

Users Guide

to

NCEMSS

The NCEM program for
the simulation of
HRTEM images

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This work was supported by the U.S. Dept. of Energy under Contract No. DE-AC03-76SF00098

<u>Section</u>	<u>Page</u>
1. Introduction to the simulation process	1
1.1 Why simulate images ?	1
1.2 Describing the transmission electron microscope	1
1.3 Simplifying the description of the TEM	3
1.4 Simulating TEM images	5
2. Introduction to NCEMSS	7
2.1 The three simulation steps	7
2.2 NCEMSS files	7
3. Running NCEMSS	11
3.1 Getting started	11
3.2 The SINGLE/LAYERED menu	13
3.3 The FILE-LIST menu	15
3.4 The PARAMETER or MAIN or CONTROL menu	17
3.4.1 Parameters of the PARAMETER menu	17
3.4.2 Control boxes	21
3.5 The BASIS menu	23
3.6 The SYMM-OP menu	25
3.7 The ATOM-LIST menu	27
3.8 The BUILD menu	29
3.9 The ATOM-DISPLAY menu	31
3.10 The AMPLIT menu	33
3.11 The CTF plot	35
3.12 The IMAGE-DISPLAY menu	37
3.13 The SET-UP menu	39
3.14 The SET-CONTRAST menu	43
3.15 The SET-LAYERS menu	45
Appendix A Multislice Size, PhaseGrating Size, and Maximum G	47
A.1 Reciprocal-space multislice	47
A.2 Fourier-transform Multislice	47
A.3 Real-space multislice	49
A.4 Storage requirements	51
Appendix B HOLZ interactions	57
B.1 Identical slices with only one sub-slice per unit cell repeat distance	57
B.2 Identical sub-slices with n sub-slices per unit cell repeat distance	57
B.3 Sub-slices based on atom positions	57
B.4 Sub-slices based on the three-dimensional potential	57
B.5 NCEMSS sub-slicing	59
B.6 Other methods	59

Figures

The SINGLE/LAYERED Menu	12
The FILE-LIST Menu	14
The MAIN Menu	16
The MAIN Menu	18
The MAIN Menu	20
The BASIS Menu	22
The SYMMTRY-OPERATOR Menu	24
The Atom List Menu	26
The ATOM-DISPLAY Menu	30
The AMPLIT Menu	32
The IMAGE-DISPLAY Menu	36
The SET-UP Menu	38
The SET-UP Menu	40
The Set Contrast Menu	42

NCEMSS - a program for simulation of HRTEM images

1. Introduction to the simulation process

1.1 Why simulate images ?

Image simulation grew out of an attempt to explain why electron microscope images of complex oxides sometimes showed black dots in patterns corresponding to the patterns of heavy metal sites in complex oxides, and yet other images sometimes showed white dots in the same patterns. This first application was therefore to characterize the experimental images, that is to relate the image character (the patterns of light and dark dots) to known features in the structure.

Most simulations today are carried out for similar reasons, or even as a means of structure determination. Given a number of possible models for the structure under investigation, images are simulated from these models and compared with experimental images obtained on a high-resolution electron microscope. In this way, some of the postulated models can be ruled out until only one remains. If all possible models have been examined, then the remaining model is the correct one for the structure. For this process to produce a correct result, the investigator must ensure that all possible models have been examined, and compared with experimental images over a wide range of crystal thickness and microscope defocus. It is also a good idea to match simulations and experimental images for more than one orientation.

Some simulations are done in order to thoroughly explore one particular image by “freeze-framing” the imaging process in the computer. In this way, we can obtain information that is not observable experimentally, such as the electron wave amplitude at the exit surface of the specimen, the magnitude and phase of each component of the image intensity spectrum, or even the amplitude contributed to the intensity spectrum by each pair of diffracted-beam interferences.

The simulation programs can also be used to study the imaging process itself. By simulating images for imaginary electron microscopes, we can look for ways in which to improve the performance of present-day instruments, or even find that the performance of an existing electron microscope can be improved significantly by minor changes in some instrumental parameter. Alternatively, based on imaging requirements revealed by test simulations, we can adjust the electron microscope to produce suitable images of some particular specimen, or even of some particular feature in a particular specimen.

1.2 Describing the transmission electron microscope

In order to simulate an electron microscope image, we need firstly to be able to describe the electron microscope in such a way that we can model the manner in which it produces the image. As a first step, we can consider the usual geometrical optics depiction of the transmission electron microscope (TEM).

The Electron Microscope

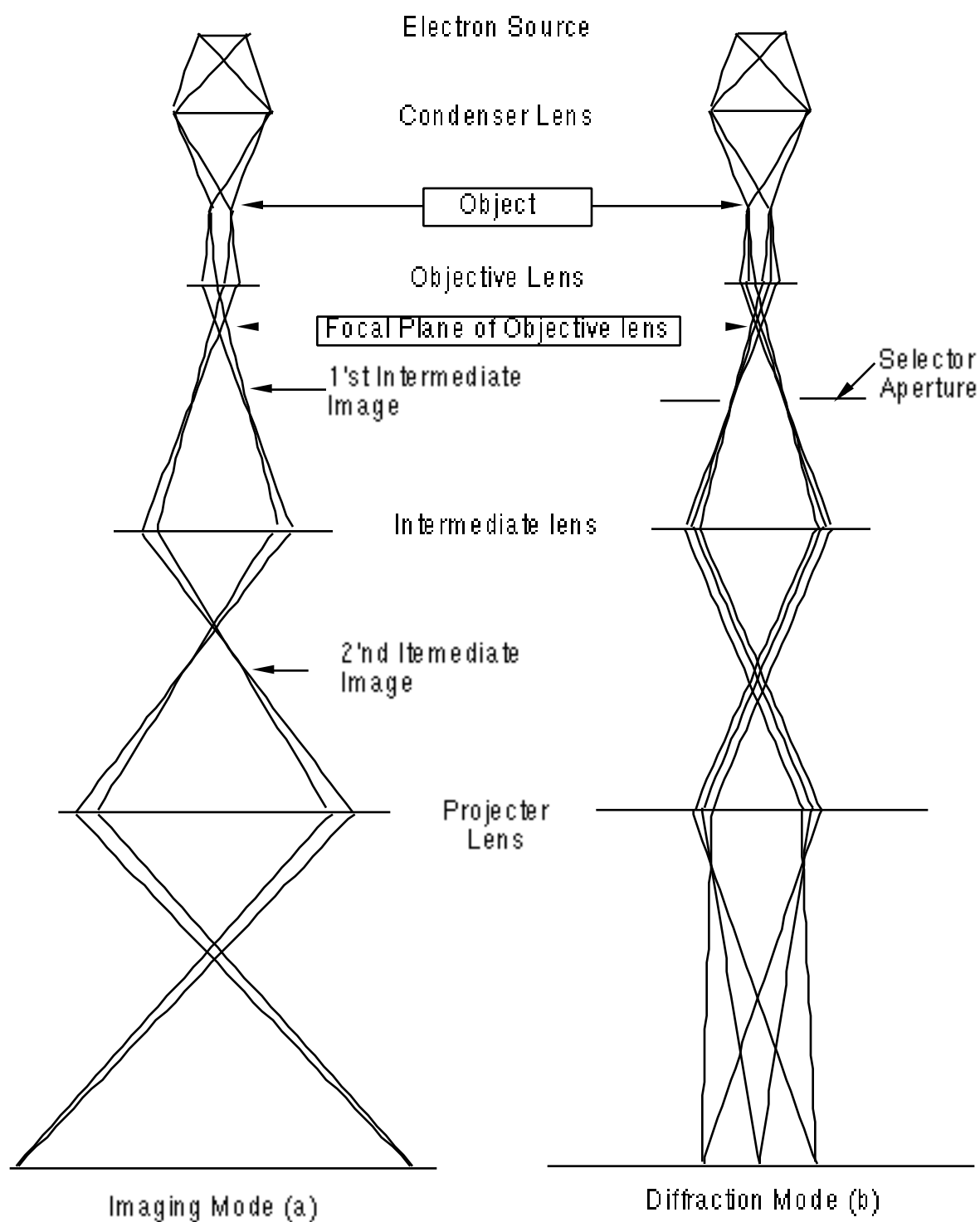


Fig.1 Geometrical optics representation of the TEM in imaging mode (a), and diffraction mode (b).

Figure 1 shows such a diagram of a TEM operated in two distinct modes, set up for microscopy (a), and for diffraction (b). In microscopy mode we see that the TEM consists of an electron source producing a beam of electrons that are focused by a condenser lens onto the specimen; electrons passing through the specimen are focused by the objective lens to form an image called the first intermediate image (I1); this first intermediate image forms the “object” for the next lens, the intermediate lens, which produces a magnified image of it called the second intermediate image (I2); in turn, this second intermediate image becomes the “object” for the projector lens; the projector lens forms the greatly-magnified final image on the viewing screen of the microscope. In microscopy mode, electrons that emerge from the same point on the specimen exit surface are brought together at the same point in the final image.

At the focal plane of the objective lens, we see that electrons are brought together that have left the specimen at different points but at the same angle. The diffraction pattern that is formed at the focal plane of the objective lens can be viewed on the viewing screen of the TEM by weakening the intermediate lens to place the microscope in diffraction mode (b).

1.3 Simplifying the description of the TEM

Consideration of the description of the electron microscope in figure 1 shows that the projector lens and the intermediate lens (or lenses) merely magnify the original image (I1) formed by the objective lens. For the purposes of image simulation we can reduce the TEM to three essential components; (1) an electron beam that passes through (2) a specimen, and then through (3) an objective lens (fig.2).

Our next step in describing the electron microscope for image simulation is to move from the geometrical optics description of the TEM to a description based on wave optics. In this description of the microscope we examine the amplitude of the electron wavefield on various planes within the TEM, and attempt to determine how the wavefield at the viewing screen comes to contain an image of our specimen.

By treating the electrons as waves, and considering our simplified electron microscope (fig.2), we see that there are three planes in the TEM at which we need to be able to compute the (complex) amplitude of the electron wavefield.

(1) The image plane:

Working backwards, we start with our desired information, the electron wavefield at the image plane; this wavefield is derived from the wavefield at the focal plane of the objective lens by applying the effects of the objective aperture and the phase changes introduced by the objective lens.

(2) The focal plane of the objective lens:

In turn, the electron wavefield at the focal plane of the lens is derived from the wavefield at the exit surface of the specimen by a simple Fourier transformation.

The Reduced Electron Microscope

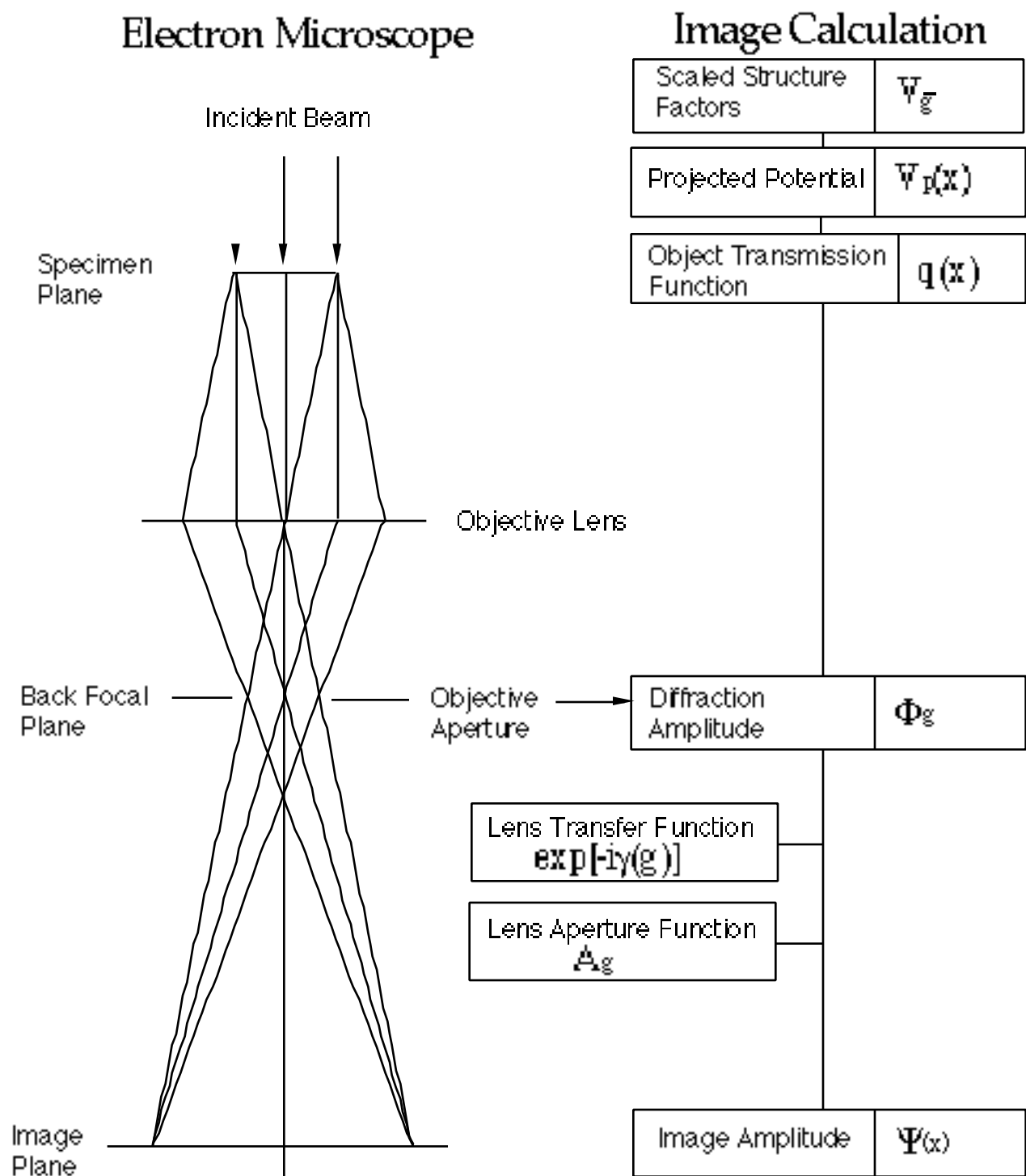


Fig. 2. The simplified TEM (left) and the calculations required for an image simulation (right). The three principal planes are marked.

(3) The specimen exit surface:

In order to know the exit-surface wavefield, we must know with which physical property of the specimen the wave interacts, and describe that physical property for our particular specimen.

Cowley and Moodie (1957) showed that the interaction of an electron beam with a specimen could be described by the so-called multislice approximation, in which electrons propagate through the specimen and scatter from the crystal potential; the electron scattering is described by the so-called phase-grating function, a complex function of the potential, and the electron propagation is computed with a propagation function dependent on the electron wavelength.

1.4 Simulating TEM images

The problem of simulating images thus becomes a problem of computing the electron wavefields at the three microscope planes. Currently, the best way to produce simulated images is to divide the overall calculation into three parts:

- (1) Model the specimen structure to find its potential in the direction of the incident beam.
- (2) Produce the exit-surface wavefield by considering the interaction of the incident electron wave on the specimen potential.
- (3) Compute the image-plane wavefield by imposing the effects of the objective lens on the specimen exit surface wave.

Cowley J.M. & Moodie A.F. (1957) The scattering of electrons by atoms and crystals. I. A new theoretical approach. *Acta Cryst.* 10, 609.

2. Introduction to NCEMSS

2.1 The three simulation steps

Since the simulation problem divides neatly into three parts, NCEMSS treats these three parts with three sub-programs -

- (1) **PHSGRT** - a program to generate the part of the crystal potential that produces electron scattering; input is from a file containing structural data about the specimen, including unit cell dimensions, symmetries, and atom positions, occupancies, and temperature factors.
- (2) **MSLICE** - a program to generate the electron wavefield at the specimen exit surface; it uses PHSGRT data combined with information about the accelerating voltage of the electron microscope, and the specimen thickness and tilt.
- (3) **IMAGE** - a program to generate the image intensity at the microscope image plane; the effects of objective lens phase changes and resolution-limiting aberrations are included via parameters like defocus, spherical aberration, incident beam convergence, spread-of-focus, and the position and size of the objective aperture.

Thus PHSGRT considers only the specimen structure, MSLICE treats the interaction of the specimen with the electron wave, and IMAGE simulates how the wave leaving the specimen interacts with the lens system of the electron microscope. Once a simulation has been made, any additional simulation will usually not require a full re-simulation; any change in microscope parameters will not affect the results of the PHSGRT and MSLICE programs, and only IMAGE will need to be re-run; any change in microscope voltage or in specimen thickness or tilt will not affect the results of PHSGRT, but MSLICE and IMAGE will need to be re-run. Of course, any change in the specimen structure will require the re-running of all three subprograms.

2.2 NCEMSS files

Supplied files: NCEMSS uses four data files to store supplied information not normally altered by the user:

- (1) **spcgrp.dat** stores information on all 230 space groups for generation of crystal symmetry operators as required by the input specimen structures.
- (2) **scatt.dat** stores information on atomic scattering factors for the first 98 elements.

- (3) **microscopes.dat** stores information on the imaging parameters of various high-resolution electron microscopes. Note that the user has the option of adding additional microscopes to the table stored in MICROSCOPES.DAT.
- (4) **lprint.ps** stores a set of Postscript definitions that are used in order to print images to a Postscript Laserprinter.

Generated files: NCEMSS generates and stores various data files in the course of a simulation. The five data files are:

- (1) **name.at** stores all the structure and microscope information needed to run the simulation. This information is derived from user input and the supplied data files. In particular, the string “**name**” is a unique name for the structure, input by the user when creating the structure file.
- (2) **name.pout** is the result of running the PHSGRT subprogram from the information stored in *name.at*; it contains the specimen potential in the direction of the electron beam.
- (3) **name.mout** is the result of running the MSLICE subprogram using the data in *name.pout* with those in *name.at*; it contains the exit-surface wave at one or more selected specimen thicknesses.
- (4) **name.iout** is the result of running the IMAGE subprogram to apply the effects of the microscope parameters in the *name.at* file to the exit-surface wave; it contains one or more images ready to be displayed.
- (5) **name.aout** contains the complex amplitudes of several diffracted beams at one-slice increments in specimen thickness. The beams are specified by the user in the main menu, and can be plotted as a function of specimen thickness.

In addition, two print files are produced (but rarely printed) just in case additional information about a computation is required by the user. These files are:

- (6) **name.p_prnt** contains information about the way in which the PHSGRT subprogram processed the *name.at* data to produce the specimen potential.
- (7) **name.m_prnt** contains information about the way in which the MSLICE subprogram processed the *name.pout* data with *name.at* data to produce the exit-surface wave; that is, it contains information on the multislice computation.

Since NCEMSS images are stored in a file for interactive display, the user has the option of writing any image to the display screen with any selected number of unit cells, with any selected value of contrast and brightness, and at any selected magnification. In addition, the user may elect to display (i.e. write to the screen) real-space functions like the projected crystal potential, the exit-surface electron wavefunction, or a drawing of the atom positions; in addition, reciprocal-space functions such as the diffraction intensities and the image power spectrum (“optical” diffractogram) may be displayed and indexed.

3. Running NCEMSS

Note on Platform dependency:

NCEMSS was originally written for a terminal emulating tektronix 4014 commands. The menus were written to the terminal and the images were displayed on a framestore. The code was executing on a Digital Equipment Corporation microVax II computer under the VMS operating systems. The code has since been ported to other platforms and will run on DEC VMS and Ultrix workstations and on various flavors of Unix running X-windows. However, because of the origin of the program, it still an old style layout dictated by the tektronix terminal. The program uses two windows. One looking like a graphics window displaying push-button style menus and one window for displaying graphics output such as images, diffraction patterns and views of unit cells. The program does not have a modern style interface with a menubar and pull down menus.

NCEMSS is run interactively at a graphics screen using a mouse or other pointing device. The graphics screen may be a workstation console, an X-window terminal or any computer running as an x-window server. Commands are issued to NCEMSS by moving a cursor to select an appropriate item from a menu. Sometimes, selecting an item from a menu will produce another menu with additional options.

Because of constant changes, the menus mentioned in this manual may not always correspond to the current version of the program for a particular platform. The text will be appropriate for the UNIX version of the program.

3.1 Getting started

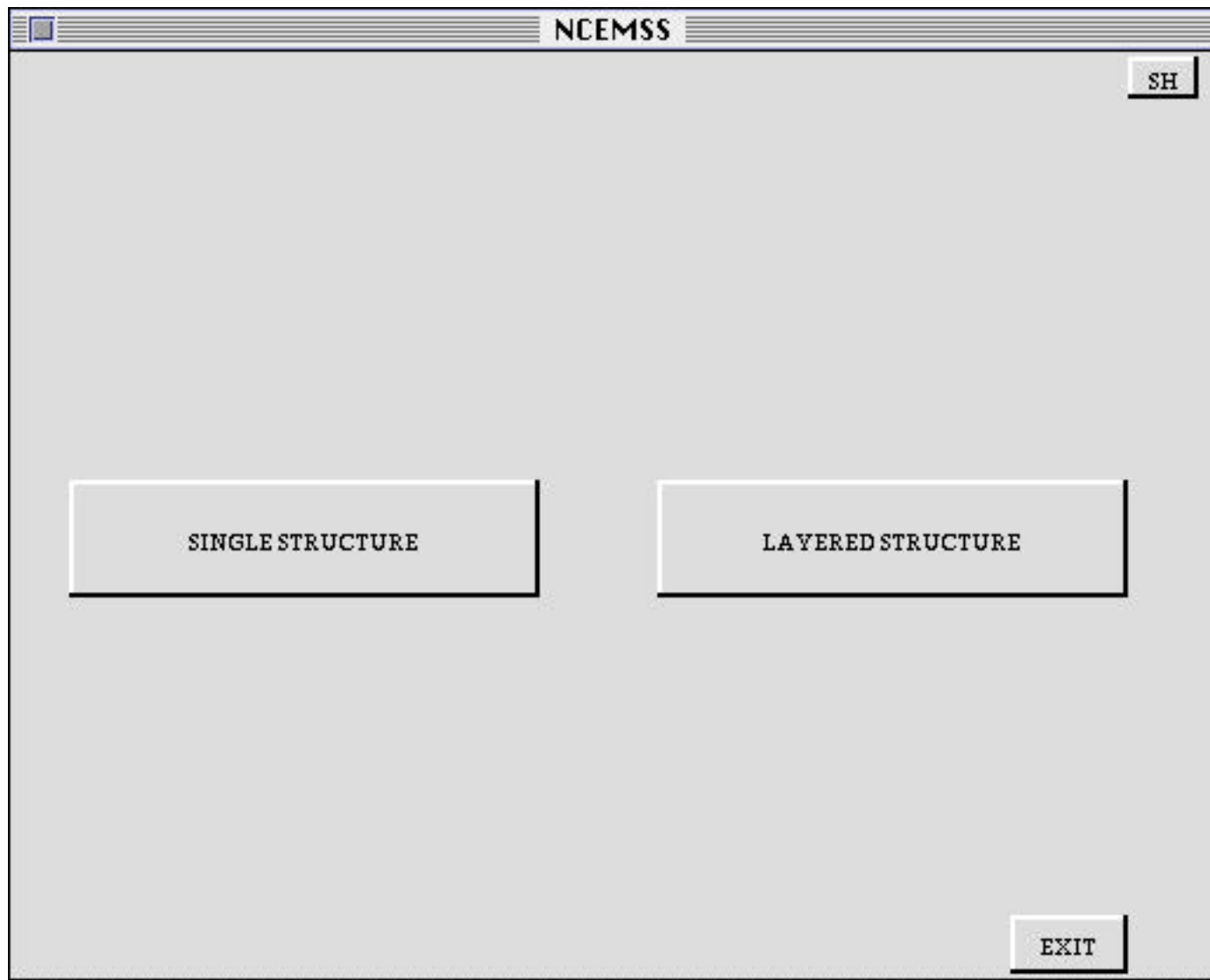
If started from an X-terminal, first type **setenv DISPLAY <IP address>** to set the output to the X-window terminal.

Start NCEMSS by typing **ncemss** followed by a carriage return:

ncemss (return)

this action will produce the SINGLE/LAYERED menu (page 12), by opening two windows on the workstation screen, one being the menu (control) window, the other the image window.

The SINGLE/LAYERED Menu



3.2 The SINGLE/LAYERED menu

The first menu encountered by the user on starting to work with NCEMSS consists of three labeled boxes. Any one of these boxes or buttons can be activated by using the mouse to move the screen cursor into the area of the screen within the box, and then pressing the LEFT button on the mouse. At the lower right of the window is the EXIT box, or button. Selecting this box will cause the program to exit and return to the system prompt.

The two major boxes allow the user to specify a choice of either a SINGLE STRUCTURE calculation, or a calculation of the images arising from a LAYERED STRUCTURE. A SINGLE STRUCTURE calculation is one where the specimen structure repeats regularly in the direction of the electron beam, and is the usual type of image simulation. A LAYERED STRUCTURE calculation is a simulation in which the specimen structure is built up of a number of different structural layers in the electron beam direction, so that the computation requires the use of more than one crystal structure file. Selecting the LAYERED STRUCTURE box produces the SET LAYERS menu (page 46). Selecting SINGLE STRUCTURE produces the FILE-LIST menu (page 14).

The FILE-LIST Menu

NCEMSS				
PERSONAL	COMMON	PREV. PAGE	NEXT PAGE	SH
inp	ltest	test	newtest	
lay1	lay2	new	s30203	
s60203	qian	qian2	s60	
s30				

USE DISPLAYED FILE	CREATE NEW FILE	RETURN
--------------------	-----------------	--------

3.3 The FILE-LIST menu

The FILE-LIST menu lists the user's structure files on the screen. In addition, there are four boxes across the top of the menu, and three boxes across the bottom. The four top boxes control the listing of the structure names; the right hand pair allow the user to "page" through the list, displaying subsequent pages of structure file names.

The top left boxes can be used to select lists of files from either the user's PERSONAL collection of structure files, or from a COMMON collection available to all users on the system. The files in the COMMON collection can often serve as useful templates for modification to the user's needs. On entry to the FILE-LIST menu, the PERSONAL box is selected automatically. To obtain the COMMON list, move the cursor to the COMMON box and press the LEFT button on the mouse. To return to your PERSONAL file collection, move the cursor to the PERSONAL box and press the button.

The three boxes at the bottom of the menu are used to proceed from the current menu. The rightmost box is the RETURN box, and is used to go back to the previous menu. Note that many menus have this facility, with the RETURN box situated in the bottom right corner of the menu. The bottom left box is used to notify NCEMSS that the user wishes to use one of the displayed structure files. Moving the cursor to this USE DISPLAYED FILE box and selecting it by clicking the mouse button removes all the other boxes, and allows the user to select one of the displayed files by moving the cursor to the correct filename and clicking the mouse button. Selecting a structure filename causes NCEMSS to read the file and display its parameters in the PARAMETER menu (often referred to as the MAIN or CONTROL menu, because it is the one from which the NCEMSS computation is controlled by the user). The CONTROL menu is shown on page 16.

The CREATE NEW FILE box is selected when the user desires to input a new structural file. Selecting this box with the cursor causes NCEMSS to ask for a unique name for the structure. Entry of the name then produces a PARAMETER menu with no parameter values, and a series of prompts from NCEMSS explaining each parameter needed for input.

HELP: If this is your first use of NCEMSS, it may be helpful to try moving the cursor to each box in turn, asking for the HELP facility by clicking the CENTER button on the mouse as each box is reached. The HELP facility is available for every command box on every menu, and should provide enough information that you will need to consult this Guide only infrequently.

The MAIN Menu

NCEMSS					
INPUT FOR : copper			SPACE GROUP #225		SH
A = 3.61			ALPHA = 90.00		
B = 3.61			BETA = 90.00		
C = 3.61			GAMMA = 90.00		
Gmax = 2.00			Zone Axis : 0 0 1		
No. of Symmetry Operators : 192			No. of slices per unit cell : 1		
No. of atoms in the basis : 1			No. of different atoms : 1		
Microscope : ARM			Foil Thickness : 40(40)120		
	Cs = 2.80		Amplit. output for plotting : yes		
	Del = 100.00		The indices are : h k l		
	Th. = 0.60			0 0 0	
Volt. = 1000.00				2 0 0	
Cent. of Laue circle: h = 0.00				2 2 0	
	k = 0.00				
Defocus : -300(-300)-1500					
Aperture Radius : 0.70					
Cent. of Obj. Aprt. : h = 0.00			Cent. of Optic Axis : h = 0.00		
	k = 0.00			k = 0.00	
CHANGE		SHOW BASIS		PHSGRT	
RUN		SHOW ATOMS		MSLICE	
		IMAGE		DISPLAY	
		AMPLIT		VIEW FILE	
				CTF	
				RETURN	

3.4 The PARAMETER or MAIN or CONTROL menu

The main CONTROL menu lists a summary of the control parameters for the current simulation as well as twelve boxes for control of the computation.

When the CREATE NEW FILE option of the FILE-LIST menu (page 14) is selected, an empty PARAMETER menu (with no control boxes) is presented, and NCEMSS prompts for parameters. These parameters have the same form as those presented in the PARAMETER menu when a structure filename is selected from the FILE-LIST menu. When every parameter has been entered, NCEMSS re-presents the PARAMETER menu with the control boxes drawn in and available for use.

3.4.1 Parameters of the PARAMETER menu

INPUT FOR: The parameter displayed next to this prompt is a short title for the structure.

SPACE GROUP #: NCEMSS generates symmetry operators for any one of the 230 space groups, when given the number of the space group required (listed in the International Tables for Crystallography). If the space group required is not one listed in the Tables, a value of zero can be entered.

A, B, C, ALPHA, BETA, GAMMA: These are the unit cell dimensions in Angstrom units, and the unit cell angles in degrees.

GMAX: The maximum value (in reciprocal Angstrom units) of g to be considered in the multislice diffraction calculation. This value imposes an “aperture” on the diffracted beams included in the dynamic scattering process. It should be large enough to ensure that all significant beam interactions are included. For light atoms and thin crystals, values as low as 2.0 are adequate. For structures with heavy atoms and large crystal thicknesses, values of 3.0 to 4.0 are to be preferred. Note that NCEMSS will compute phase-grating coefficients out to twice GMAX in order to include dynamical interactions correctly (Appendix A).

ZONE AXIS: Specimen orientation is selected by specifying the zone axis desired. Three indices are entered with one space between each.

NO. OF SYMMETRY OPERATORS: If a space group has been selected, the correct value for this parameter will have been entered by NCEMSS. If a value of zero has been entered for the SPACE GROUP #, then the correct number of operators must be entered here.

NO. OF SLICES PER UNIT CELL: For unit cells with large repeat distances in the beam direction, moderate values of GMAX may allow the Ewald sphere to approach the so-called pseudo-upper-layer line that the multislice allows at the reciprocal of the chosen slice thickness. In this case NCEMSS will sub-divide the slice into two or more subslices. How this is done depends upon the potential setting chosen in the SET-UP menu (page 40).

The MAIN Menu

NCEMSS					
INPUT FOR : copper			SPACE GROUP #225		SH
A = 3.61			ALPHA = 90.00		
B = 3.61			BETA = 90.00		
C = 3.61			GAMMA = 90.00		
Gmax = 2.00			Zone Axis : 0 0 1		
No. of Symmetry Operators : 192			No. of slices per unit cell : 1		
No. of atoms in the basis : 1			No. of different atoms : 1		
Microscope : ARM			Foil Thickness : 40(40)120		
	Cs = 2.80		Amplit. output for plotting : yes		
	Del = 100.00		The indices are : h k l		
	Th. = 0.60			0 0 0	
Volt. = 1000.00				2 0 0	
Cent. of Laue circle: h= 0.00				2 2 0	
	k= 0.00				
Defocus : -300(-300)-1500					
Aperture Radius : 0.70					
Cent. of Obj. Aprt. : h= 0.00			Cent. of Optic Axis : h= 0.00		
	k= 0.00			k= 0.00	
CHANGE		SHOW BASIS		PHSGRT	
RUN		SHOW ATOMS		MSLICE	
		IMAGE		DISPLAY	
		AMPLIT		VIEW FILE	
				CTF	
				RETURN	

NO. OF ATOMS IN THE BASIS: This value is the number of independent atom positions in the basis or asymmetric unit of the cell. When operated on by the symmetry operators, the basis generates all the atom positions within the cell.

NO. OF DIFFERENT ATOMS: This value is the number of different types of atoms in the specimen structure; difference is due to a different Debye-Waller factor or different atomic number.

MICROSCOPE: The type of electron microscope used to generate the imaging parameters. If a type known to NCEMSS is entered, then NCEMSS provide values for CS, the spherical aberration coefficient of the objective lens (in mm.); DEL, the halfwidth of a Gaussian spread of focus due to chromatic aberration (in Angstrom units); TH., the semi-angle of incident beam convergence (in milliradian). If the type of microscope is unknown to NCEMSS, the above values must be entered separately (or the data file MICROSCOPES.DAT may be edited to include an appropriate microscope type).

FOIL THICKNESS: The thickness of the specimen foil may be entered as one single number representing the thickness in Angstrom units, or as a series of thicknesses represented by the upper and lower bounds and a thickness step; e.g. 100(50)250 will cause NCEMSS to store the exit wavefield at specimen thicknesses of 100Å to 250Å in steps of 50Å (a total of four thicknesses).

AMPLIT. OUTPUT FOR PLOTTING: A number of diffracted beams may be selected for plotting of their intensity and phase variation as a function of specimen thickness. If YES is answered to the NCEMSS prompt, the number of beams and their indices may be entered.

VOLT.: The electron microscope accelerating voltage in kilovolts.

CENT. OF LAUE CIRCLE: Specimen tilt is specified by entering the center of the Laue circle in units of the h and k indices of the projected two-dimensional reciprocal-space unit cell.

DEFOCUS: The defocus of the objective lens is entered in Angstrom units with a negative value representing underfocus (weakening of the lens current). As for the FOIL THICKNESS parameter, a single value of defocus may be entered, or a range specified by the upper and lower bounds and the interval; -300(-200)-1100 means defocus values of -300Å, -500Å, -700Å, -900Å and -1100Å.

APERTURE RADIUS: The radius of the objective aperture is specified in reciprocal Angstrom units.

CENT. OF OBJ. APRT.: The center of the objective aperture is defined in units of the h and k indices of the two-dimensional reciprocal-space unit cell, as for the Laue circle center.

CENT. OF OPTIC AXIS: The center of the optic axis of the electron microscope is specified in terms of the h and k indices of the two-dimensional reciprocal-space unit cell, just as for the Laue circle center and the aperture center.

The MAIN Menu

NCEMSS					
INPUT FOR : copper			SPACE GROUP #225		SH
A = 3.61			ALPHA = 90.00		
B = 3.61			BETA = 90.00		
C = 3.61			GAMMA = 90.00		
Gmax = 2.00			Zone Axis : 0 0 1		
No. of Symmetry Operators : 192			No. of slices per unit cell : 1		
No. of atoms in the basis : 1			No. of different atoms : 1		
Microscope : ARM			Foil Thickness : 40(40)120		
	Cs = 2.80		Amplit. output for plotting : yes		
	Del = 100.00		The indices are : h k l		
	Th. = 0.60			0 0 0	
Volt. = 1000.00				2 0 0	
Cent. of Laue circle: h= 0.00				2 2 0	
	k= 0.00				
Defocus : -300(-300)-1500					
Aperture Radius : 0.70					
Cent. of Obj. Apert. : h= 0.00			Cent. of Optic Axis : h= 0.00		
	k= 0.00			k= 0.00	
CHANGE		SHOW BASIS		PHSGRT	
RUN		SHOW ATOMS		MSLICE	
		IMAGE		DISPLAY	
		AMPLIT		VIEW FILE	
				CTF	
				RETURN	

3.4.2 Control boxes

CHANGE: When the CHANGE box is activated by clicking the mouse with the cursor within the CHANGE box boundaries, any parameter value may be changed simply by moving the cursor to the parameter position, clicking the mouse and entering the new value from the keyboard in response to the NCEMSS prompt. To leave CHANGE mode, deactivate the CHANGE box by clicking the mouse with the cursor once again positioned over the CHANGE box.

RUN: Activating the RUN box will cause NCEMSS to run an image simulation for the current values of the parameters shown in the PARAMETER menu. NCEMSS will automatically run the least required computation, starting with the PHSVRT program only if a structure parameter has been changed since the last run of this data, and starting with the IMAGE program if the only change has been in the electron microscope imaging parameters.

SHOW BASIS: This box will cause NCEMSS to display the BASIS menu, a list of the atom positions making up the basis (page 22).

SHOW ATOMS: this box will cause NCEMSS to display the ATOM-LIST menu, a list of all the atom positions in the unit cell (page 26).

PHSVRT: Activating the PHSVRT control box will run the PHSVRT sub-program for the current parameter values.

MSLICE: Activating the MSLICE control box will run the MSLICE sub-program for the current parameter values.

IMAGE: Activating the IMAGE control box will run the IMAGE sub-program for the current parameter values.

AMPLIT: Activating the AMPLIT control box will open up a plotting window (page 34), and ask the user which of the stored diffracted beam amplitudes to plot (assuming that some diffracted beams were stored by specifying their indices before the MSLICE was run).

DISPLAY: This control box is used to activate the IMAGE-DISPLAY menu (page 38) for writing images to the display screen.

VIEW FILE: Activating this control box causes NCEMSS to ask which print file to display, then to display it.

CTF: Activating this control box produces a linear-image Contrast Transfer Function under the imaging conditions specified by the current parameter values (page 36).

RETURN: Return to previous FILE-LIST menu.

he BASIS Menu

#	TYPE	NAME	X	Y	Z	DW	OCC
1	1	Cu	0.0000	0.0000	0.0000	0.5000	1.00

SH

PAGE +

PAGE -

PAGE #

CHANGE

ADD

DELETE

SHOW SYMM. OP

RETURN

3.5 The BASIS menu

The BASIS menu shows a list of the atom positions making up the basis; when operated upon by the symmetry operators, the basis yields the full set of unit cell atom positions. The BASIS menu displays the atom positions, showing the chemical symbol (NAME) for each atom, its fractional coordinates (X,Y,Z), the Debye-Waller factor, and the site occupancy. Subsequent pages of long lists can be viewed with the three right-hand control boxes.

CHANGE: The value of any parameter can be changed by activating the CHANGE box, then moving the cursor to the parameter position, clicking the mouse and entering the replacement value.

ADD: Additional atom positions may be added by activating the ADD box and entering parameter values in response to prompts.

DELETE: Activating the DELETE box, then moving the cursor to the appropriate line, will delete the line.

SHOW SYMM. OP: A list of the symmetry operators may be obtained by activating this control box in order to bring up the SYMM-OP menu (page 24).

RETURN: Return to previous MAIN menu.

The SYMMTRY-OPERATOR Menu

# SYMMETRY OPERATOR		# SYMMETRY OPERATOR	
1	x, y, z	21	$z, -x, -y$
2	$x, y+1/2, z+1/2$	22	$z+1/2, -x, -y+1/2$
3	$x+1/2, y, z+1/2$	23	$z+1/2, -x+1/2, -y$
4	$x+1/2, y+1/2, z$	24	$z, -x+1/2, -y+1/2$
5	$-x, -y, z$	25	$-z, -x, y$
6	$-x, -y+1/2, z+1/2$	26	$-z+1/2, -x, y+1/2$
7	$-x+1/2, -y, z+1/2$	27	$-z+1/2, -x+1/2, y$
8	$-x+1/2, -y+1/2, z$	28	$-z, -x+1/2, y+1/2$
9	$-x, y, -z$	29	$-z, x, -y$
10	$-x, y+1/2, -z+1/2$	30	$-z+1/2, x, -y+1/2$
11	$-x+1/2, y, -z+1/2$	31	$-z+1/2, x+1/2, -y$
12	$-x+1/2, y+1/2, -z$	32	$-z, x+1/2, -y+1/2$
13	$x, -y, -z$	33	y, z, x
14	$x, -y+1/2, -z+1/2$	34	$y+1/2, z+1/2, x$
15	$x+1/2, -y, -z+1/2$	35	$y, z+1/2, x+1/2$
16	$x+1/2, -y+1/2, -z$	36	$y+1/2, z, x+1/2$
17	z, x, y	37	$-y, z, -x$
18	$z+1/2, x, y+1/2$	38	$-y+1/2, z+1/2, -x$
19	$z+1/2, x+1/2, y$	39	$-y, z+1/2, -x+1/2$
20	$z, x+1/2, y+1/2$	40	$-y+1/2, z, -x+1/2$

3.6 The SYMM-OP menu

The SYMM-OP menu shows a list of the symmetry operators generated by the chosen space group (or input by the user when a space group number of zero is entered in the MAIN menu - see page 20). The right-hand control boxes are used to page through long lists of symmetry operators.

CHANGE: Any operator may be replaced by activating the CHANGE box, clicking the mouse over the appropriate line, and entering the new operator.

ADD SYMMOP: Activating this control box enables the user to add a new operator to the list.

DELETE SYMMOP: Activating this box, then placing the cursor over any operator and clicking the mouse, will delete that operator.

RETURN: Return to previous BASIS menu.

The Atom List Menu

#	TYPE	NAME	X	Y	Z	DW	OCC
1	1	Cu	0.0000	0.0000	0.0000	0.5000	1.00
2	1	Cu	0.0000	0.5000	0.5000	0.5000	1.00
3	1	Cu	0.5000	0.0000	0.5000	0.5000	1.00
4	1	Cu	0.5000	0.5000	0.0000	0.5000	1.00

SH

PAGE +

PAGE -

PAGE #

DISPLAY

RETURN

3.7 The ATOM-LIST menu

The ATOM-LIST menu shows a list of the atom positions making up the unit cell. The list displays the atom positions one per line, showing the chemical symbol (NAME) for each atom, its fractional coordinates (X,Y,Z), the Debye-Waller factor (DW), and the site occupancy (OCC). Subsequent pages of long lists of atom position parameters can be viewed with the three right-hand control boxes.

BUILD CELL (not implemented on Unix Versions): Activating the BUILD control box brings up the BUILD menu (page 28) with the facility of generating defect cells.

DISPLAY: Activating this control box brings up the ATOM-DISPLAY menu (page 30), for the purpose of drawing an atom model of the current structure (page 32).

RETURN: Return to previous MAIN menu.

3.8 The BUILD menu

The BUILD menu is used to create defect cells visually with the aid of the cursor. The menu has a right-hand column of control buttons, activated in the usual way.

INCR X: This button is used to increment the unit cell in the x direction. The INCR_Y button does the same in the y direction. When the INCR_X button is activated, NCEMSS will ask for the additional number of repeats to be input from the keyboard. Note that the total length of the new cell in the x-direction will be the original length plus the number of increments specified.

DISPLAY: This control box is used to display the current defect cell, and should be used on entering the menu, and after each change made to the defect cell.

INSERT: To insert an atom, activate this box and move the cursor to the required position. Note the changes in the fractional coordinates displayed in the bottom line of the menu as the cursor is moved. NCEMSS will prompt for parameter values.

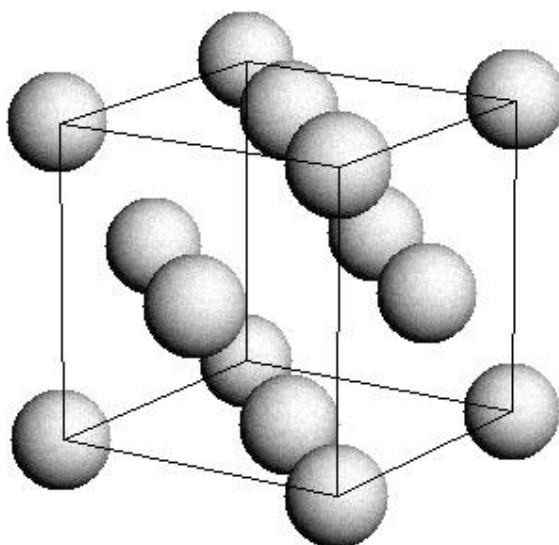
REMOVE: To remove an atom, activate this box and move the cursor to the appropriate atom, then click the mouse.

MOVE: To move an atom, activate this box, move the cursor to an atom position, click the mouse, move the mouse to the new position (note the fractional coordinates), and click again.

CHANGE: To change the atomic number of an atom, activate this box, and click the mouse at the atom position.

RETURN: Return to previous ATOM-LIST menu.

The ATOM-DISPLAY Menu



NCEMSS							
#	TYPE	NAME	X	Y	Z	DW	OCC
1	1	Cu	0.0000	0.0000	0.0000	0.5000	1.00
2	1	Cu	0.0000	0.5000	0.5000	0.5000	1.00
3	1	Cu	0.5000	0.0000	0.5000	0.5000	1.00
4	1	Cu	0.5000	0.5000	0.0000	0.5000	1.00

UNIT CELL

NEW UNIT CELL

UNIMPLEMENTED

RETURN

3.9 The ATOM-DISPLAY menu

When DISPLAY is selected in the ATOM-LIST menu (page 26), most of the control buttons are replaced to produce the ATOM-DISPLAY menu. The ATOM-DISPLAY menu has only four control boxes.

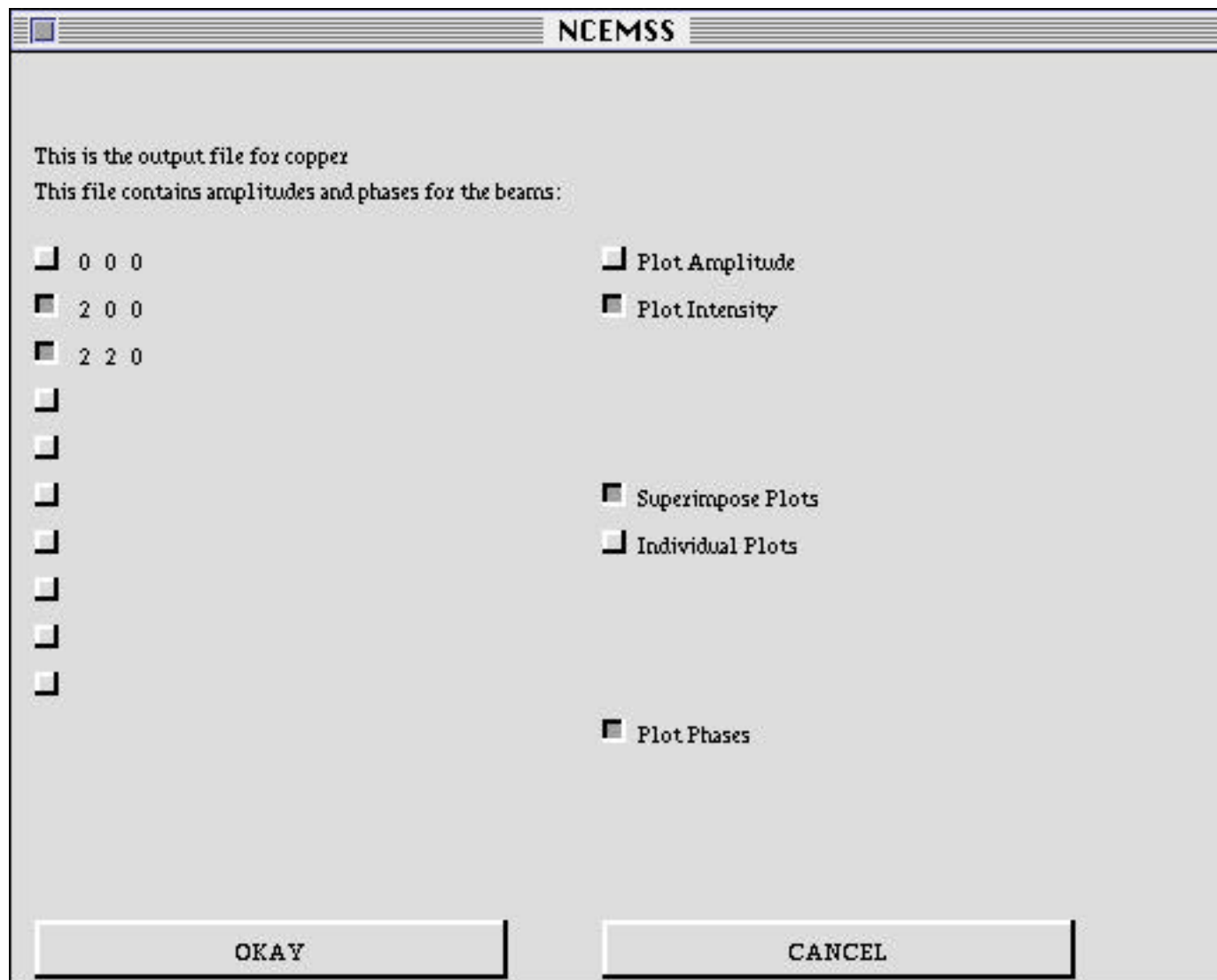
UNIT CELL: Activating this box splits it in two. Selecting either option causes NCEMSS to ask for the viewing direction indices to be input from the keyboard; NCEMSS then draws the unit cell, either with or without perspective (page 32).

NEW UNIT CELL: As for UNIT CELL, but for drawing any new unit cell produced with the BUILD menu (page 28).

3-D ATOM DISPLAY: This control box initiates a three-dimensional atom drawing routine based on a routine written by W.O. Saxton. It can be used to produce publication-quality atom model drawings with a wide range of different lighting conditions. This procedure is not implemented on most versions of NCEMSS, specifically all unix version

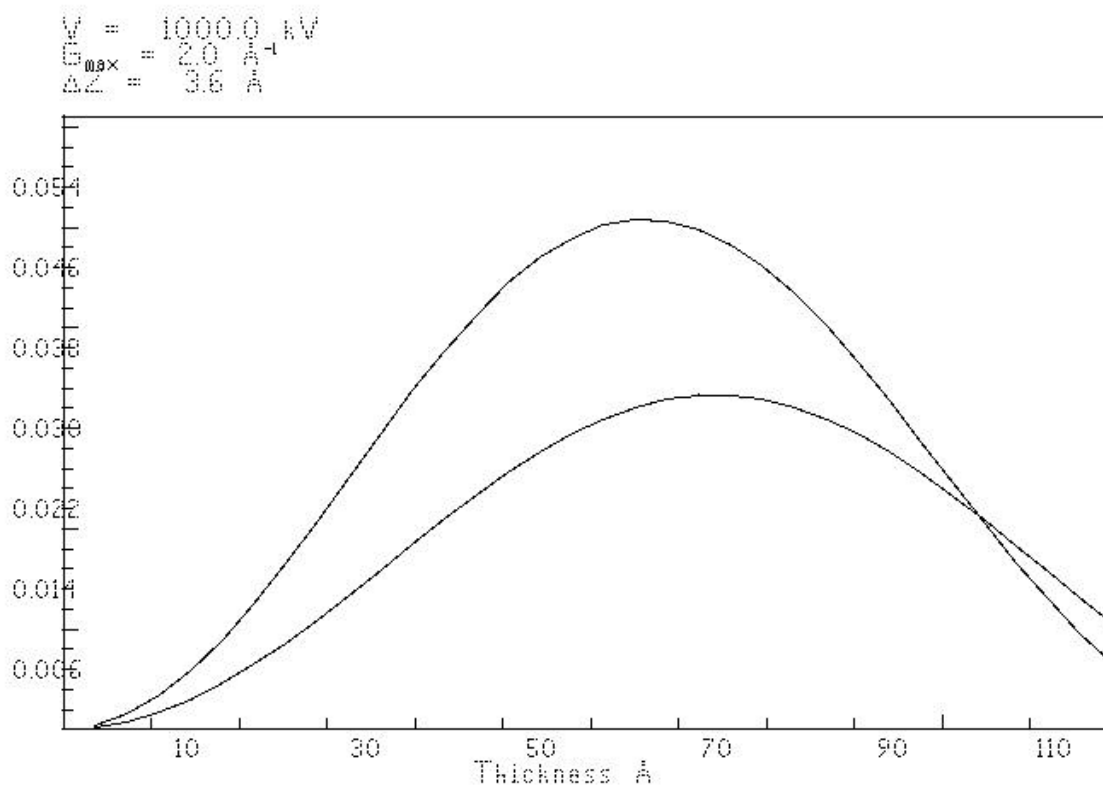
RETURN: Return to previous ATOM-LIST menu.

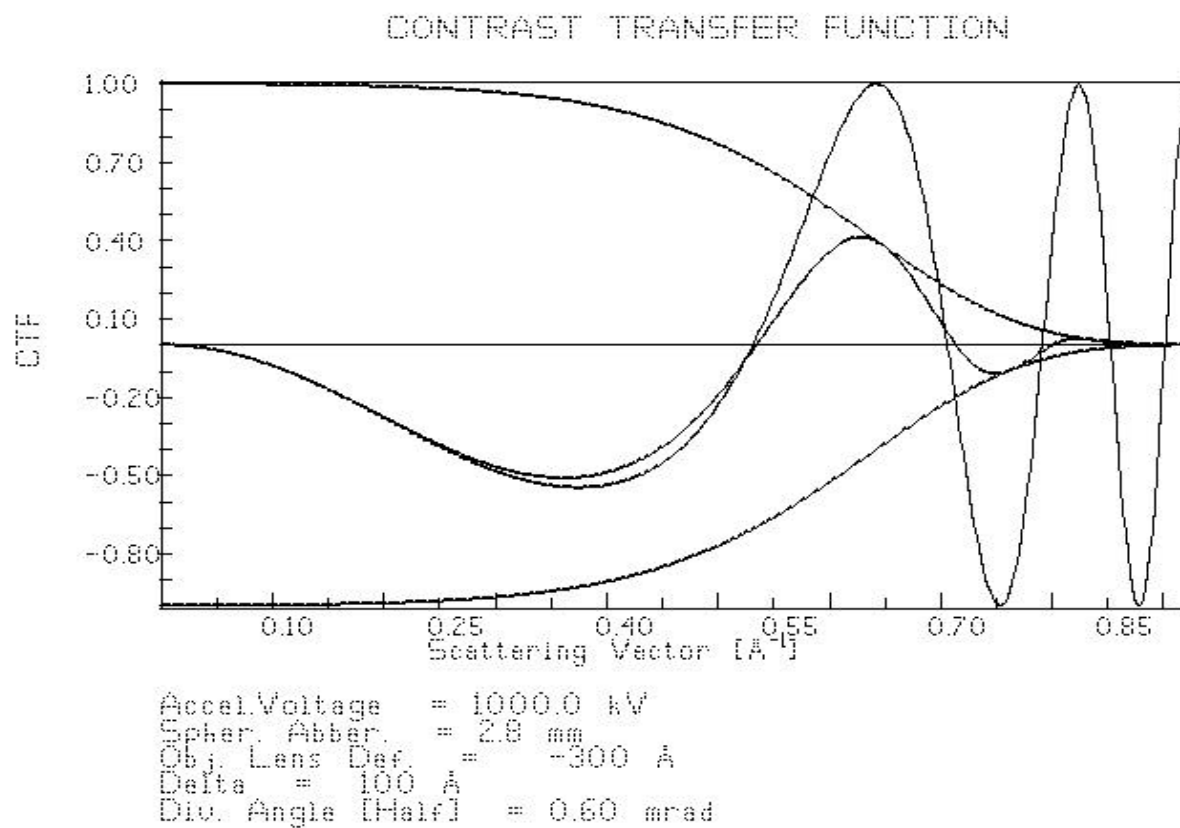
The AMPLIT Menu



3.10 The AMPLIT menu

On activating the AMPLIT control box on the MAIN menu, the user will be presented with a list of the diffracted beams for which the complex amplitudes are currently stored as a function of specimen thickness. NCEMSS will ask the user to select which beams to plot, whether to superimpose the plots, and whether to include phase plots. The plots will be drawn with thickness horizontal and marked in Angstrom units. The various curves can be marked with the appropriate beam indices by using the TEXT option of the SET-UP menu (page 38).

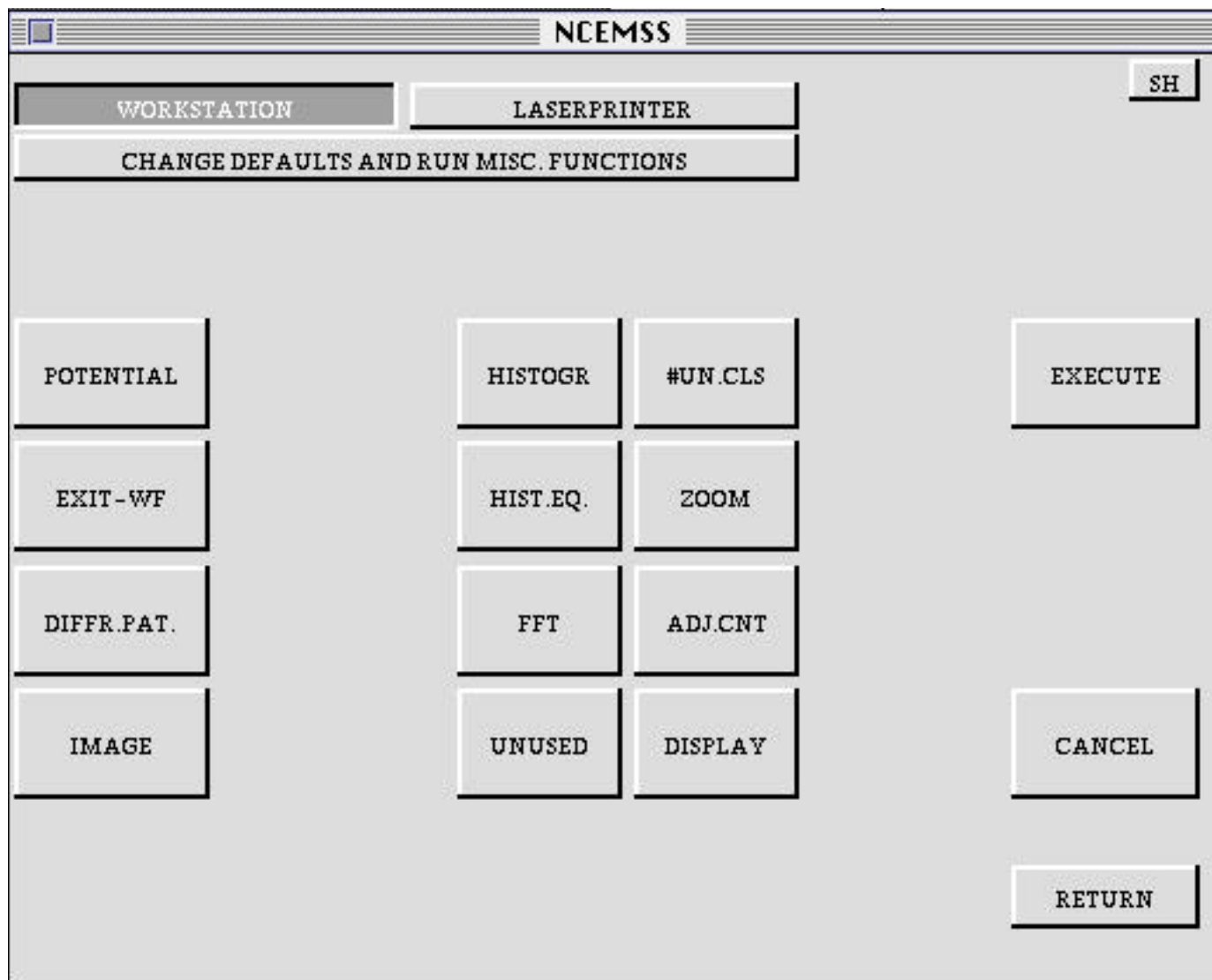




3.11 The CTF plot

The result of activating the CTF control button on the MAIN menu is a plot of the linear-image Contrast Transfer Function. This function is first plotted as the undamped sine part of the complex phase change due to the objective lens spherical aberration and defocus. The damping curves due to the effects of spatial and temporal coherence (incident beam convergence and spread of defocus) are plotted next, then finally the result of imposing the damping on the sine curve. Remember that this curve is only useful for estimating the linear contribution to the image of the diffracted beams exiting a thin crystal (one in which they have suffered only essentially kinematic scattering).

The IMAGE-DISPLAY Menu



3.12 The IMAGE-DISPLAY menu

When DISPLAY is selected in the MAIN or CONTROL menu (page 16), NCEMSS brings up the IMAGE-DISPLAY menu. This menu consists of 21 control buttons. The top three are used to select various options that remain until reset. The left-hand column is used to select the function to be displayed. Other control boxes select the actions to be taken.

WORKSTATION/LASERPRINTER: These two boxes are mutually exclusive and are used to select the output device for the image display.

CHANGE DEFAULTS AND RUN MISC. FUNCTIONS: This control is used to bring up the SET-UP menu (page 40) where various imaging options and defaults may be set.

POTENTIAL: Selecting this input produces a display of the unit cell potential projected in the incident electron beam direction.

EXIT-WF: The electron wavefield at the crystal exit surface may be displayed by selecting this input function.

DIFFR.PAT.: Selects the diffraction pattern for display.

IMAGE: Selects the current image for display.

HISTOGR: Produces a histogram of the intensity values in the function selected from column one.

HIST.EQ.: Stretches the image contrast by performing a histogram equalization operation before display.

ADJ.CNT: Brings up the SET-CONTRAST menu (page 44) for selection of contrast parameters before display.

FFT: Performs a fast Fourier transform on the selected function and squares the result before display. (Performed on the image, FFT produces the image power spectrum or “optical diffractogram”).

#UN.CLS: Enables input of the number of unit cells desired in the displayed image.

ZOOM: Asks for a factor to use in magnification the image.

DISPLAY: Directs the output to the display device.

EXECUTE: Takes the selected function, applies the selected operations, and outputs the picture.

CANCEL: Cancels the selected options, usually because one was selected by mistake.

The SET-UP Menu

NCEMSS			
SET ERASE	SET NOERASE	ERASE THE DISPLAY	
SET NOMONTAGE	SET MONTAGE	WRITE TEXT ON THE DISPLAY	
SET NOREQ POS	SET REQ POS	STORE PARTS OF THE DISPLAY	
NOMONT-SPACE	MONTAGE-SPACE	DISPLAY STORED IMAGE	
INT.AUTO-SCALE	INT.ABS-SCALE	PRINT A STORED IMAGE	
CTF-AUTOSCALE	CTF-ABS.SCALE	PRINT THE SCREEN	
PG-REC SP	PG-REAL SP	LIST STORED IMAGE-FILES	
APERTURE	NO APERTURE	SET CONTRAST FOR LASERWRITER	
TITLES	NO TITLES	SET DIV.ANGLE FOR DP	
2D-POT.SLICE	3D-POT.SLICE	IMAGE ONLY	OVERLAY ATOMS
SET MIN. INTENSITY (LENS)		AUTOSCALE	FIXED
SET MIN.INT.TO DISPLAY(FFT)		DISPLAY	PRINT
SET CAMERA LENGTH		REL.PHASE	PHASE
INDEX DIFFR.PT.		ASCII FILE	BINARY FILE
CHANGE CENTER OF DIFFR.PT.		OUT->PRINTER	OUT->FILE
READ THE CURSOR POSITION		NORM. MONT.	CUSTOM
RETURN			

3.13 The SET-UP menu

Opting to change the various defaults by selecting the CHANGE box in the IMAGE-DISPLAY menu (page 38), brings up the SET-UP menu. This menu is used to change the default settings of some “hard” parameters, and to manipulate the image display. The nine two-way switches on the left of the menu are normally set to default to the left-hand setting.

SET ERASE<>NOERASE: When ERASE is set, the display screen will be erased before each new image is displayed (except see MONTAGE).

SET NOMONTAGE<>MONTAGE: When NOMONTAGE is set, only one image will be displayed for each activation of the EXECUTE command from the IMAGE-DISPLAY menu (page 38). When MONTAGE is set, then a full through-thickness and/or through-focus series of images will be displayed at one EXECUTE command (assuming the calculation was carried out for such a series by setting the appropriate parameter values in the PARAMETER menu (page 16)). Note that a MONTAGE will erase the screen before display, regardless of the ERASE setting.

SET NOREQ-POS<>REQ-POS: When NOREQ_POS is set, individual images will be written to the center of the display screen (assuming that NOMONTAGE is set). When REQ_POS is set, the user will be prompted for the coordinates at which the image is to be displayed.

NOMONT-SPACE<>MONTAGE-SPACE: is used to set the desired spacing between the montaged images.

INT.AUTO-SCALE<>INT.ABS-SCALE: To see the most detail in any image, set INT.AUTO-SCALE to display the image with its minimum set to black and its maximum to white. To intercompare images, it is better to use INT.ABS-SCALE to choose the same absolute scale for all the images.

CTF-AUTOSCALE<>CTF-ABS.SCALE: Can be used to scale a CTF plot (page 36) by fixing the maximum g value considered. In AUTOSCALE mode the CTF is drawn to where it approaches zero.

PG-REC SP<>PG-REAL SP: determines whether or not the calculation is done in reciprocal space or in real space. This switch should be set to reciprocal space since the real space calculation is not debugged yet.

APERTURE<>NO-APERTURE: determines whether or not the current objective aperture radius is drawn on a displayed diffraction pattern.

TITLES<>NO TITLES: determines whether titles are written under each displayed image. Notice that MONTAGE will suppress titles, but a title for the montaged series may be added using WRITE TEXT.

2D-POT.SLICE<>3D-POT.SLICE: When the number of slices per unit cell exceeds one in the MAIN menu (page 16), NCEMSS will sub-slice the unit cell in one of two ways. When 2D-POT is set, the total potential within the cell will be projected, and a portion assigned to each sub-slice. A more-accurate method is to approximate the upper-layer zones by sub-slicing a three-dimensional potential into the required number of sub-slices. In this way the variation of the specimen structure in the electron beam direction is included in the simulation. Of course, it takes longer in 3-D).

SET MIN. INTENSITY (LENS): sets the minimum diffracted beam intensity that will be considered to pass through the objective lens; this minimum can be set to exclude very low intensity beams from large defect unit cells, and so speed up the image calculation.

SET MIN.INT.TO DISPLAY(FFT): determines down to what intensity diffracted beams will be drawn in a diffraction pattern display.

he SET-UP Menu

NCEMSS			
SET ERASE	SET NOERASE	ERASE THE DISPLAY	
SET NOMONTAGE	SET MONTAGE	WRITE TEXT ON THE DISPLAY	
SET NOREQ POS	SET REQ POS	STORE PARTS OF THE DISPLAY	
NOMONT-SPACE	MONTAGE-SPACE	DISPLAY STORED IMAGE	
INT.AUTO-SCALE	INT.ABS-SCALE	PRINT A STORED IMAGE	
CTF-AUTOSCALE	CTF-ABS.SCALE	PRINT THE SCREEN	
PG-REC SP	PG-REAL SP	LIST STORED IMAGE-FILES	
APERTURE	NO APERTURE	SET CONTRAST FOR LASERWRITER	
TITLES	NO TITLES	SET DIV.ANGLE FOR DP	
2D-POT.SLICE	3D-POT.SLICE	IMAGE ONLY	OVERLAY ATOMS
SET MIN.INTENSITY (LENS)		AUTOSCALE	FIXED
SET MIN.INT.TO DISPLAY (FFT)		DISPLAY	PRINT
SET CAMERA LENGTH		REL.PHASE	PHASE
INDEX DIFFR.PT.		ASCII FILE	BINARY FILE
CHANGE CENTER OF DIFFR.PT.		OUT->PRINTER	OUT->FILE
READ THE CURSOR POSITION		NORM. MONT.	CUSTOM
RETURN			

SET CAMERA LENGTH: is used to adjust the magnification of the diffraction pattern display. The value is input in mm., and has a default setting of 520mm.

INDEX DIFFR.PT.: is used to index a diffraction pattern. On moving the cursor to the selected diffraction spot and clicking the mouse, the indices are written next to the spot.

CHANGE CENTER OF DIFFR.PT.: The center of the displayed diffraction pattern can be changed by selecting this command and using the mouse to click on the desired position in the image display window.

READ THE CURSOR POSITION: reads the cursor position within an image.

ERASE THE DISPLAY: does just that.

WRITE TEXT ON THE DISPLAY: is used to write text at the cursor position.

STORE PARTS OF THE DISPLAY: after selecting this command, mark the corners of an area of the display window (image) to be stored and the image will be saved in a file. The user is prompted for a name and the program will automatically add the extension .at

DISPLAY STORED IMAGE: use this command to displayed a stored image of the type <name>.at created by the previous command.

PRINT STORED IMAGE FILE: sends the content of the file <name>.at to a connected laserprinter. The program creates a file "laserprinter.ps" and uses the command "lpr laserprinter.ps" to send the file to the printer. It is up to the user to set up the appropriate redirection of the output to a valid printer.

PRINT THE SCREEN: sends the content of the image window to a connected laserprinter. It otherwise works identical to the command above.

LIST STORED IMAGE-FILES: sends the command "ls *.im" to the operating system. The output list of stored image files is displayed in the terminal session window.

SET CONTRAST FOR LASERWRITER: allows the user to change the values of brightness (normally 0.5) and contrast (normally 1.0) of the printed image

SET DIV.ANGLE FOR DP: use this to change the size of the displayed diffraction spots in case the size is not optimal for viewing.

IMAGE ONLY<>OVERLAY ATOMS: controls whether atom positions are overlaid on the image or not.

AUTOSCALE-FIXED: use this to either let the computer choose black and white levels automatically or to use fixed values input by the user.

DISPLAY<>PRINT: in the display position, anything "DISPLAYED" goes to the image window. In the PRINT position, the actual numeric data is sent to a file in a format that depends on the setting of the switch ascii/binary below.

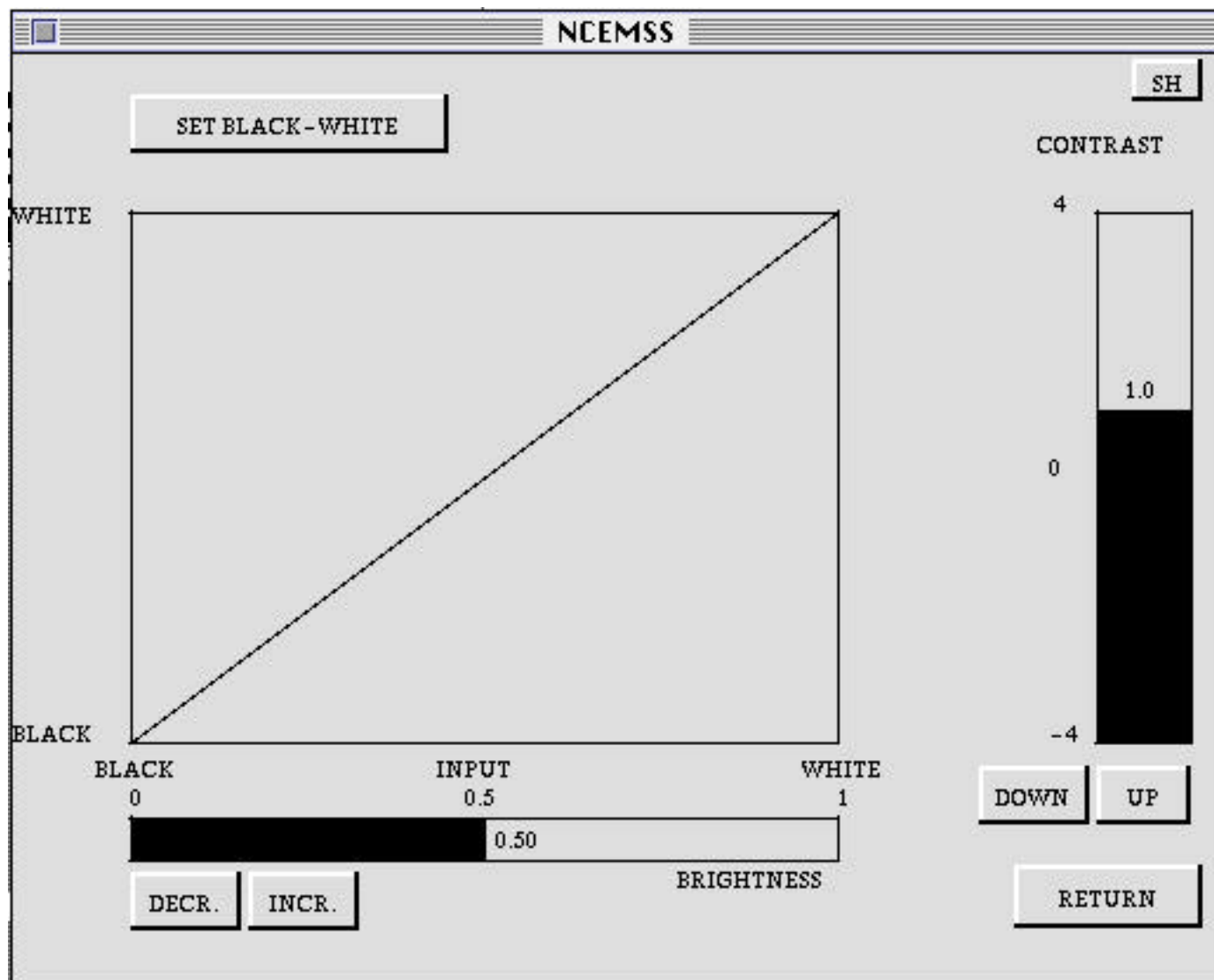
REL PHASE <> PHASE: determines if the phases reported for diffracted beams include the phasechange due to the mean inner potential of the crystal

ASCII FILE<>BINARY FILE: determines if the numeric output data for an image, projected potential or complex wavefunction is in ascii or binary.

OUT->PRINTER<>OUT->FILE: normally when you reroute the output to the printer, the program executes the command "lpr laserprinter.ps". Selecting OUT->FILE will create a named postscript file that can be saved and printed at any time later.

NORM.MONT<>CUSTOM: allows extra control on the layout of montaged images.

The Set Contrast Menu



3.14 The SET-CONTRAST menu

When the ADJ.CNT box of the IMAGE-DISPLAY menu (page 38) is activated, it brings up the SET-CONTRAST menu. This menu displays the current contrast and brightness settings graphically. The straight line shows the mapping of the image intensity values (horizontal axis) into the displayed output intensity values (vertical axis). For a one-to-one mapping, the values of contrast (vertical bar-graph) and brightness (horizontal bar-graph) should be 1.0 and 0.5 respectively.

To increase (or decrease) the contrast used to display the image, tap the mouse with the cursor positioned over the UP (or DOWN) boxes underneath the vertical bar-graph. The contrast-transfer graph will pivot about its mid-point as the contrast is changed, providing a plot of how input grey levels are mapped into output greyscale levels. Note that a contrast value of less than zero will produce a negative image.

To increase (or decrease) the image brightness, use the INCR. and DECR. boxes to move the mid-point of the contrast-transfer graph to the left or right.

The contrast-transfer curve may be set directly, by activating the SET BLACK-WHITE box, then clicking the mouse after positioning the cursor at one end-point of the desired line, then clicking at the other endpoint. These end-points need not be exactly on the lines forming the box enclosing the contrast-transfer graph.

NCEMSS

***** Construct Phase-grating sequence *****

SH

LAYER#	NAME	DZ(A)	LAYER#	NAME	DZ(A)
1	lay1	4.00			
2	lay2	4.00			

DEF LAY

DEL LAY

DEPOSIT

INSERT

REPEAT

TOP - 0.00 A

4.00

8.00

12.00

16.00

20.00

24.00

28.00

32.00

36.00

40.00

BOTTOM - 40.00 A

RESET

REMOVE

PHASE-GRATING SEQUENCE :
1 2 1 2 1 2 1 2 1 2

lay1

lay2

RETURN

3.15 The SET-LAYERS menu

If the LAYERED STRUCTURE option is selected from the SINGLE/LAYERED menu (page 12), then the SET-LAYERS menu appears. This menu can be used to “construct” a specimen consisting of multiple layers of different single structures.

DEF LAY: To include a structure in the phase-grating sequence that will comprise the final layered structure, use the DEF LAY box and enter the name of the structure as it appears in the FILE-LIST menu (p.14). Up to six different structures may be used to make up the layered structure. Note that a PHSGRT calculation (p.21) must be carried out for any structure before it can be included in a layered calculation. Also note that, as well as existing, all the phase-gratings used to build a layered structure must be the same shape and size; i.e. each phase-grating must have the same values for the projected (two-dimensional) cell axes and cell angle, and also be computed out to the same scattering parameter, GMAX.

DEL LAY: This box is used to remove a previously-defined layer name from consideration.

DEPOSIT: The layered structure can be built up by depositing layers of any member structure that was defined earlier using DEF LAY. Each deposition is made by clicking on the DEPOSIT box, then on the appropriate LAYER symbol, then entering the layer thickness desired. The final structure is built from the top down; i.e. each subsequent layer is deposited onto the bottom of any existing sequence. A graphical representation of the structure appears on the left of the menu, and the phase-grating sequence is also listed.

INSERT: In addition to depositing a specified thickness of a chosen layer, it is possible to insert a specified thickness at any chosen thickness of the final structure. Clicking on this button, followed by the appropriate LAYER symbol, causes NCEMSS to ask for a layer thickness to be inserted, and the structure thickness at which to insert it.

REPEAT: This button is used to repeat a defined sequence a chosen number of times in order to build up a periodic layer structure.

RESET: This button zeros everything in preparation for another try.

REMOVE: The phase-grating sequence can be operated on directly to remove single slices, one at a time, by activating this button and clicking on the offending phase-grating in the sequence.

Appendix A Multislice Size, PhaseGrating Size, and Maximum G

The “size” of a multislice calculation is defined conveniently by the size of the largest array (the $Q(k)$ or $q(x)$ array). For an array size of $2n \times 2m$, the multislice is said to be a “parameter $n+m$ ” multislice; thus a parameter-16 multislice will have a $Q(k)$ array size of 256×256 , (or 512×128 , or 1024×64 , or 2048×32 , or 4096×16 , depending upon the shape of the unit cell used in the computation). This size parameter must apply to all multislice programs, regardless of which of the three current algorithms (reciprocal-space, Fourier-transform, or real-space) is employed by the program.

A.1 Reciprocal-space multislice

As introduced by Goodman and Moodie (1974), the basic recursive form of the multislice description of dynamical diffraction can be written as

$$\psi_{n+1}(\mathbf{k}) = [\psi_n(\mathbf{k}) \cdot P_{n+1}(\mathbf{k})] * Q_{n+1}(\mathbf{k}) \quad (A1)$$

That is, $\psi_{n+1}(\mathbf{k})$, the wave function (given in reciprocal space) at the exit surface of the $(n+1)$ th slice, is obtained by multiplying the wave function at the exit surface of the n th slice by $P_{n+1}(\mathbf{k})$, the propagator for the $(n+1)$ th slice, followed by the convolution of this result by $Q_{n+1}(\mathbf{k})$, the phase-grating function (given in reciprocal space) for the $(n+1)$ th slice.

In multislice computer programs that use the above reciprocal-space formulation, the three functions, $\psi(\mathbf{k})$, $P(\mathbf{k})$, and $Q(\mathbf{k})$ are represented by two-dimensional arrays containing terms with indices that can be regarded as those of the diffracted beams within the diffracting specimen. In order to impose no extra symmetry on the computation, a “circular aperture” is usually placed on the terms in the arrays, so that terms beyond a certain distance in reciprocal space are set to zero. Note that the $Q(\mathbf{k})$ array must extend out to twice as far in reciprocal space as the $\psi(\mathbf{k})$ and $P(\mathbf{k})$ arrays in order to correctly include all physical scatterings to each diffracted beam. Figure A1 shows how this doubled phase-grating requirement arises because $Q(\mathbf{k})$ is a “probability map” of terms that determine how much of each diffracted beam is to be scattered through the angle corresponding to the term. Thus, in order to compute the scattering of diffracted beams out to $k = \pm(h,k)$, the $\psi(\mathbf{k})$ and $P(\mathbf{k})$ must be $(2h+1) \times (2k+1)$ in size, and $Q(\mathbf{k})$ must be $(4h+1) \times (4k+1)$. For example, the SHRLI80 programs used a 128×128 array for $Q(\mathbf{k})$, making SHRLI80 a parameter-14 multislice and giving a maximum (h,k) value of $(31,31)$; this limits the number of diffracted beams to less than 4096, adequate for most perfect-crystal computations, but too small for simulation of many defect structures (O’Keefe et al, 1978).

A.2 Fourier-transform Multislice

For larger arrays (and thus larger numbers of diffracted beams), it is faster to compute the multislice by recasting (A1) into a form where the convolution is replaced by two Fourier transforms and a multiply operation, as was done by early users of multislice in the Melbourne group. Then

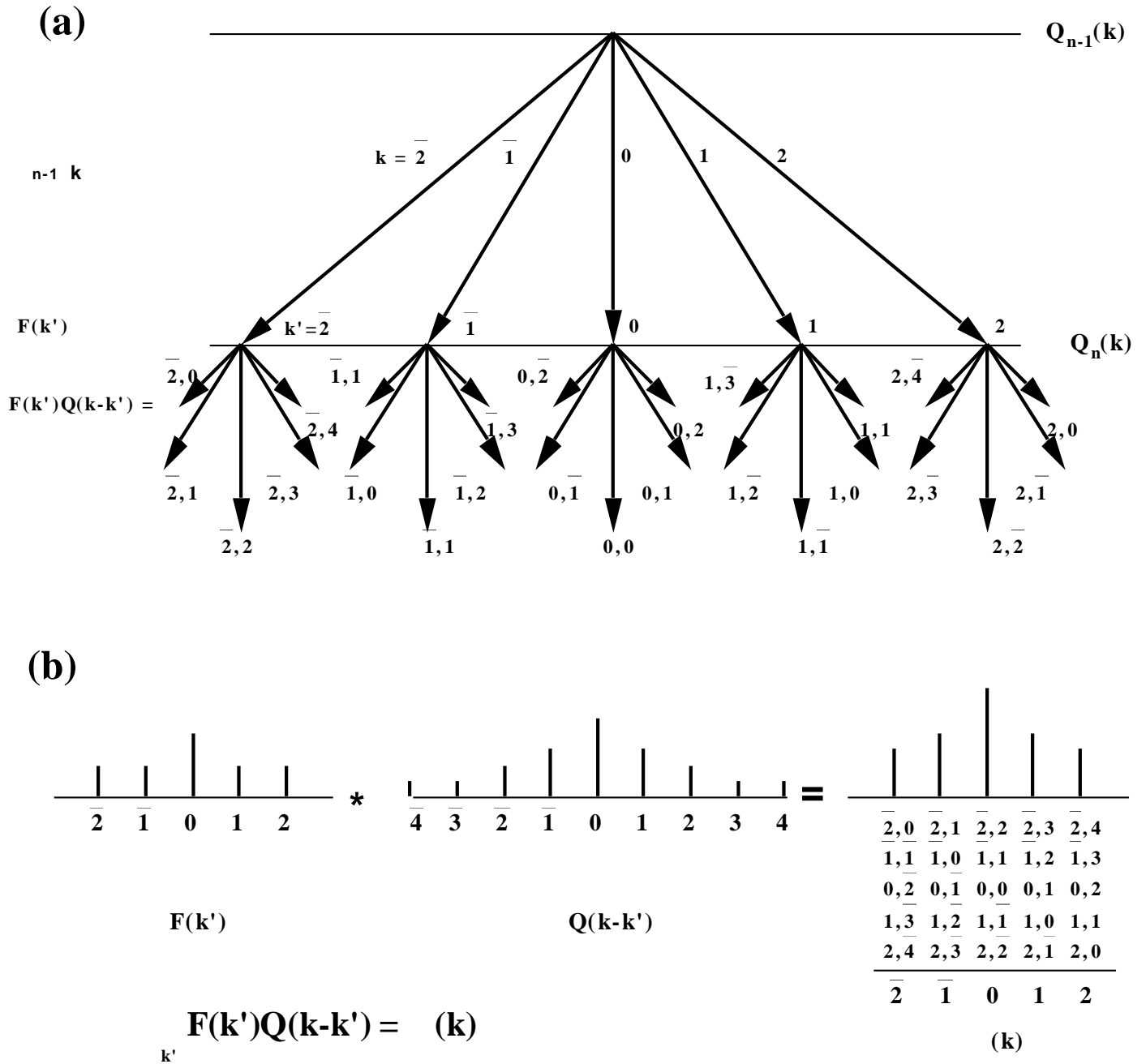


Fig. A1. Convolution description of multiple scattering. In order to include all scattering contributions to the dynamic electron wavefield (k) , the phase-grating coefficients $Q(k)$ must extend out twice as far in reciprocal space as do the coefficients of the wavefield. For the five depicted diffracted beams (k) , (where $|k| = -2, -1, 0, 1, 2$), the convolution requires nine phase-grating coefficients $Q(k)$, (where $|k| = -4$ to 4).

(a) sketch of the contributions to the five diffracted beam directions; note that (e.g.) the contribution of the incoming (2) beam to the outgoing (-2) beam requires the presence of the $Q(-4)$ phase-grating coefficient.

(b) Delta-function representation of the scattering process, showing each $F(k') \cdot Q(k-k')$ term contributing to the outgoing (k) , $|k| = -2$ to 2 . Here the incoming function $F(k)$ is equal to the product $(k) \cdot P(k)$ in equation (A1). Note the presence of the $Q(\pm 3)$ and $Q(\pm 4)$ coefficients in the table of interactions; except for (0) , every outgoing (k) contains a contribution from these outer coefficients, and would be in error without them.

$$q_{n+1}(\mathbf{k}) = F [F^{-1} [n(\mathbf{k}) \cdot P_{n+1}(\mathbf{k})] \cdot q_{n+1}(\mathbf{x})] \quad (\text{A2})$$

Here the F represents the Fourier transform operation, and $q(\mathbf{x})$ is the real-space form of $Q(\mathbf{k})$, i.e. the (inverse) Fourier transform of $Q(\mathbf{k})$. Experience with the SHRLI programs has produced the not-surprising result that, in order to obtain the same results with (A2) as with (A1), $q(\mathbf{x})$ must be formed from a $Q(\mathbf{k})$ that extends twice as far in reciprocal space as do $n(\mathbf{k})$ and $P(\mathbf{k})$.

Note that, as well as correctly describing the physics of the scattering process by ensuring that all contributions from all the diffracted beams leaving the previous slice to each diffracted beam from the current slice are included, the doubled phase-grating also neatly eliminates the possibility of any “aliasing” arising from the necessary sampling of the real-space functions. Unfortunately, in their description of the FFT multislice, Ishizuka and Uyeda (1977) stated that the number of diffracted beams must be no less than the number of phase-grating coefficients; under their condition, the effects of aliasing will produce incorrect scattering results if array sizes are not made large enough to produce essentially zero electron amplitude over the outer five-ninths of the phase-grating and wave-amplitude arrays. This confusion appears to have arisen when the concept of FFT multislice was introduced to the Kyoto group by a visiting researcher familiar with its use in the Physics Department of Melbourne University. At Melbourne, it had been found that aliasing occurred when the convolution step of the reciprocal-space multislice (equation A1) was replaced by a forward/inverse Fourier transform sequence. This aliasing boosted the amplitudes of the outer beams in the calculation until “knock off” parameters were introduced to set the outer beam amplitudes to zero after each slice. However, even after this procedure eliminated the aliasing effect, results from the FFT multislice did not exactly match ones from the “standard” reciprocal-space formulation (O’Keefe, 1972). For this reason, the SHRLI80 programs (O’Keefe et al, 1978) continued to use the (slower) reciprocal-space form of the multislice. Experiments with various scattering algorithms (Self et al, 1983) led to the testing of different ways of avoiding aliasing in FFT multislice. It was realized that one such method was by choosing a $q(\mathbf{x})$ formed from $Q(\mathbf{k})$ terms that extended only 2/3 of the way to the array edges, provided that only the same number of diffracted beams was used in $Y(\mathbf{k})$, with the outer 5/9 of the diffracted beam array reset to zero after every slice. A better method was to ensure that $q(\mathbf{x})$ was formed from a $Q(\mathbf{k})$ that extended out to twice the scattering angle as $n(\mathbf{k})$, and to reset the outer 3/4 diffracted beams to zero after each slice. This latter method conforms to the physics of the scattering process (fig.A1), and proved to yield the same results as the reciprocal-space multislice. A multislice program using this method was incorporated into the SHRLI81 suite, and this method is used in the NCEMSS multislice program (O’Keefe and Kilaas, 1988).

A.3 Real-space multislice

A third method of computing the multislice is to carry out the calculation completely in real space; this is an alternative to computing in reciprocal-space (as in equation A1), or in both real and reciprocal-space (as in equation A2). Fourier transformation of (A1) gives

$$y_{n+1}(x) = [y_n(x) * p_{n+1}(x)] \cdot q_{n+1}(x) \quad (A3)$$

In this formulation the real-space wave function $y_n(x)$ is convolved by a real-space propagator $p_{n+1}(x)$ and the result multiplied by the real-space phase-grating. Van Dyck (1983) has developed this method and shown that the convolution step need not be carried out with the full $2^n \times 2^m$ $p(x)$ array, but only with a such smaller array (since $p(x)$ is sharply peaked in the forward direction for high energy scattering). Since the modified $p(x)$ array is so much smaller, the computation time should take less time than either of the reciprocal-space multislice (A1) or the FFT multislice (A2); however, tests (e.g. Kilaas and Gronsky, 1983) have shown that the original formulation of the method required more beams and smaller slices to achieve the same precision as either the reciprocal-space multislice or the FFT multislice, resulting in a longer time to produce the wavefield at the same total specimen thickness. Van Dyck and Coene (1984) have since proposed a modified implementation of the real-space multislice into a workable algorithm, with results that approach those produced by the multislice formulations of equations A1 and A2 (Coene and Van Dyck, 1984). Since the $p(x)$ array is much smaller, procedure (A3) does produce some saving in memory over the other multislice formulations.

A.4 Storage requirements

All three formulations of the multislice procedure require the computer (or array processor) to store three different complex arrays corresponding to the phasegrating function in real or reciprocal space ($q(x)$ or $Q(k)$), the electron wavefield in real or reciprocal space ($y(x)$ or $Y(k)$), and the propagator function in real or reciprocal space ($p(x)$ or $P(k)$).

With a reciprocal-space phasegrating $Q(k)$, of $2^n \times 2^m$ terms, a parameter-($n+m$) reciprocal-space multislice (equation A1), requires a reciprocal-space wavefield array (or set of diffracted beams), $Y(k)$, of $2^{n-1} \times 2^{m-1}$ terms, and a reciprocal-space propagator array $P(k)$, of $2^{n-1} \times 2^{m-1}$ terms.

An equivalent parameter-($n+m$) FFT multislice (equation A2) requires a real-space phase-grating array $q(x)$, of $2^n \times 2^m$ terms, an electron wavefield array $y(x)$, of $2^n \times 2^m$ terms, and a reciprocal-space propagator array $P(k)$, of $2^{n-1} \times 2^{m-1}$ terms.

For a real-space parameter-($n+m$) multislice (equation A3), both the $y(x)$ and $q(x)$ arrays need to hold $2^n \times 2^m$ terms, whereas $p(x)$ may be as small as thirteen (Kilaas & Gronsky, 1983), giving a total requirement of slightly over $2 \times 2^{n+m}$ terms. In implementing the real-space multislice it is important that the $2^n \times 2^m$ $q(x)$ array should be formed from a full $2^n \times 2^m$ $Q(k)$ terms, whereas the $2^n \times 2^m$ $y(x)$ array should be formed from only $2^{n-1} \times 2^{m-1}$ $Y(k)$ terms in order to include correctly all the physical scattering contributions to each diffracted beam and to avoid aliasing problems (fig A1).

Any (correctly implemented) multislice of size $2^n \times 2^m$ (parameter $n+m$) thus includes the effects of only $2^{n-1} \times 2^{m-1}$ diffracted beams. This is true for all three formulations of the multislice: the reciprocal-space method (equation A1), the FFT method (equation A2), and the real-space multislice (equation A3).

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Appendix BHOLZ interactions

With suitable algorithms, it is possible to include in the diffraction calculation the effects of out-of-zone scatterings, or non-zero (or higher-order) Laue zone (HOLZ) interactions. Basically, there are four ways to produce the set of phasegratings (or projected potentials) that describe the “multisliced” crystal. For structures with short repeat distances in the beam direction, the simplest method is to use one slice per unit cell. For structures with large repeats in the beam direction, several methods may be used, three of which rely on sub-dividing the slice into “sub-slices”. Any of the four methods can be used in NCEMSS.

B.1 Identical slices with only one sub-slice per unit cell repeat distance

A multislice computation in which every slice is identical contains no information about the variation in structure along the incident beam direction, and includes scattering interactions with only the zero-order Laue zone (ZOLZ) layers. For structures with short repeat distances in the beam direction such a computation is adequate, since the Ewald sphere will not approach the (relatively distant) high-order zones.

B.2 Identical sub-slices with n sub-slices per unit cell repeat distance

For structures with large repeats in the beam direction, a method of sub-dividing the slice is required in order to compute the electron scattering with sufficient accuracy. The simplest, but most approximate method, is to compute the projected potential for the full repeat period then use $1/n$ of the projected potential to form a phase-grating function that can be applied n times to complete the slice. This method avoids interaction with any “pseudo-upper-layer-line” (Goodman and Moodie, 1974), but ignores real HOLZ layers.

B.3 Sub-slices based on atom positions

An improvement on sub-dividing the projected potential is to sub-divide the unit cell atom positions. In this procedure the list of atom positions within the unit cell is divided into n groups depending upon the atom position in the incident beam direction. From these sub-sliced groups, different projected potentials are produced to form n different phase-gratings, which are applied successively to produce the scattering from the full slice.

B.4 Sub-slices based on the three-dimensional potential

A further improvement on sub-dividing the atom positions, is to sub-divide the three-dimensional potential of the full slice, since an atom with a position within one sub-slice can have a potential field that extends into the next sub-slice. Rather than compute a full three-dimensional potential and then integrate over appropriate sub-slic-

es (a 128x128x128 potential would require over two million samples to be stored), it is possible to derive an analytical expression for the potential within the sub-slice $z_0 \pm Dz$ projected onto the plane at z_0 (Self et al., 1983). It is possible to apply this method routinely to structures with large repeats in the beam direction, thus generating several different phase-gratings for successive application, and even to structures (perhaps with defects) that are aperiodic in the beam direction and require a large number of individual non-repeating phase-gratings (Kilaas et al., 1987).

B.5 NCEMSS sub-slicing

While ensuring that the calculation remains sufficiently accurate, NCEMSS will normally choose the simplest (and quickest) method of specifying how slices are defined for any particular combination of specimen, zone axis, accelerating voltage, and maximum g . To this end, the user can choose to neglect HOLZ interactions if these are judged to be unimportant. If HOLZ interactions are important, then the user should select the “3D-POT.SLICE” box in the SET-UP menu (p 41), rather than the “2D-POT.SLICE” box.

When a two-dimensional calculation is selected, NCEMSS will use one slice per cell if the cell repeat distance in the beam direction is small (B.1). If the repeat distance is too large for one slice per unit cell, NCEMSS will avoid pseudo-upper-layer-lines by producing n identical sub-slices (B.2).

When a three-dimensional calculation is selected, (3D-POT.SLICE activated), NCEMSS uses a sub-divided three-dimensional potential (B.4) when the repeat distance is large, and defaults to one slice per cell if the distance is small enough. Note that the number of sub-slices per unit cell can be forced to be greater than one by setting it explicitly in the MAIN menu (p 16); this will ensure that any HOLZ interactions are included even for small repeat distances. Of course, if the repeat distance is very small, leading to a distant HOLZ in reciprocal space, both the calculation and the experiment it is modeling will interact only very weakly with the HOLZ reflections.

Use of the LAYERED STRUCTURE option (p 12) to produce the scattering from a structure that is layered or aperiodic in the incident beam direction is effectively an application of the method of sub-slicing based on atom positions (B.3). Thus the user could create a number of sub-slices by assigning selected atoms to different structure files, then forming a phasegrating for each sub-slice, and using the SET-LAYERS menu (p 46) to specify how the sub-slices are to be used to describe the specimen structure. Normally, of course, the use of the B.4 option is to be preferred, as it produces a superior result, and is far easier to use.

B.6 Other methods

Van Dyck has proposed other methods to include the effects of HOLZ layers, including the second-order multislice with potential eccentricity (Van Dyck, 1980) and the improved phase-grating method (Van Dyck, 1983). Tests of these procedures show that the extra computation involved in using potential eccentricity may be worthwhile, but that the improved phase-grating method diverges too easily to be useful.

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