after running option "L" which computes refined parameters for the 2D reciprocal lattice (AX,AY,BX,BY in TSU), for a^* and b^* , the two principal lattice vectors). The lattice coordinates are normally stored in the file FFTLAT.DAT, which is read back by this routine. It is thus IMPERATIVE that the correct FFTLAT.DAT file be read in. You also have the option of entering the reciprocal lattice coordinates by hand.

Alternatively, this option can be used after using EMCORAVG (correlation averaging) if one wants to feed into the Fourier-based software routines. EMCORAVG.DAT contains the required reciprocal lattice coordinates. Because EMCORAVG is often run in the mode which forces the reciprocal space lattice coordinates to occur at integer transform sample unit positions, (enabling peaks of the reflections to be exactly sampled in the FFT), this routine uses the ORIGINAL refined lattice coordinates for determining a^* , b^* , c^* , α^* , β^* , γ^* , d^* , etc., but uses the "enforced" coordinates to extract the structure factor measurements. The ORIGINAL lattice dimensions are retained in the header records of the structure factor file in order to override the distortions imposed when forcing the reciprocal lattice to exact TSU positions.

Begin by specifying a filename and header text for the SF output file.

Structure factors are computed in one of two ways:

- 1) Transform intensity data, obtained within a circular or

elliptical window, which is centered about the ideal reciprocal lattice position for each reflection, are INTEGRATED with each transform sample point weighted by a Gaussian function whose magnitude is proportional to the distance from the calculated lattice position to the sample point as given below:

The intensity at each sample point is weighted by W^{*2} , where

$$W = \exp \left(\frac{-d*d}{2.0*r*r} \right)$$

with d = distance (in TSU) of the sample point from the ideal lattice position.
 r = radius of the window (in TSU).

For example, with $r = 1.00$

d	=	0.00	0.50	1.00	1.50	2.00
W	=	1.00	0.88	0.61	0.32	0.14
W^{*2}	=	1.00	0.78	0.37	0.11	0.02

Choose the window shape (DEFAULT=circular) and RADIUS (DEFAULT=1.0 TSU: this must be large enough to include the entire spot) and set the cutoff variable, CUT (DEFAULT=2.0). CUT determines the actual dimensions of the window used for integration and background calculations. Intensities are integrated inside a window with a radius = RADIUS*CUT and background measurements are determined from within an annulus whose inner and outer radii are RADIUS*CUT and 2*RADIUS*CUT, respectively. If you choose not to subtract backgrounds, CUT is set automatically = 2.0. Applying the background correction to the structure factor measurements helps to reduce the noise, especially for the higher resolution data. The background value at each lattice point is estimated from the average intensity in an annular region outside the integration window. **WARNING:** Choose RADIUS and CUT with care to avoid artifacts produced when peaks of neighboring spots are erroneously included in the background area.

The structure factor amplitude is computed as the square root of the (weighted) integrated intensity. Measurements are then scaled down by an arbitrary factor of 1000.0 to help avoid overflows in the formatted output file.

The structure factor phase for each reflection is obtained by interpolation of the four sample points adjacent to the calculated

lattice position. Phase measurements cannot be computed by integration of all the sample points inside the reflection window mainly because the phase term shows large fluctuations across and just outside the the reflection peak due to the $\text{SIN}(X)/(X)$ influence from the edges of the boxed (and floated), digitized micrograph.

- 2) Structure factor amplitudes may be computed by interpolation as is done to obtain phases. If this option is used, there is no need to set a window shape or size, and the option to subtract backgrounds is not available. This option is mainly useful for extracting structure factor data from models or from the Fourier transforms of image averages after running the correlation analysis procedures (where there should be little or no noise surrounding the reflections).

Specify the Miller indices of the two principal lattice vectors (DEFAULTS = 1,0,0 and 0,1,0). This option is really only important for correctly identifying the spot indices for a three-dimensional data set such as from several tilt series from orthogonal sections of a Three-dimensional crystal. The [hkl] indices for the two principal lattice vectors in the two-dimensional projection data provides a transformation matrix which is used in subsequent programs (eg. EMSF2DBT) to identify the orientation of the data when processed. For example, assume we had an [h0l] projection such that the c* direction was horizontal and a* was vertical in the FFT. Since the lattice refinement routines ("L" option) use the convention a* = near horizontal vector and b* = near vertical vector, then the two principal lattice directions would be identified as [hkl] = 0,0,1 for a* and [hkl] = 1,0,0 for b*. Thus, to transform from the 2D h'k' indices used in option "L" to 3D [hkl] indices output by this routine, the following transformation matrix algebra is performed:

$$\text{hkl} = \text{h}'\text{k}' * \text{T} \quad \text{where} \quad \text{T} = \begin{vmatrix} \text{a11} & \text{a12} & \text{a13} \\ \text{a21} & \text{a22} & \text{a23} \end{vmatrix}$$

$$\begin{aligned} \text{Thus, } h &= h' * \text{a11} + k' * \text{a21} \\ k &= h' * \text{a12} + k' * \text{a22} \\ l &= h' * \text{a13} + k' * \text{a23} \end{aligned}$$

Example for $T = \begin{vmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix} :$

h' k'	h	k	l	
1 0	0	0	1	
0 1	1	0	0	
1 1	1	0	1	
2 3	3	0	2	
-5 9	9	0	-5	etc.

The SF output file contains information on the unit cell parameters, the transformation matrix, and the structure factor data (amplitudes and phases) in the format given in [TSB.FOR]EMPROGS.DOC. The SF data can be refined using EMSFREF and back transformed using EMSF2DBT (or EMSF3DBT) to produce MAP files which can be displayed with EMMAP.

This routine also generates a temporary file (FFTSPT.TMP) which contains a listing of several of the parameters used to compute the structure factors as well as the structure factor data.

You also have the option (DEFAULT=N) to create a file (FFTBOXES.TMP) that lists the 9 by 9 arrays of amplitudes and phases for each spot, in a format similar to that used in the EMFFT option "L" (sub-option "B"). Be sure to print out the file on the line or laserprinter in LANDSCAPE (NOT PORTRAIT) mode, otherwise much of the file will not print out on the page. The data as printed out in the FFTBOXES.TMP file may differ slightly from the data output in the structure factor and FFTSPT.TMP files because some parameters (e.g. RADIUS=1.0; CUT=2.0) are fixed.

OPTION K: Fix values in FFT

Option not yet available.
Documentation needs to be written.

OPTION L: LATTICE refinement

"L" allows you to refine two-dimensional crystalline lattice parameters. Before running this option, you must be sure that you have displayed the FFT to maximum size on the graphics device. You are given one of the two following warning messages depending on which graphics device you are using:

WARNING: FFT must be displayed at 1024x1024 size and centered at 640,512

WARNING: FFT must be displayed at 512x512 size and centered at 320,256

"L" currently has provides two separate sub-options in the following touch-key menu:

EMFFT_LATREF TOUCH-KEY OPTIONS

- A Use overlay grid to refine lattice
B Least squares fit of individual spots
E EXIT routine

SUB-OPTION A: Use overlay grid to refine lattice

This allows you to select two spots of known indices with the data tablet puck and the program then draws a reciprocal lattice net over the displayed FFT. You can then reenter either or both spots and keep redrawing the lattice net until you are satisfied that the net accurately fits the lattice reflections. This method is somewhat more subject to error than sub-option "B" (below) which does a least squares fit on the basis of as many input spots as you care to identify.

First enter the densitometer pixel size in nanometers (DEFAULT=0.51nm which corresponds to 25 micron sampling of a micrograph at 49,000 magnification). This is only used for giving real-space lattice statistics while you are fitting the net. Thus, if you aren't interested in accurate real-space parameters, you can just ignore this by hitting the <CR> key. Next enter the Miller indices for the two spots, [H1,K1] and [H2,K2], you plan to select with the tablet puck (4I FORMAT). If you misindex these spots, the reciprocal lattice net and lattice parameters will be incorrect and you will be unable to build a proper filter mask with option "F", for example. Choose the R,G,B color of the overlay grid (3I FORMAT: DEFAULT=150,150,150=light grey). At this point control is transferred to the data tablet puck and the following menu appears on the terminal screen:

Mark two spots with tablet cursor:

YELLOW = enter new position
WHITE = keep old position
BLUE = turn grid on/off
GREEN = EXIT

ASTAR BSTAR GAMSTR ADIM BDIM GAMMA

Carefully select the positions of the [H1,K1] and [H2,K2] spots (in that order) with the YELLOW puck button. After entering these two positions, the overlay reciprocal lattice net is drawn. Use the BLUE puck button to toggle the net off and on. To change the lattice, you must always enter two spots. Use WHITE to accept the

previous position and YELLOW to select a new position. Hit GREEN to exit from the selection process after which you are allowed to restart or finish the session. If you choose to restart, the routine will again prompt you for the pixel size, grid overlay color, etc. as before.

If you want to exit the routine completely, you have the option to save the reciprocal lattice parameters in the file FFTLAT.DAT (DEFAULT=N). This file stores the X and Y coordinates (in TSU) for the [1,0] and [0,1] lattice vectors. These two vectors can then be used in subsequent EMFFT routines such as "F" to build filter masks with holes positioned at the points of an ideal lattice defined by these principal vectors.

SUB-OPTION B: Least squares fit of individual spots

This option helps determine the lattice parameters of diffraction patterns. The LEXIDATA TABLET cursor is used to pick out spots for a least-squares determination of a crystalline lattice. The optional end product of the routine is a file (FFTLAT.DAT) containing the coordinates (in transform sample point units) of the [10] and [01] lattice vectors.

CRYSTAL LATTICE REFINEMENT STEPS

1. Choose a cursor type and color.
2. Mark two reference spots with the Lexidata tablet cursor and enter the H,K index for each. Be certain that the two spots do not both lie on a line which intersects the origin of the diffraction pattern. WARNING: the indexing must conform to usual crystallographic conventions in order for certain options in the refinement program "EMSFREF" to work correctly. Also, it is highly recommended that you choose two reference spots which have reasonably high indices (i.e. don't just mark the [10] and [01] spots) since this will give a better initial estimate of the reciprocal lattice parameters. If you are somewhat sloppy at this step, the indexing of high resolution spots may be wrong due to the magnification of small errors made when low resolution spots are used as reference.
3. Choose the maximum number of contour intervals (default NC = 25; range = 5-25) and the maximum contour value (default CLIM = 999.0; range = 0.0-999.0) to scale the contoured amplitude displays. If the amplitudes cover a large dynamic range, it is best to set NC = 25 and CLIM < 999., otherwise some of the weaker, high resolution spots that are important for accurate lattice refinement may not show up in the display because they won't be contoured at the lowest level.

4. Pick spots using the YELLOW puck button. 9x9 amplitude and phase arrays will be displayed at the terminal and a contour display of the amplitude array will be appear on the LEXIDATA (the diffraction pattern will disappear from the graphics screen at this point).
5. Place the tablet cursor over the spot center and hit the YELLOW button to accept the position. WARNING: Try not to be overinfluenced by sharp peaks; mark the center of gravity of the WHOLE spot. DX,DY, listed at the terminal, identifies the position you have chosen, measured in coordinates relative to the center of the 9x9 array (+X to the RIGHT and +Y UP). If you wish to bypass the spot, hit either the WHITE, BLUE or GREEN buttons.
6. After a minimum of two spots have been successfully entered, the current values for the lattice parameters can be obtained by hitting either the WHITE, BLUE or GREEN button. After the lattice parameters are listed, you have the option (Y,W or B) to delete measurements by hand, or to continue (G). To delete spots, type the H,K index (2I format) for each spot followed by a <CR>. A second <CR> will return you to the program where you may then EXIT the routine or start entering additional spots. Please note that, depending on which option you choose at this part of the routine, you may be required to enter subsequent options either from the data tablet puck or from the terminal keyboard. Thus, if you hit the GREEN button to bypass deleting spots by hand, then your next option is answered through the puck, NOT at the terminal keyboard. This helps insure that you don't have to needlessly keep moving your hand from the tablet puck to the terminal and vice versa. Likewise, if you hit Y,W or B to delete spots, then your next option will be answered from the terminal keyboard unless you resume picking out new spots for refinement.
7. When the routine is exited, you are given the option to store The x,y coordinates (in transform sample point units) of the [10] and [01] lattice vectors in the ASCII file FFTLAT.DAT. This is then used by EMFFT option "G".

ADDITIONAL NOTES: Experience with samples such as catalase crystals and gap junction membranes indicates that the lattice parameters should be considered valid if at least 10 or more well resolved spots can be refined so that none deviate more than .75-1.0 transform sample point from the ideal lattice. Treat with caution any spots that deviate more than 1 sample point.

OPTION O: OPEN an existing FFT stored on disk

"O" allows you to read in an FFT stored on disk.

OPTION R: READ and transform IMAGE data

"R" allows you to read in an IMAGE and Fourier transform it for use by the remaining EMFFT options. The DEFAULT size of the FFT will be the smallest power of two in each dimension with a minimum size limit of 128 by 128. Thus, if your IMAGE is 63 by 513 pixels (NCOL,NROW), then the DEFAULT FFT size is 128 by 1024. You may INCREASE either FFT dimension up to a maximum of 1024 TSU.

OPTION S: Get FFT STATISTICS

"S" is used to obtain the current values of FFT_AVG, FFT_STD, and FFT_MAX.

OPTION W: WRITE the current FFT to disk or line printer

"W" allows you to save the current FFT (including any changes that have been applied) to a disk file with the standard FFT file format (DEFAULT) or a file that is ASCII formatted for dumping to the lineprinter ("1").

The lineprinter-type output file contains the FFT amplitudes and/or phases in a format suitable for dumping to a lineprinter or laserprinter. Currently, the output is restricted to the central 128 TSU, centered about the Y-axis (meridian) of the FFT. This is completely adequate for displaying 128x128 up to 256x1024 FFT files, but may leave out significant data from FFT data with IDIM1>256. With this option you can output amplitudes and/or phases. If you output phases, you may change the FFT origin (FFT_ORIGX,FFT_ORIGY) if you wish. The amplitudes are normalized to a LOG2 scale with a maximum value of 9. Phases are coded using the characters 0-9,A-Z to represent 0-360 degrees in 10 degree steps.

After using "W", you MUST select "O" or "R" to continue.

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The FORTRAN code for EMFFT is in

JUSTEM\$DKA0:[TSB.FOR]EMFFT.FOR, .SUBS.

This documentation is in JUSTEM\$DKA0:[TSB.DOC]EMFFT.DOC 5-Mar-92

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