

ONED.DOC

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CONTENTS

- A. INTRODUCTION
- B. CONSTRUCTING A MOTIF INTERACTIVELY
- C. USING AN EXISTING MOTIF
- D. SAMPLING THE MOTIF
- E. SPECIFYING THE NUMBER OF REPEATS
- F. FLOATING THE DATA
- G. APPLYING A TEMPERATURE FACTOR
- H. ADDING NOISE TO THE DATA
- I. FILTERING THE DATA
- J. FLOW CHART FOR ONED PROGRAM

A. INTRODUCTION

ONED is useful for illustrating in one-dimension the principles of diffraction theory. One can build simple 1D motif structures by Fourier summation and perform various Fourier analysis operations on a single motif or a periodic array of motifs. ONED requires the use of a Lexidata graphics device (either the 1280x1024 pixel resolution device in LILY B-131 or the 640x512 device in LILY B-403). This program operates with several "TOUCH-KEY" options which require you to enter your choice (e.g. a "Y" or "N" to answer yes or no) by merely pressing the appropriate keyboard character WITHOUT hitting the <CR> key.

The program begins with the building up of a 1D motif structure. This is accomplished either by reading in an existing motif stored as a disk file or by constructing one with the interactive graphics device.

B. CONSTRUCTING A MOTIF INTERACTIVELY

To build a new motif, type a "1" followed by <CR> at the first prompt and then enter values for as many sinusoidal waves as you wish. Enter the wave number (frequency), amplitude, and phase for each wave. **NOTE:** be careful to enter the values as an integer (wave #) followed by two floating point numbers (amplitude, phase) and with the numbers separated by commas. Each time you enter another wave, the current motif is displayed on the graphics screen as a green-colored curve. The white line identifies the zero density level. As a simple example one might enter the following values:

```
1, 100., 0.  
2, 50., 90.  
3, 50., 180.  
0, 160., 0.
```

NOTE: Wave #0 just adds a constant density to the motif, consequently its phase is meaningless.

Continue adding as many waves as you like (you may even subtract waves by specifying negative amplitudes but this option may still have bugs!) and finish by hitting a <CR>. At this point you have the option of saving your work of art as a disk file to show friends and family at an appropriate later date, or you can start over (and over and over) to get the desired result, or you can continue with what you have built.

C. USING AN EXISTING MOTIF

If you already have a motif stored in a disk file, hit <CR> at the first program prompt and then type the name of the file.

D. SAMPLING THE MOTIF

Each motif is stored in computer memory or on disk as a smooth function consisting of 128 evenly-spaced points (pixels). The intensity at each pixel is the density of the motif at that point. If you have created an ASCII file of a motif, try typing the file contents (this must be done outside the program, for example by typing "TYPE filename") to see how the 128 data points are stored (16 rows of eight pixels each).

ONED allows you to construct large, periodic objects (1D crystals), up to 256 pixels long by stringing together multiple copies of the motif. You must first decide how coarsely or finely to sample the 128-point motif (NSAMPL). Typically, one might sample the motif with 16.0 or 32.0 points (this involves simple interpolation of the 128-point function). **NOTE:** NSAMPL (DEFAULT = 32.0) is a floating point value!

E. SPECIFYING THE NUMBER OF REPEATS

Enter NMOTIF, to specify the number of motifs in the 1D crystal. **NOTE:** NMOTIF is entered as a floating point value, so crystals with a non-integral number of unit cells can be made. Note also that your crystal can not exceed 256 pixels in length. Depending on what value you choose for NSAMPL, a DEFAULT value for

NMOTIF will be given that produces a crystal of 256 points. Only values of NMOTIF that are less than or equal to the DEFAULT are acceptable.

F. FLOATING THE DATA

You have the option of floating (Y) or not floating (N) the data. Floating refers to the process of subtracting from every point in the object the average background value. Floating is generally necessary in computing FTs from discrete data otherwise spurious ripples occur in the Fourier transform as a result of strong diffraction from sharp discontinuities in the object. The DEFAULT answer is "Y" (type a "Y" or a <CR>).

G. APPLYING A TEMPERATURE FACTOR

A temperature factor applies a smooth exponential falloff to the Fourier transform. If you choose "Y" to apply the temperature factor (DEFAULT = "N"), then enter a value for TFAC in units of inverse pixels to specify at what point the temperature factor function reaches a value equal to $1.0/\exp$ (≈ 0.368). For TFAC = 0.5, the amplitudes in the object Fourier transform will be downweighted by $1.0/\exp$ at the edge of the transform. For TFAC = 0.25, the amplitudes drop to $1.0/\exp$ of their original values half-way out in the transform. **NOTE:** If you apply the temperature factor more than once, the effect is MULTIPLICATIVE.

H. ADDING NOISE TO THE DATA

If you choose to add shot noise to the crystal (DEFAULT = "N") you can specify a desired signal-to-noise ratio (SN_RATIO) within the range 0.01 to 1000.0.

I. FILTERING THE DATA

If you choose to filter the crystal (DEFAULT = "N") you have the following touch-key menu options:

```
Touch-key Filtering Options
-----
B  BACK transform data
M  MASK transform data
R  Set RESOLUTION limits
T  Apply TEMPERATURE factor
E  EXIT routine
```

Choice:

"B" is used to BACK-transform the current Fourier transform. The original, noise-free object is displayed in yellow dots above the current object (displayed in red).

"M" is used to define values for building a filter mask to block out portions of the Fourier transform. The mask consists of a series of holes of diameter, HOLE_DIAM (<CR>=1.0) that are evenly spaced LSPACE (<CR>=256.0/NMOTIF) transform pixel units (1 TPU is one step in the discrete, 256-point transform). The program gives a DEFAULT value for LSPACE that positions the holes with respect to the IDEAL positions of the reciprocal lattice of the crystal. Try altering LSPACE and note the bizarre effects that can result. As HOLE_DIAM is reduced, the amount of averaging increases. "Infinite" averaging occurs when HOLE_DIAM = 1.0 (DEFAULT).

"R" is used to impose RESOLUTION limits (RMIN,RMAX) on the Fourier transform data. RMIN and RMAX are specified in inverse pixel units to define an annulus (inner and outer limits) within which the Fourier transform is zeroed. Usual practice is to set RMAX < 0.5 (low-pass filter) and RMIN = 0.0 (NO high-pass filtering). High-pass filtering (RMIN > 0.0) will knock-out low-resolution terms and enhance high resolution features (but may create bizarre effects!).

"T" is used to apply a TEMPERATURE factor in the same way as described above. The temperature factor applied is displayed in light blue next to the Fourier transform.

J. FLOW CHART FOR ONED PROGRAM

* MAIN *

* (ONED.FOR) *

*

*-- LX_INIT

*

*-- LX_ZOOM

*

*-- LX_CTSET

*

|-- PIRADDEG

*-- ONED_INIT |-- LX_ERASE

* |-- LX_VEC

*-- ONED_BLD -- |-- GET_YESNO

* |-- LX_CHAN

* |-- LX_ZOOM

* |-- ONED_INIT

*

|-- GET_YESNO

*-- ONED_INFO ----- |-- BELL

*

*-- ONED_TERP

*

*-- ONED_TFAC -- ONED_FFT -- FORT

*

*-- ONED_NOIS ----- |-- ONED_FFT -- FORT

* |-- SEED

*-- ONED_FLOT -- ONED_FFT -- FORT

*

|-- ONED_FFT -- FORT

*-- ONED_PLOT -- |-- ONED_BOX ----- |-- LX_ERASE

* |-- LX_VEC |-- LX_VEC

*

|-- GET_YESNO

* |-- READCHAR

* |-- STRING_UPPER

*-- ONED_FLT --- |-- ONED_FFT -- FORT

* |-- ONED_PLOT -- * (see above)

*-- GET_YESNO |-- ONED_MSK -- LX_VEC

*

|-- ONED_TFAC

*-- LX_CHAN