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INTERACTIVE SOFTWARE FOR SIMULATION OF HIGH RESOLUTION TEM IMAGES

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INTERACTIVE SOFTWARE FOR SIMULATION OF HIGH RESOLUTION TEM IMAGES

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INTERACTIVE SOFTWARE FOR SIMULATION OF HIGH RESOLUTION TEM IMAGES

Roar Kilaas

A new highly interactive and user friendly software package for simulation and processing of high resolution transmission electron micrographs has been developed at the National Center for Electron Microscopy (NCEM) at the Lawrence Berkeley Laboratory. Designed to be used by scientific visitors to the Center, the software is completely menu driven from a graphics terminal with a mouse and requires little to no computer knowledge for proper usage. Although the software is written to ensure maximum performance using hardware available at the NCEM, hardware dependent code is kept in separate modules that are easily modified. The new software package combines an unparalleled ease of use with the latest theory in the field of simulation of high resolution transmission electron micrographs.

Introduction

There has been a tremendous improvement in computer hardware in the recent years. Only a few years ago, image simulations of high resolution electron micrographs were mostly done on large mainframes and often overnight. Images were printed out the next day in the form of overprinted characters on

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The author would like to thank Dr. M.A. O'Keefe for assistance in planning screen outlays, suggesting useful options and ways to make the programs run more efficiently. Dr. O'Keefe's own SHRLI programs provided at all times useful checks as to the accuracy of CEMPAS. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

computer paper. Today it is possible to purchase a micro/mini-computer such as a MicroVax or a Sun, connect it to a small array processor and a framestore and compute images faster than it is possible on a computer costing millions of dollars and all at a cost of less than $100K. Interactive software is gaining popularity at the expense of software written to run in batch mode. With almost instantaneous results available in most cases, the user often requires the ability to immediately change input and output parameters. This is the case at the NCEM at Berkeley where a new dedicated facility for computer processing and simulation of electron micrographs has been a major project for the last two years. Hand in hand with acquisition of hardware there has also been a major effort in software development. Experience with previous software had shown that there are many factors beyond the ability to solve certain equations that determine the usefulness of a set of programs. Some of the more important factors are listed below:

i) The user interface. Apart from the ability to produce correct results this is possibly the most important feature of any type of software and likely to be overlooked, particularly in the scientific community. It determines how accessible programs are to others than the author and how quickly new problems can be tackled. There are numerous examples of powerful software packages that are never used to their potential because of the time it takes the user to become familiar with commands and options. It is also essential that some form of help is available other than through manuals.

ii) Flexibility. Beyond memory and speed considerations there should be no limit on the size and shape of the calculation that could be performed. Most existing software is built around fixed array dimensions which very often are of a wrong size and shape for many image calculations. Calculations of defects especially, require array sizes that can be varied independently in the two image dimensions and that can be made large enough to minimize boundary effects when employing periodic continuation.[1]

iii) Expansion possibilities. Earlier software packages were often written with tight constraints on computer memory and modularity of the software was often compromised. This makes it more difficult to modify these packages as to take advantage of recent developments in hardware. Hardware dependent code should be confined to a set of primitives that can easily be modified.

It was necessary to address each of the factors above during the design of the new software. These factors will be discussed further in the next paragraph. The goal was to create a set of programs that was simple to use and yet sophisticated enough to allow growth in the future. The culmination of this effort is called CEMPAS (Center for Electron Microscopy Processing and Simulation) which at this stage is primarly a simulation software package. A limited number of processing options are included and more will be added if the need arises. Most processing is currently being handled by the SEMPER software package,[2] but an integration of CEMPAS and SEMPER is also being investigated.

Design Implementation

The user interface. The choice of a user interface depends on who ultimately will be using the software and there are unfortunately no easy answers. The most common interface is the command language interpreter (CLI) where the program executes functions according to commands typed at the keyboard. Parameters associated with a given command are provided with default values that need only be specified if different values are to be used. Commands are thus quickly entered and executed. The advantage to this approach is speed and the fingers never need to leave the keyboard. The disadvantage is the time it takes for new users to learn the commands and options to take full advantage of the software.

A different approach is to provide input through the keyboard using menus. Users respond to prompts by entering their choice of command. The advantage is that the user does not need to remember any of the commands; the disadvantage is that updating menus takes time and the user needs to be prompted for any parameters.

The interface chosen for CEMPAS makes extensive use of menus, but instead of typing a response from the keyboard, the user responds by moving the cursor to a region associated with the command and presses one of the buttons on a mouse. The keyboard is used for input of data. Again the advantage is that the time required to learn to run the software is reduced to almost zero and the graphics screen used with the menus can be used for drawing curves, crystalline unit cells, etc., providing a very pleasing environment. The disadvantage is that experienced users might find it easier and faster to input data from the keyboard.

Another problem which is not related to how commands are input, is determining what information to display, what kind of commands to build into the program, etc. Unfortunately new users always find they need features that are not included and thus the software is always changing.

Flexibility. Some simulation software restricts the user to use arrays of fixed dimensions in their calculations. Typical dimension is a 128 by 128 point array. This limits the largest dimension in a calculation to 32Å if the potential is to be sampled every 0.25Å. To avoid aliasing the propagator should only extend out as far as 1/2 of the phasegrating and this results in a calculation that only includes diffracted beams out to $1Å^{-1}$. Instead of using fixed dimensions, CEMPAS uses variable array dimensions which are limited only by the amount of memory available. Thus if the unit cell is 16A by 128A, the program might choose an array of 64 by 512 points. Presently the maximum array dimensions are determined by the product of the two dimensions and cannot exceed 256K (512*512,256*1024, etc.).

Expansion possibilities. It is only to be expected that more efficient and accurate algorithms will be developed in the future and that progress in hardware development will continue to further reduce computation times. Given sufficient money new hardware can quickly be acquired; however development of software takes time, and changes in hardware should preferably only require minor modifications to a program. CEMPAS is written such that every menu option has a subroutine associated with it. This means that only subroutines need to be modified when algorithms change. Likewise device dependent code is limited to a set of primitives and only the codes required to draw a line between two points, to read the cursor position e.g., need to be modified in the case of a change in the display hardware. The penalty in overhead associated with transfer in and out of subroutines is offset by the ease of maintenance.

Accuracy of the calculations. CEMPAS has been written to include recent development in imaging theory to ensure accuracy. Presently most dynamical scattering calculations employ Fourier transforms, although there has been some research into newer algorithms.[3,4] However these new algorithms do not presently offer a practical alternative to the use of Fourier transforms.[5,6] CEMPAS uses a method originally published by Ishizuka and Uyeda[7] with the option to include potential eccentricity.[5] For accurate subslicing of the unit cell the program will automatically incorporate upper Laue layer interactions.[8] In the formation of the image, second order imaging effects are included to further ensure accurate results.[9]

Description of the hardware. The hardware at the NCEM will be described in detail in a forthcoming paper and only the part that is relevant to the operation of CEMPAS is presented below. A complete diagram of the system is given in Fig. 1.

The heart of the system is a MicroVax with 7 MB of memory soon to be expanded to 13 MB. Intensive vector operations, such as operations on large arrays, are performed in the CSPI MM+4 array processor. The CSPI MM+4 consists of 4 array processors that can be run in parallel giving a performance enhancement over the stand alone MicroVax of a factor of 20 to 80, depending on the number of array processors that are employed in the calculation. Images are displayed on TV monitors connected to a dual user GOULD 9527 image processor; hardcopy is provided on an Apple LaserWriter. Images are stored on a 500 MB formatted Fujitsu Eagle II Winchester disk drive. Archiving and backup is onto 6250 bpi magnetic tape using a Kennedy tape drive.

Description of CEMPAS. CEMPAS consists presently of about 14000 lines of computer code and is continually being improved and expanded as enhancements are needed. Approximately 35% is written in FORTRAN, 64% in C and 1% in VAX11 MACRO. The user interface is written entirely in C, while most of the number crunching routines are written in FORTRAN. A few routines were written in ASSEMBLER to increase speed.

As previously mentioned, the use of menus and a pointing device makes CEMPAS extremely easy to use. Several users of the NCEM facilities have already made use of the software without the need to consult a manual. The use of menus eliminates the need to remember commands and displays all options in plain view. To obtain help on a specific command, the user need only point at the command and press "h" on the keyboard to produce a help message. Input is simplified by the fact that scattering factors for the first 98 elements and crystallographic data on all 230 space groups are stored in the program, and the user is being prompted for any other necessary information. The program automatically creates the proper input files such that the user is not

required to learn how to edit files. All parameters needed in a calculation are visible to the user and can immediately be changed. To ensure that the program has the correct data there are several ways of drawing the unit cell with the atomic content. Images, diffraction patterns, "optical" diffractograms, Pendellosung plots, Contrast Transfer Function plots, etc. are easily calculated and promptly displayed. Images can be zoomed in or out, histogram equalized, Fourier transformed, intensity transformed, filtered and compared, again all with the use of the mouse. The list below gives some of the more important features of CEMPAS.

Input of crystallographic data facilitated by a database of the 230 crystallographic spacegroups and/or the use of any supplied set of symmetry operators. In addition there are menu driven operations that will expand an existing unit cell in any particular direction to create a large supercell and to create defects such as interstitials or vacancies. Atoms can be visually moved around in the unit cell and deposited anywhere. Further facilities for creating defects, such as shearing of subsections, twinning about a given plane, etc., will be added in the near future.

Viewing of the crystallographic cell from any direction, both with or without perspective view. Additionally the structure can be viewed from a given direction with a specified field of view with options of measuring distances between atoms, marking 2-d or 3-d unit cell, highlighting of specific atoms, specifying lighting conditions, etc.

Automatic calculation of a projected 2-d or true 3-d unit cell perpendicular to the incoming electron beam direction for use in the image simulation program. This unit cell is again viewable with or without perspective.

Automatic selection of correct array dimensions for the specified model to use in the multislice calculation up to x*y=256K. The ability to vary the

array dimensions independently is invaluable for simulating defects such as grainboundaries which often has a short periodicity along the boundary, e.g., though a 16384*16 point calculation.

Visual compositional display of the specimen when creating a structure that varies in the direction of the electron beam. Compositional layers are easily inserted, depositing and deleted from the structure.

Display of projected potentials and Fourier coefficients (structure factors).

Computation and display of simulated high resolution electron microscope images.

Choice of output ranging from the graphic terminal screen to one of 3 framestores or the laser printer.

Provision for inclusion of upper Laue layer interactions though proper subslicing of the unit cell potential. Automatic subslicing of the unit cell potential if the periodicity along the incident beam direction is too large.

Inclusion of second order effects in the image formation.

Computation and display of dynamical diffraction patterns. Options include indexing of patterns, modifying the convergence angle and the camera constant.

Plotting of amplitudes/intensities and phases vs. thickness of any number of selected beams.

Plotting of Electron Microscope Contrast Transfer Functions.

Positive or negative interpolative zoom of images, histogram equalization, histogram calculation and specification, contrast and brightness adjustments.

Fourier transforms of images or diffractograms, high and lowpass filters and specification of frequency windows.

Multislice calculations involving 64K beams with 256K interactions in approx. 2 s/slice.

Examples

The use of CEMPAS is best demonstrated by presenting a subset of the available screens and menus that the user has access to. Figures 3-15 show a typical session with CEMPAS where a simulation of a limited through-focus through-thickness set of images has been calculated for orthorhombic ZrO_2. In addition two screens that aid the user in creating structures with defects are shown in Figs. 14 and 15. Figure 13 shows the quality of images available from the terminal screen in the absence of a frame store.

References

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3. D. Van Dyck, J. Microscopy 119 (1980) 141.
4. D. Van Dyck, J. Microscopy 132 (1983) 31.
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6. R. Kilaas, Ultramicroscopy 19 (1986) 23.
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9. M.A. O'Keefe, Proc. EMSA 37 (1979) 556.

Figure Captions

Fig. 1 Schematic diagram showing the NCEM computer system for simulation and processing of transmission electron micrographs. TK50: 95 MB cartridge tape; RX50: dual floppy disk drives; RD53: 71 MB fixed disk; QDA50/61: controller with 503 MB formatted capacity Winchester Disk; CSPI MM+4: 4 individual array processors; GOULD IP9527: dual user image processor. The second MicroVax is used in real time data acquisition.

Fig. 2 Display of a section of the orthorhombic ZrO_2 structure viewed down the 110 direction. Output routine courtesy of W.O. Saxton. This is the atomic model used in the calculation of the images in Fig. 3.

Fig. 3. A limited through-focus/through-thickness series of computed images of the orthrhombic phase of ZrO_2. Images were first displayed on the Gould framestore and subsequently printed on the Apple LaserWriter.

Fig. 4. CEMPAS menu showing existing structure files belonging to a user. Additional structures are available from the space marked "COMMON". These are Center files made available to all users.

Fig. 5. CEMAS menu showing pertinent information regarding simulation of a particular structure. The most important structural data together with microscope data are displayed in this menu. Multislice calculations are run from here.

Fig. 6. Display of atom positions generated by applying the symmetry operators to the basis atoms. Orthorhombic phase of ZrO_2.

Fig. 7. Display of the symmetry operators associated with a particular space group. These symmetry operators are maintained in a data base which provide information on all 230 space groups. Symmetry operators are easily customized from the menu.

Fig. 8. Display of a ZrO_2 unit cell viewed from the 542 direction. Small spheres represent the oxygen atoms.

Fig. 9. Contrast transfer function with and without damping.

Fig. 10. A CEMPAS menu indicating how the user can choose to select a sequence of operations to be performed on a selected source, image, diffraction-pattern, etc., and display the result.

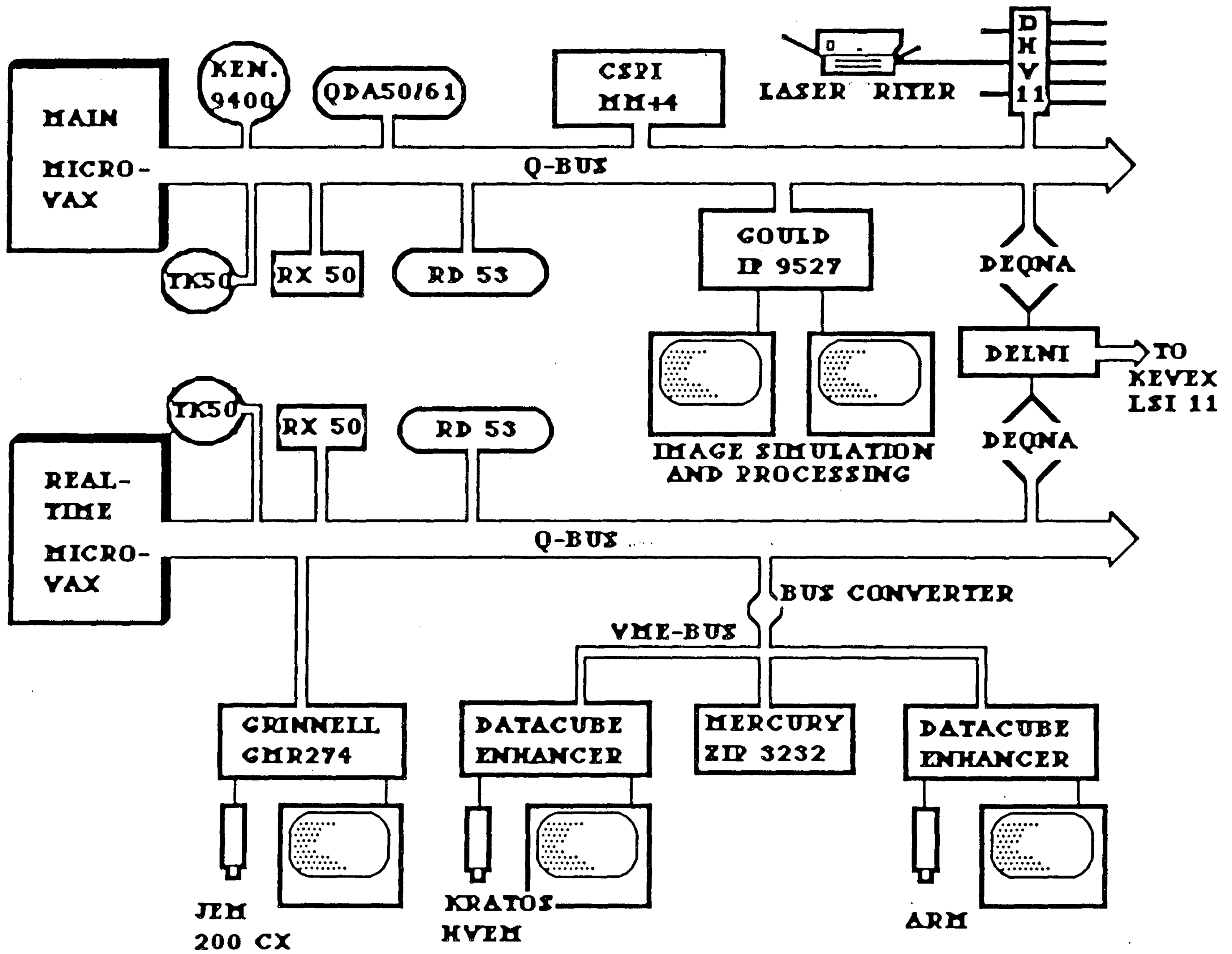
Fig. 11. Menu showing current setting of image brightness and contrast with options to change these settings.

Fig. 12. Computed dynamical diffraction pattern (left) and the computed power spectrum of the corresponding image (Fig. 13).

Fig. 13. Print of the terminal screen showing a halftone image; each image-point is represented by a square of 5*5 pixels.

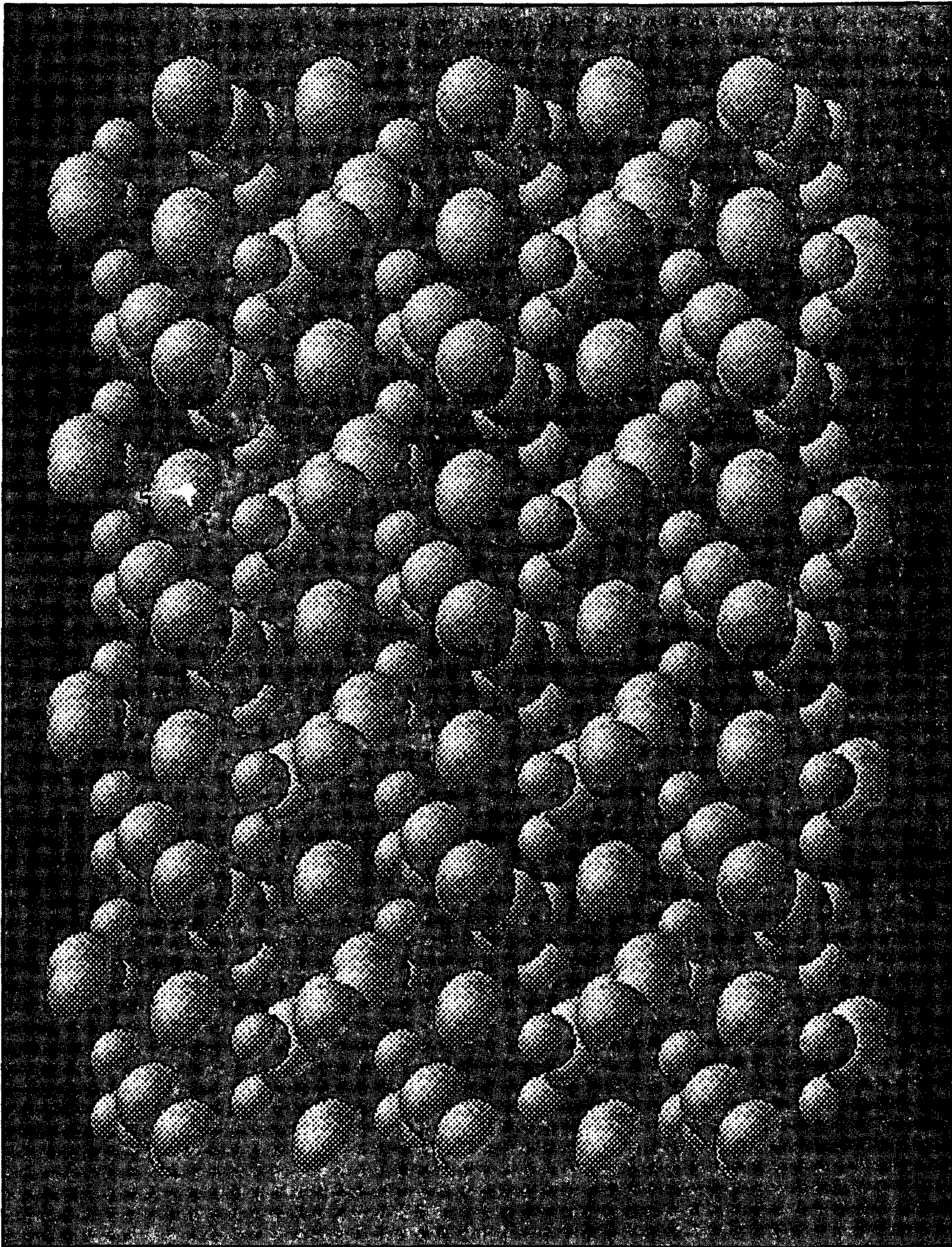
Fig. 14. CEMPAS menu indicating how the user can construct a unit cell for use in an image calculation.

Fig. 15. Menu used to construct a specimen where the composition varies along the incident beam direction.



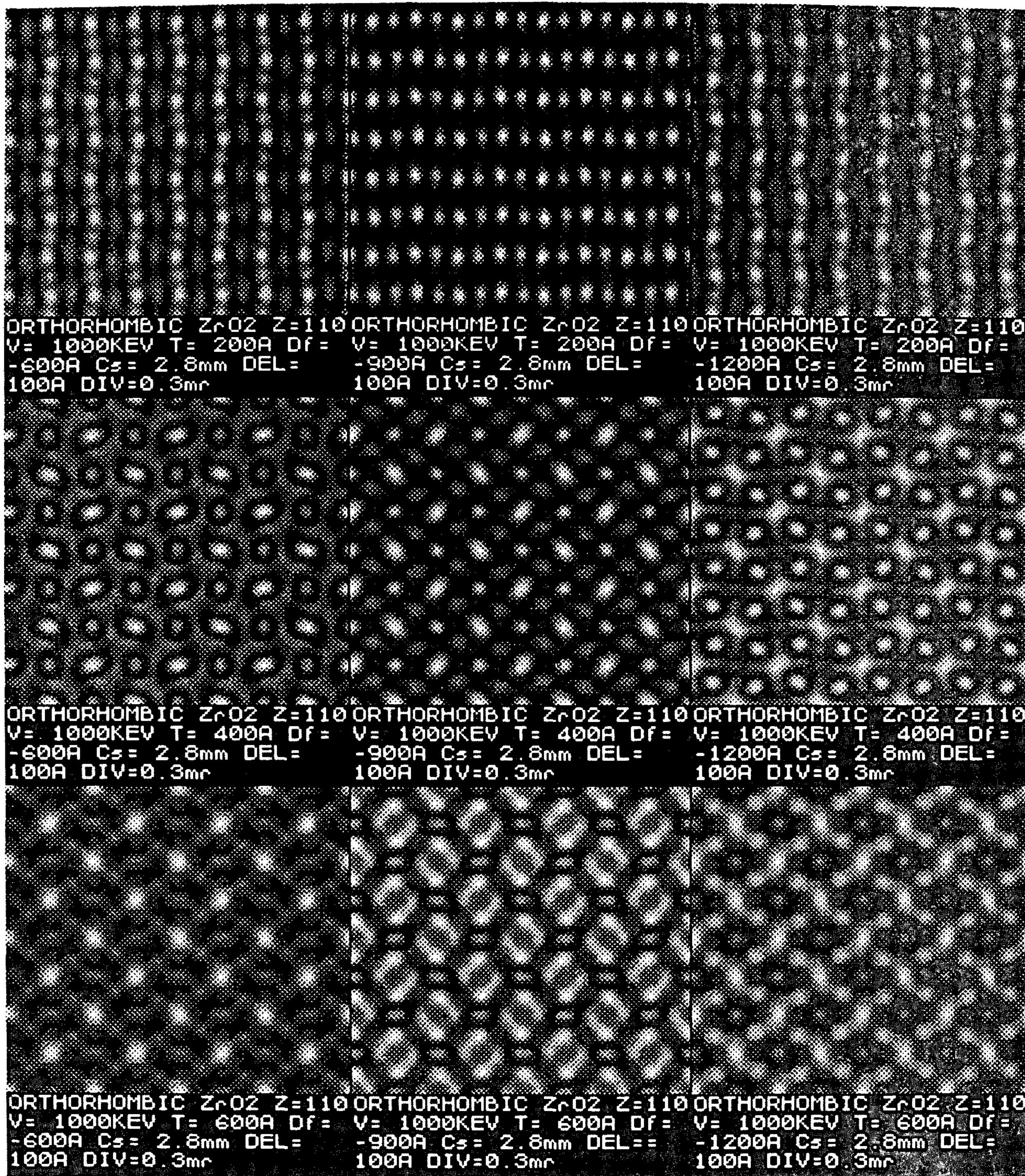
XBL 8611-4756

Fig. 1



- XBL 874-1625 -

Fig. 2



- XBL 874-1626 -

Fig. 3

PERSONAL | COMMON | NEXT PAGE | PREV. PAGE | DCL

AL2O3	AL3LI	AL3LIVAC	ALUMINUM
ANATESE	BATI2O5	BATIO3	BITE
BITE4	BITEL1	BITEL4	BTEK
BTEKNEW	CDTE	CO2SIO4	COPPER
CUBE	CUBE121	CUBELARGE	CULARGE
CUTI2	D100	DOLOM	FAUJ001
FAUJ110	FAUJPT	GAALAS	GAAS
GENBO	GOLD	INP	INTERFACE
INTERFACE1	LASRCUO4	LAYER1	LAYER2
MAGNESIUM	MOLYBDENUM	MZR	MZRO2
OCTAHEDRON	PLATINUM	QW	QWLARGE
RUTILE	SI3N4	SI3N4IFC	SICBETA
SILICON	SIO2	SIO2EXT2	SPINEL
SPINEL4	STACY	TEST	TIO2B
ZIRCON	ZSM5		

USE DISPLAYED FILE | CREATE NEW FILE | RETURN

XBL 874-1926

Fig. 4

INPUT FOR : ORTHORHOMBIC ZRO2		SPACE GROUP # 61	DCL
A = 10.01		ALPHA = 90.00	
B = 5.24		BETA = 90.00	
C = 5.05		GAMMA = 90.00	
GMAX = 2.00		ZONE AXIS : 1 1 0	
NO. OF SYMMETRY OPERATORS :	8	NO. OF SLICES PER UNIT CELL :	1
NO. OF ATOMS IN THE BASIS :	3	NO. OF DIFFERENT ATOMS :	2
MICROSCOPE : ARM		FOIL THICKNESS :	600.00
CS =	2.80	AMPLIT. OUTPUT FOR PLOTTING :	YES
DEL =	100.00	THE INDICES ARE :	H K L
TH. =	0.30		0 0 0
VOLT. = 1000.00			0 2 0
			2 0 0
CENT. OF LAUE CIRCLE: H =	0.00		
K =	0.00		
OBJ. LENS DEFOCUS : -1200.00			
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	IMAGE	DISPLAY	CTF
RUN	SHOW ATOMS	MSLICE	AMPLIT	VIEW FILE	RETURN

- XBL 874-1630 -

Fig. 5

DCL

#	TYPE	NAME	X	Y	Z	DW	OCC
1	1	ZR	0.1340	0.0334	0.2500	0.2000	1.00
2	1	ZR	0.6340	0.4666	0.7500	0.2000	1.00
3	1	ZR	0.8660	0.5334	0.2500	0.2000	1.00
4	1	ZR	0.3660	0.9666	0.7500	0.2000	1.00
5	1	ZR	0.8660	0.9666	0.7500	0.2000	1.00
6	1	ZR	0.3660	0.5334	0.2500	0.2000	1.00
7	1	ZR	0.1340	0.4666	0.7500	0.2000	1.00
8	1	ZR	0.6340	0.0334	0.2500	0.2000	1.00
9	2	O	0.0411	0.3750	0.1292	0.2000	1.00
10	2	O	0.5411	0.1250	0.8708	0.2000	1.00
11	2	O	0.9589	0.8750	0.3708	0.2000	1.00
12	2	O	0.4589	0.6250	0.6292	0.2000	1.00
13	2	O	0.9589	0.6250	0.8708	0.2000	1.00
14	2	O	0.4589	0.8750	0.1292	0.2000	1.00
15	2	O	0.0411	0.1250	0.6292	0.2000	1.00
16	2	O	0.5411	0.3750	0.3708	0.2000	1.00
17	2	O	0.2280	0.7500	0.5000	0.2000	1.00
18	2	O	0.7280	0.7500	0.5000	0.2000	1.00
19	2	O	0.7720	0.2500	0.0000	0.2000	1.00
20	2	O	0.2720	0.2500	0.0000	0.2000	1.00

PAGE +

PAGE -

PAGE *

CHANGE | ADD | DELETE | BUILD CELL | DISPLAY | RETURN

- XBL 874-1629 -

Fig. 6

#	SYMMETRY OPERATOR	#	SYMMETRY OPERATOR
1	X,Y,Z	21	1/3+Y-X,2/3+Y,1/6+Z
2	-Y,X-Y,Z	22	1/3+Y,2/3+X,1/6-Z
3	Y-X,-X,Z	23	1/3-X,2/3+Y-X,1/6-Z
4	-X,-Y,-Z	24	1/3+X-Y,2/3-Y,1/6-Z
5	Y,Y-X,-Z	25	2/3+X,1/3+Y,1/3+Z
6	X-Y,X,-Z	26	2/3-Y,1/3+X-Y,1/3+Z
7	-Y,-X,1/2+Z	27	2/3+Y-X,1/3-X,1/3+Z
8	X,X-Y,1/2+Z	28	2/3-X,1/3-Y,1/3-Z
9	Y-X,Y,1/2+Z	29	2/3+Y,1/3+Y-X,1/3-Z
10	Y,X,1/2-Z	30	2/3+X-Y,1/3+X,1/3-Z
11	-X,Y-X,1/2-Z	31	2/3-Y,1/3-X,5/6+Z
12	X-Y,-Y,1/2-Z	32	2/3+X,1/3+X-Y,5/6+Z
13	1/3+X,2/3+Y,2/3+Z	33	2/3+Y-X,1/3+Y,5/6+Z
14	1/3-Y,2/3+X-Y,2/3+Z	34	2/3+Y,1/3+X,5/6-Z
15	1/3+Y-X,2/3-X,2/3+Z	35	2/3-X,1/3+Y-X,5/6-Z
16	1/3-X,2/3-Y,2/3-Z	36	2/3+X-Y,1/3-Y,5/6-Z
17	1/3+Y,2/3+Y-X,2/3-Z		
18	1/3+X-Y,2/3+X,2/3-Z		
19	1/3-Y,2/3-X,1/6+Z		
20	1/3+X,2/3+X-Y,1/6+Z		

DCL

PAGE +

PAGE -

CHANGE SYMMOP

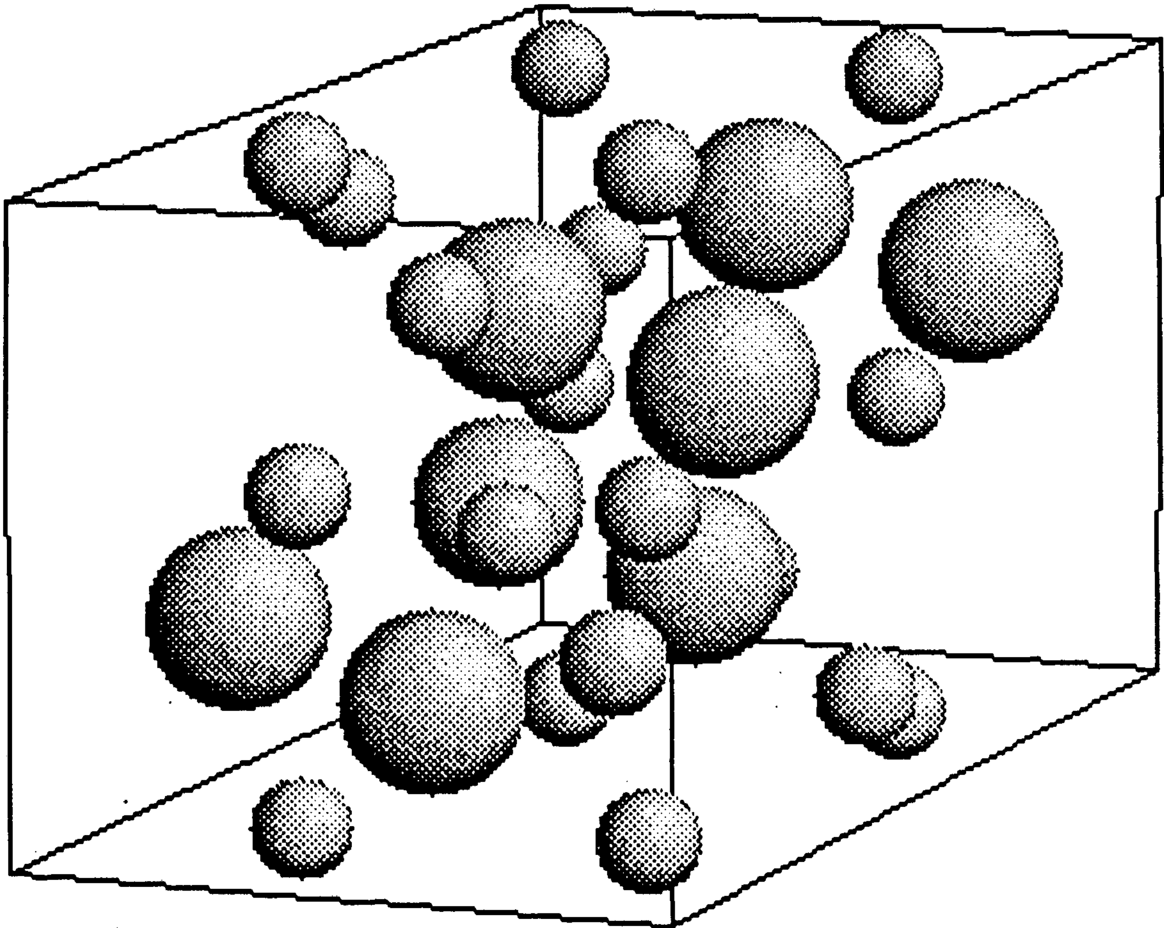
ADD SYMMOP

DELETE SYMMOP

RETURN

- XBL 874-1627 -

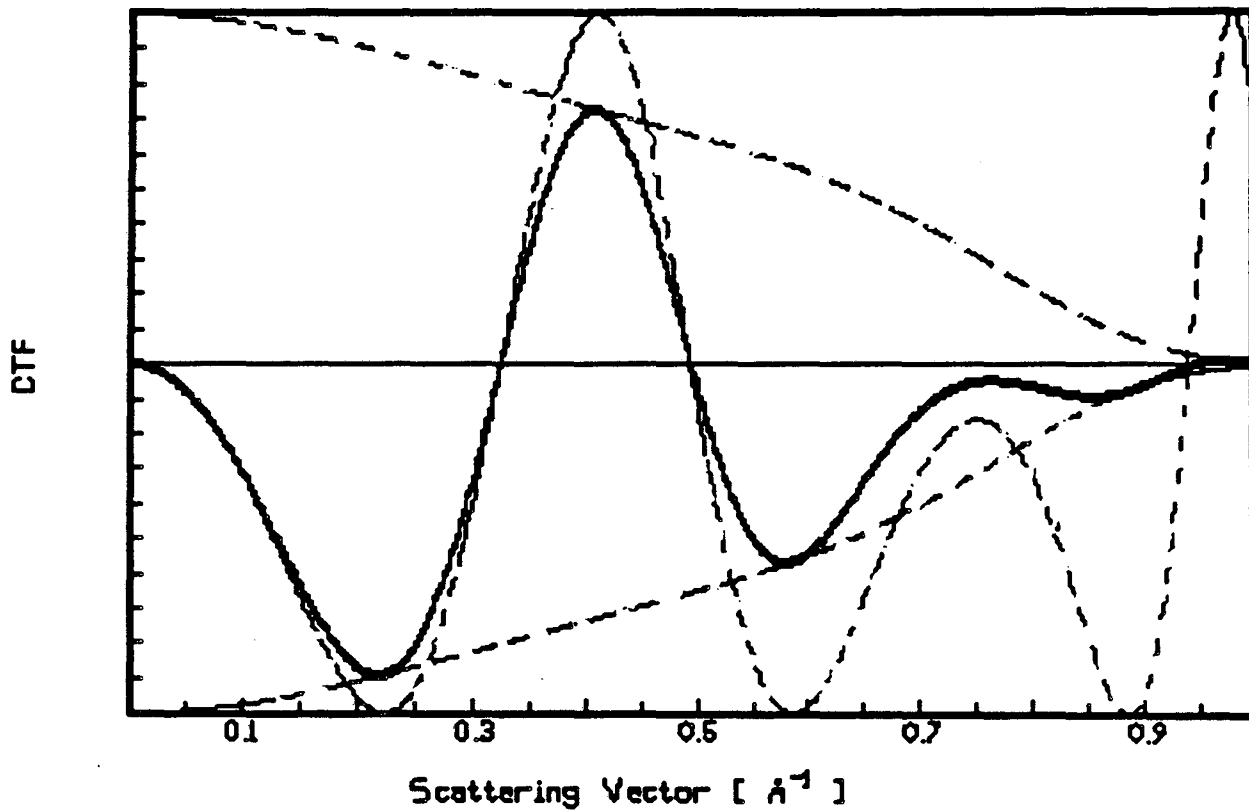
Fig. 7



- XBL 874-1633 -

Fig. 8

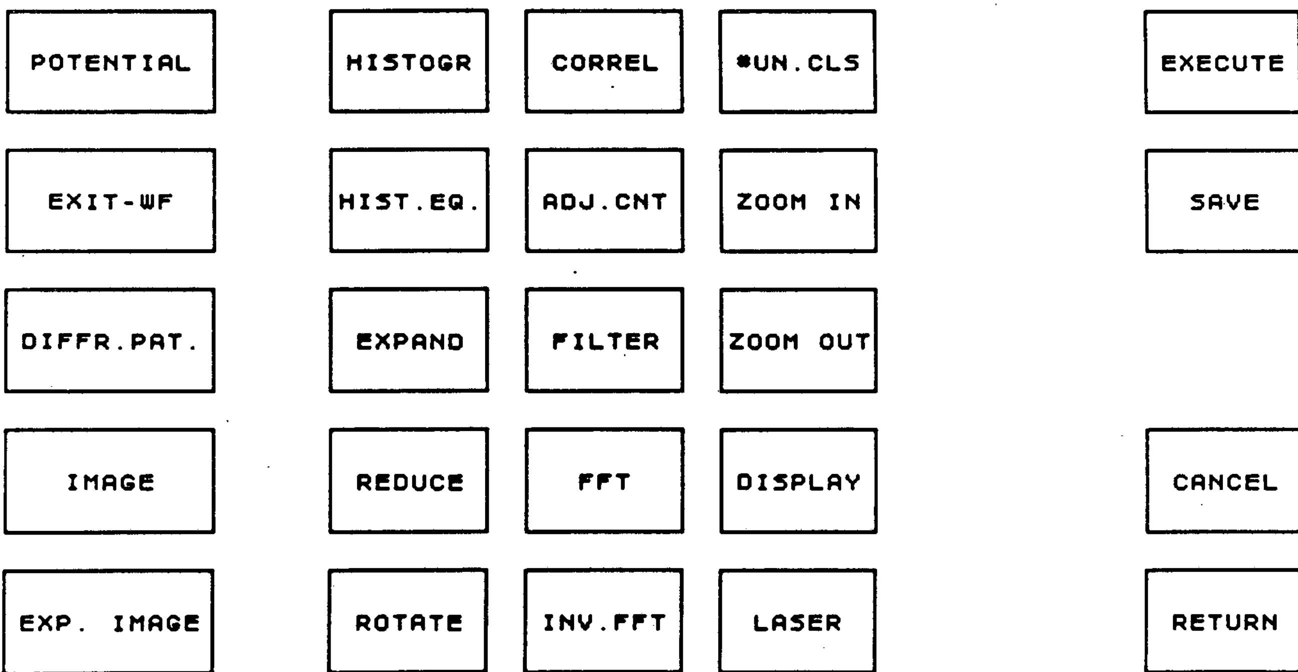
CONTRAST TRANSFER FUNCTION



Accel.Voltage = 1000.0 kV
Spher. Abber. = 2.8 mm
Obj. Lens Def. = -1200. Å
Delta = 100. Å
Div. Angle [Half] = 0.30 mrad

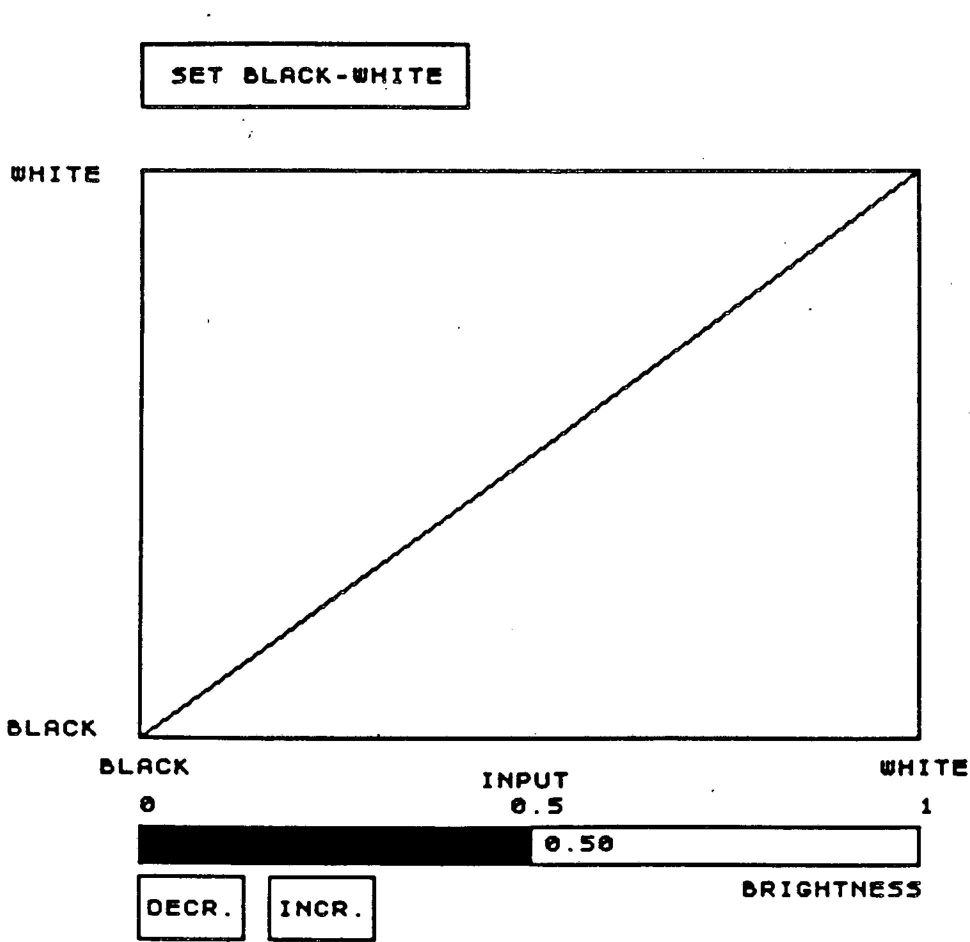
- XBL 874-1632 -

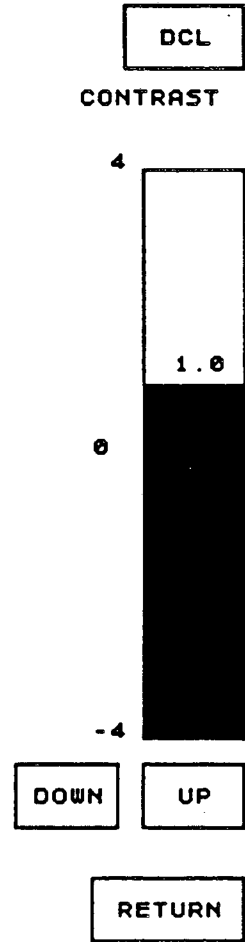
Fig. 9



- XBL 874-1628 -

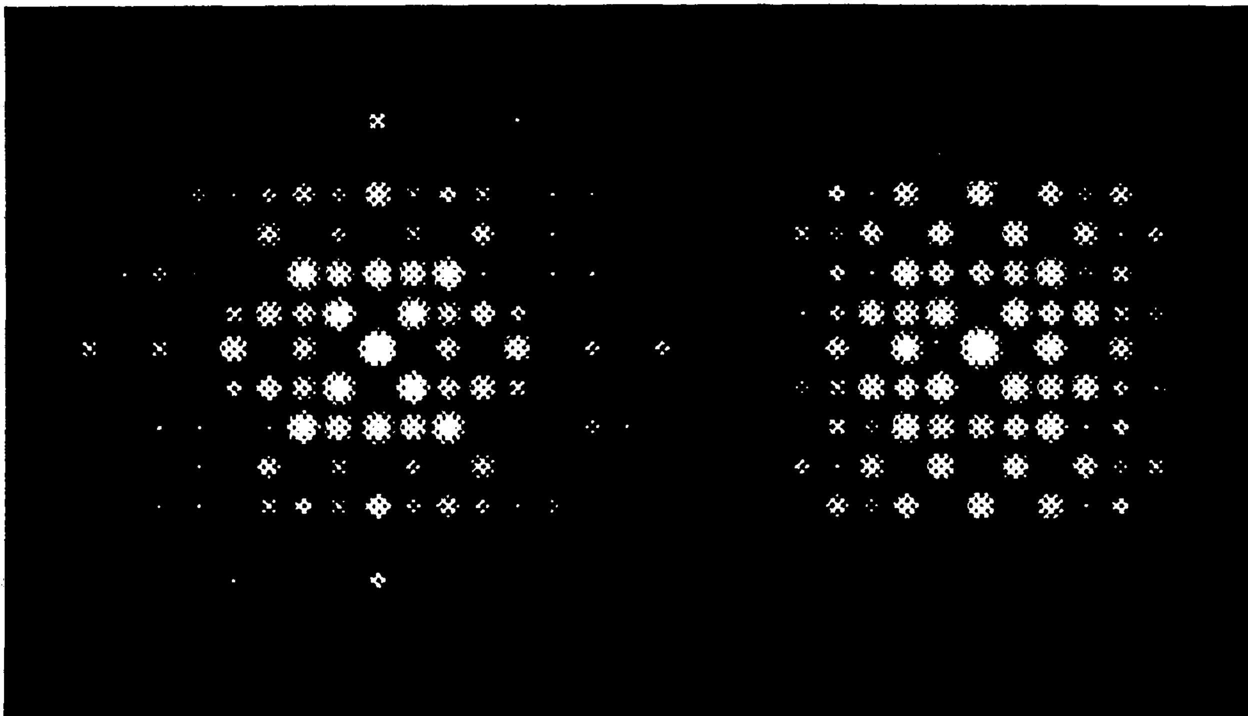
Fig. 10





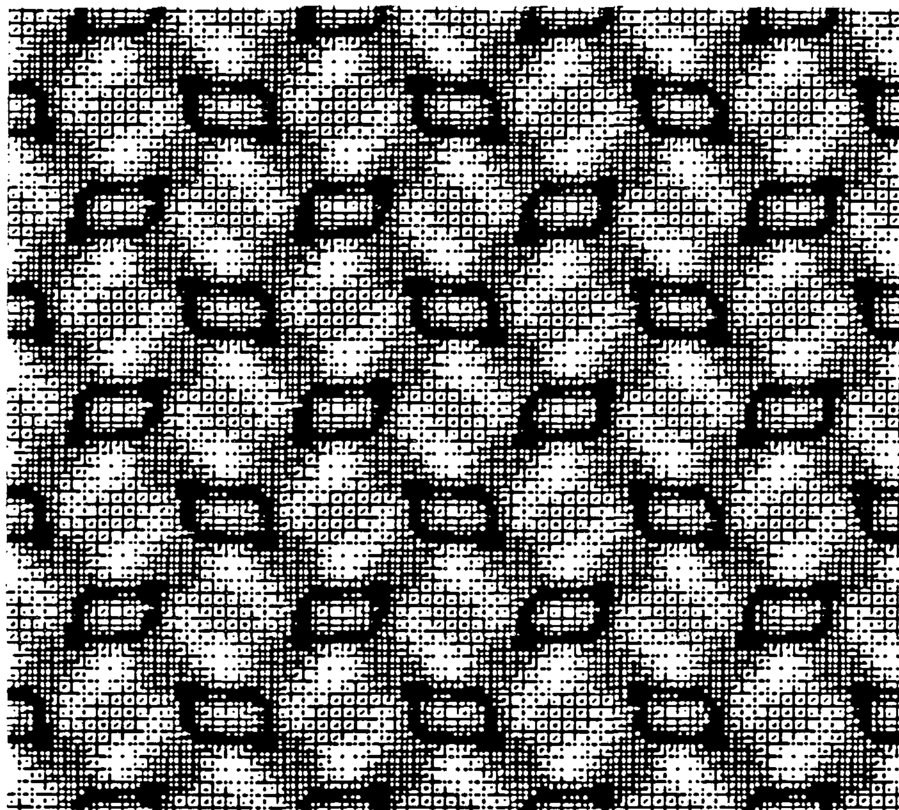
XBL 874-2927

Fig. 11



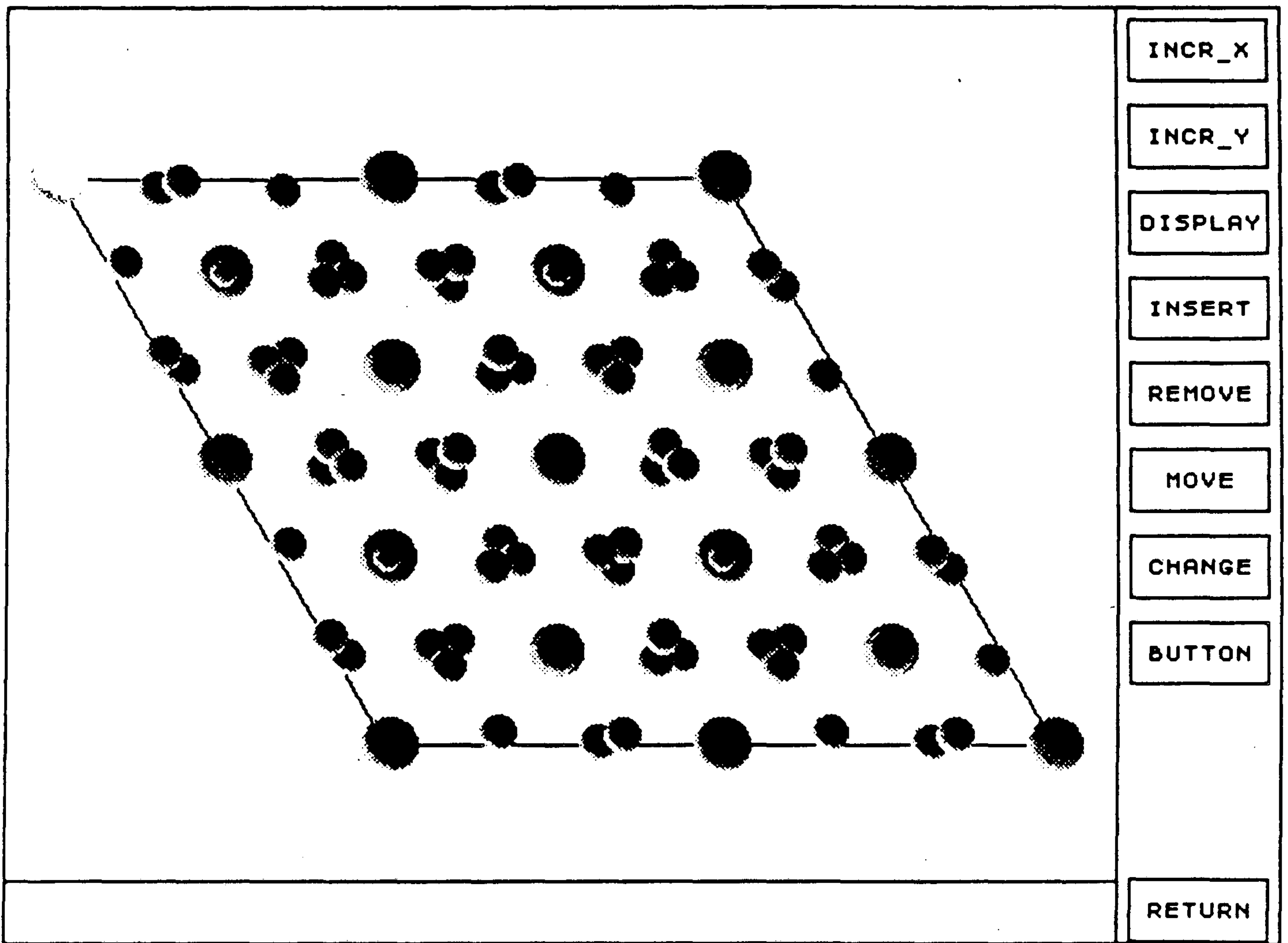
\- XBL 874-1624 -

Fig. 12



XBL 874-1928

Fig. 13



XBL 874-1623

Fig. 14

***** CONSTRUCT PHASE-GRATING SEQUENCE *****

LAYER #	NAME	UNIT CELL THICKNESS
1	LAYER1	3.00
2	LAYER2	3.00
3	LAYER3	3.00

DEF LAY

DEL LAY

TOP - 0.00 A

18.00

57.00

81.00

BOTTOM- 81.00 A

LAYER1

LAYER2

LAYER3

DEPOSIT

INSERT

RESET

REMOVE

REPEAT

PHASE-GRATING SEQUENCE :

1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3
3 3

RETURN

- XBL 874-1631 -

Fig. 15

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