14.4-12 MULTI-SLICE COMPUTATION ON A PERSONAL COMPUTER

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Computation of electron diffraction and multi-beam lattice images using the multi-slice formulation for the theory of dynamical scattering of electrons by a crystal has been realized on a personal computer programmed in FORTRAN-77. The whole package consists of four seperate programs. As many as 4 different phase gratings can be employed and the number of beams included in the computation is determined by imposing a circular aperture of chosen radius. Up to 4000 beams can be included. However, the results are meaningful for about 1000 beams within that aperture. The computation is useful for small to medium unit cells, where lattice parameters are less than 3 nm, and they contain less than 300 atoms within a unit cell. Under such a condition, the speed of computation is about 40 seconds per slice. Either the wave function or the intensity distribution at the bottom surface of crystal can be stored and the former can be recalled for forming lattice images using a suitable contrast transfer function, the latter can be recalled to compute Pendellosung or a convergent beam electron diffraction pattern. The half-tone output of images can be printed on an Epson FX-85 printer with up to 25 grey levels or transfered to special a graphics display. In our laboratory we use a Hewlett Packard 12065 video interface, which displays 16 grey levels on 576 x 455 picture points. The alternative display is achieved by encoding a picture as a simple sequence of ASCII characters and transmitting the resulting file to the HP computer.

14.4-13 IMAGE FORMATION USING STEM ELECTRON MICRO-DIFFRACTION PATTERNS STORED ON VIDEO TAPE by John Konnert and Peter D'Antonio, Laboratory for the Structure of Matter, U.S. Naval Research Laboratory, Washington, DC 20375 and J.M. Cowley, Department of Physics, Arizona State University, Tempe, Arizona 85287

Electron microdiffraction patterns may be collected from regions as small as 3Å in diameter using an HB5 STEM from VG MIcroscopes, LTD., that has been fitted with a special ultra-high resolution pole piece (Cowley, Ultramicroscopy, 1984, 14, 27-36). When the STEM is equipped with an optical system, a very large number of diffraction patterns may be collected at the rate of 30/sec and conveniently stored on video tape. The portion of data to be analyzed is transferred through a time-base corrector and recorded on an optical disc. The Panasonic recorder used in this work stores 16,000 frames on each video disc. These frames are retrieved at random, digitized and analyzed. An example is given in Figure 1, which illustrates a microdiffraction pattern obtained for a glass in this manner using a 15Å beam. Fourier transformation of the intensity (using data to $1Å^{-1}$) yielded the interatomic distance distributions shown in Figures 2 and 3. When a beam is scanned over a region of sample, the variation of all or a portion of each diffraction pattern as a function of beam position may be used to form an image. If the patterns are sufficiently accurate, the interatomic distance information in the Fourier transforms of the intensities can be used for image formation. Results of experiments being carried out at Arizona State University will be discussed.

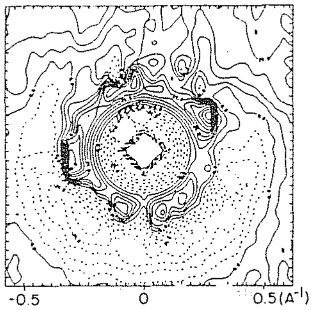

Figure 1. Microdiffraction pattern of $MgAlSi_3O_8$ glass obtained with 15Å diameter beam. A cylindrical Gaussian function representing the smoothly falling average intensity has been subtracted from the total intensity. Negative contours are dashed.

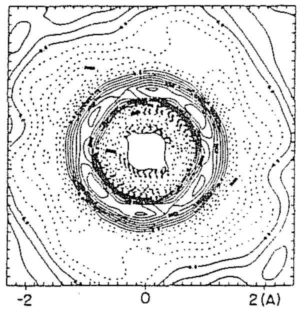

Figure 2. Real part of the Fourier transform of the intensity in Fig. 1. The ring at 1.4A represents the average projected Si-O and Al-O distances within the 15A diameter column.

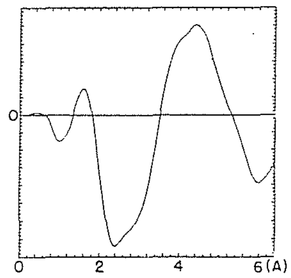

Figure 3. Integration of Fig. 2 for each projected interatomic distance. The oscillations occur about the zero line representing a material with the same density that possesses no order.