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INTERACTIVE SIMULATION OF HIGH RESOLUTION ELECTRON MICROGRAPHS

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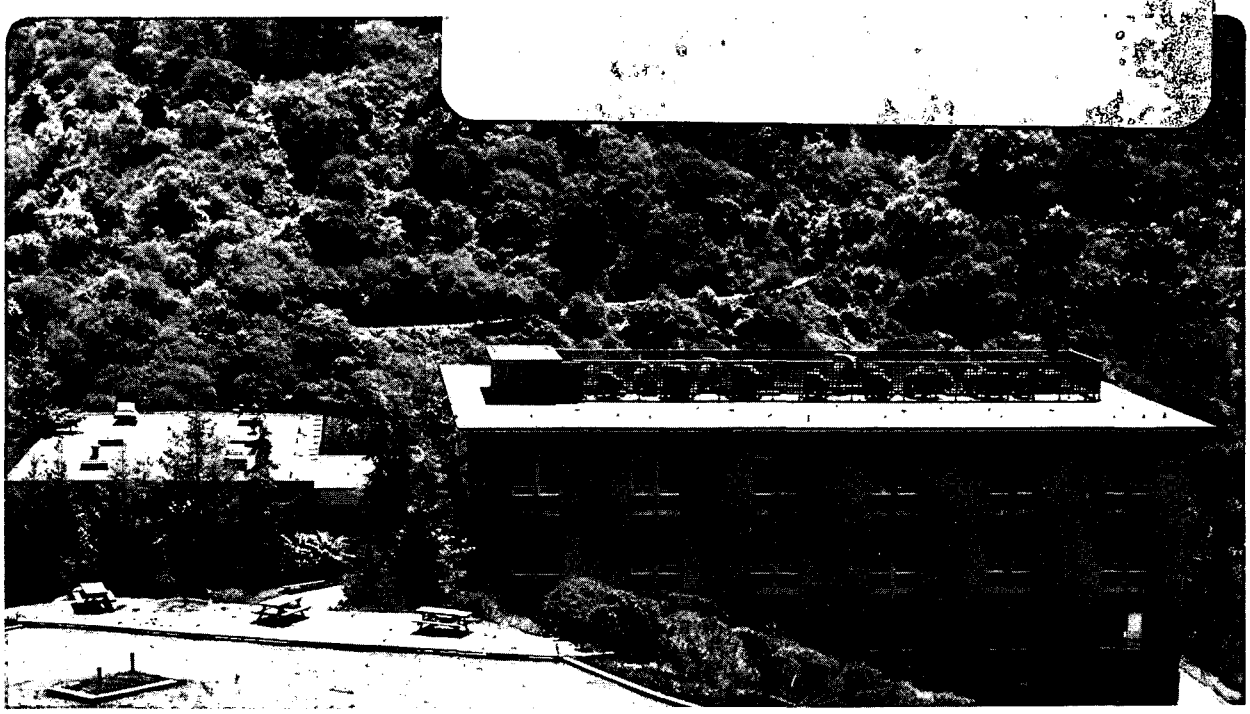

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INTERACTIVE SIMULATION OF HIGH RESOLUTION ELECTRON MICROGRAPHS

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Only a few years ago image simulation of HRTEM images were mostly carried out as low priority jobs on large mainframe computers with images available the next day as overprinted characters on computer paper. Today the same calculation can be carried out on a dedicated workstation in a matter of minutes with output on high resolution video monitors. This improvement in computer hardware has produced a shift from software primarily designed to run as batch jobs to interactive software that allows instant changes to both the atomic model and microscope parameters. In these near "real time" calculations the user interface becomes an important part of the software, since setting up the conditions for the calculation may take longer than the calculation itself.

In an attempt to create a truly interactive environment for simulation of HRTEM images, a new set of programs has been written at the National Center for Electron Microscopy (NCEM) at Berkeley. Previous experience with image simulation software has revealed several drawbacks with many existing programs and an effort has been made to make this the most powerful and user friendly program of its kind. The factors that received particular attention are as follows:

1) The user interface. There are presently several types of user interfaces available, each with its advantages and disadvantages. The most common interface is the command language interpretor (CLI) found in most computer operating systems. Commands are entered by typing the commands on the keyboard giving a powerful and efficient way of communicating with the program. This approach works well with experienced users who are familiar with the program. The inexperienced user, however, finds it difficult to remember commands and is often unaware of many powerful options. A second method is to provide menus on the screen and have the user respond by entering a keyword associated with a particular choice. 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 new software package uses menus, but rather than typing in a response at the keyboard, the user moves a mouse to direct the program to take actions. This eliminates the need to remember commands and the learning period is reduced to almost zero.

2. Flexibility. Many existing simulation programs use a fixed number of sampling points in the calculation, severely limiting the size of the unit cell. While this may not be a problem when calculating images of perfect crystals, calculations involving defects often require large unit cells in either one or both directions. This problem is overcome by using variable dimensions limited in principle only by available memory.

3. Expansion possibilities. With hardware improving daily, software needs to be flexible enough to require only minor modifications as it is run in different environments. While this new suite of programs has been written to ensure maximum performance utilizing hardware present at the NCEM, great care has been taken to separate hardware dependent code. Thus as the hardware changes, only a few routines need to be rewritten. This is also true as new algorithms are developed.

4. Accuracy. The new software includes recent improvements in image simulation theory, such as inclusion of potential eccentricity[1], second order imaging[2] and proper calculation of projected potential[3] when the slice thickness is different from the periodicity along the incident electron beam direction. The multislice program is based upon the Fourier transform method first published by Ishizuka and Uyeda[4]. There has been some research into new image simulation algorithms[1,5], but these do not presently offer a practical alternative[6,7].

As previously mentioned, the new set of programs was designed to be flexible and easy to use. The program comes with a data base consisting of scattering factors for the first 98 elements and crystallographic data on all 230 space groups. There is a separate menu that lets the user construct large unit cells and create defects. To ensure that the program has the correct data, there are several ways of drawing the unit cell with the atomic content. The parameters that go into the calculation are at all times in plain view and can be changed with a click of the mouse. In case the user needs help on any particular command, help is available by clicking a second button on the mouse. In addition to being user friendly, the program tries to include most functions that a user might need. Thus 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 figures on the next two pages illustrate some of the menus that are available to the user and some typical output. Figure 1a shows the main menu from which the multislice programs are run. Any parameter in this screen can be changed by activating the CHANGE command. Likewise, any atom coordinate shown in Fig. 1c can be changed with a click of the mouse. Figure 1d shows the menu from which images are manipulated and displayed. Images can be directed to a framebuffer for display on a video monitor or they can be displayed directly on the local terminal screen. When the image is displayed on the terminal screen each image point is usually made up of 4*4 or 5*5 pixels giving either 17 or 26 grey levels. Workstations like SUN and MicroVax, configured with color, however, are capable of displaying each image point as one pixel in 256 shades of grey.

References

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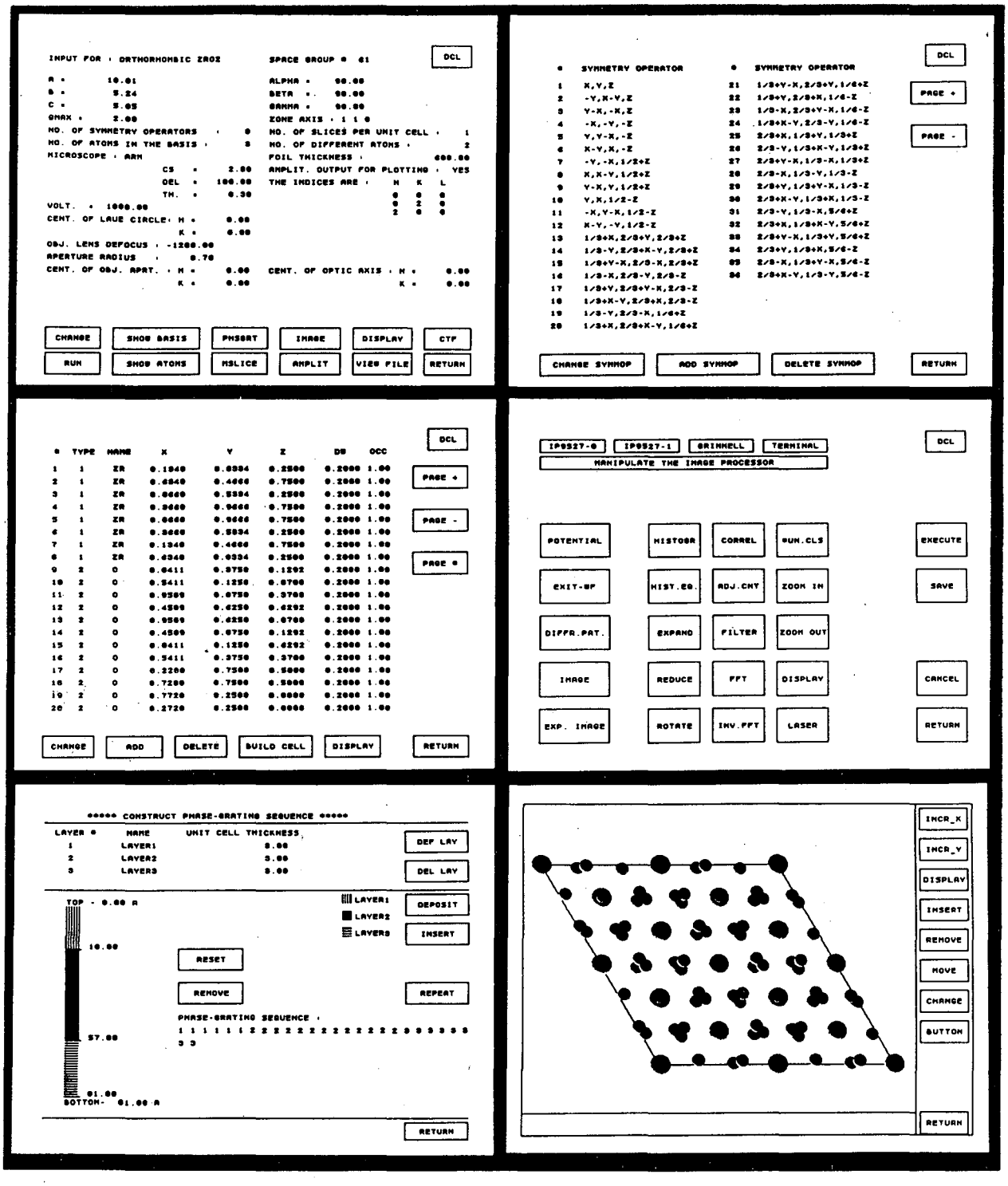

Fig. 1. Examples of screens and menus available to the user. a) Main menu from which multislice calculations are run. b) Screen displaying all symmetry operators associated with a choice of space group. c) Display of atom coordinates. d) Menu controlling display of images, diffraction patterns, etc. The left row indicates the input source to the actions represented by the middle row of commands. e) Menu for defining a structure that varies along the incident electron beam direction. f) Menu designed to help the user during the construction of large unit cells with defects. (a-XBL 874-1630, b-XBL 874-1627, c-XBL 874-1629, d-XBL 874-1628, e-XBL 874-1631, f-XBL 874-1623)

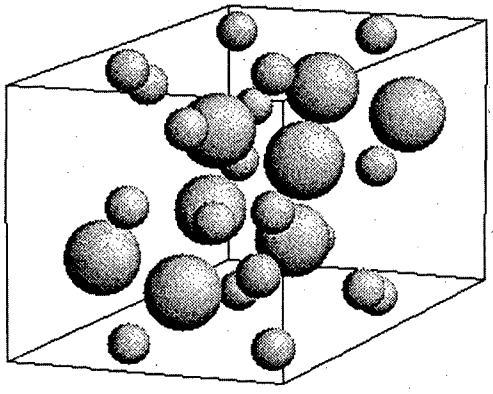

Fig. 2. Perspective view of the basic unit cell showing the atomic content. The cell can be viewed from any direction. XBL 874-1633

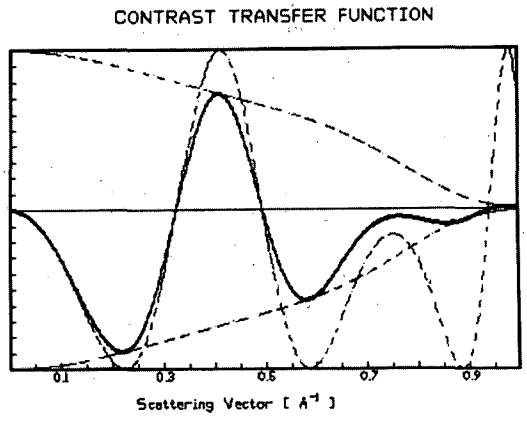

Fig. 3. Plot of the contrast transfer function. Parameters are taken from the main menu (1a). XBL 874-1632

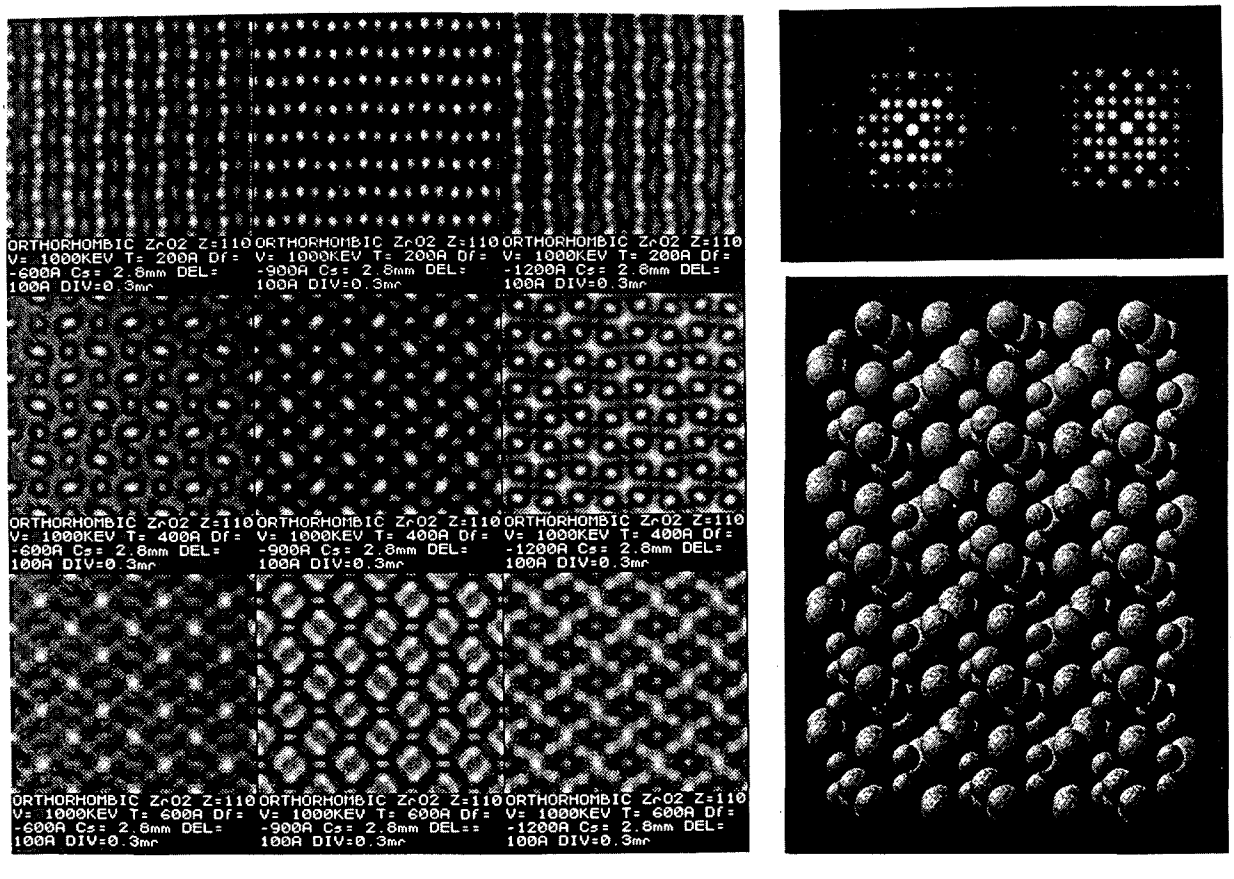

Fig. 4. Typical output. a) Limited through thickness and through Focus series of computed images. b) Dynamical diffraction pattern (left) and "optical diffractogram". c) Drawing of a section of the specimen. Atom drawing routine courtesy of W.O. Saxton.
(a- XBL 874-1626, b- XBL 874-1624, c- XBL 874-1625)

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