

Three-dimensional Reconstruction from Radiographs and Electron Micrographs: Application of Convolutions instead of Fourier Transforms

(computer time/accuracy/x-ray/shadowgraphs)

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ABSTRACT A new technique is proposed for the mathematical process of reconstruction of a three-dimensional object from its transmission shadowgraphs; it uses convolutions with functions defined in the real space of the object, without using Fourier transforms. The object is rotated about an axis at right angles to the direction of a parallel beam of radiation, and sections of it normal to the axis are reconstructed from data obtained by scanning the corresponding linear strips in the shadowgraphs at different angular settings.

Since the formulae in the convolution method involve only summations over one variable at a time, while a two-dimensional reconstruction with the Fourier transform technique requires double summations, the convolution method is much faster (typically by a factor of 30); the relative increase in speed is larger where greater resolution is required. Tests of the convolution method with computer-simulated shadowgraphs show that it is also more accurate than the Fourier transform method. It has good potentialities for application in electron microscopy and x-radiography. A new method of reconstructing helical structures by this technique is also suggested.

The problem of reconstructing the three-dimensional distribution of the optical density of an object from electron micrographs has been studied by several workers. The methods previously suggested involve the use of Fourier transforms [see ref. 1]. Recently, the senior author suggested in the first paper of this series [2] that this method of reconstruction is more generally applicable to various techniques of biophysical interest, such as medical radiography, autoradiography, and in industrial radiography. In that connection, a simplified procedure of three-dimensional reconstruction *via* two-dimensional sections was also proposed [2] that greatly reduces the computational times involved, since only two-dimensional Fourier sums are computed. In this paper, we present a still further improvement of the technique, using convolutions instead of Fourier transforms, in which all integrals or sums to be evaluated are one-dimensional, involving only one variable at a time. The resultant further reduction in computational time is also accompanied by appreciable improvement in the accuracy of reproduction. As a consequence, it appears possible to obtain reasonably good reproduction with only a small number (about 3-12) of transmission photographs (or shadowgraphs). The basic mathematics of the method is discussed in the next section, followed by simulated examples that show the power of the method.

Abbreviations: F.T. = Fourier transform; FTP = polar coordinate Fourier transform method; FTC = Cartesian coordinate Fourier series method; CON = convolution method, newly proposed.

MATHEMATICAL THEORY

The first step in the solution of the problem consists of replacing the three-dimensional (optical) density distribution by a set of two-dimensional density functions in a series of sections perpendicular to, say, the z -axis, as shown in Fig. 1. The object is placed in a parallel beam of radiation, incident normal to the z -axis, and shadowgraphs (in two dimensions) are obtained by rotating the object about the z -axis, which is also equivalent to rotating the imaging system, consisting of the source and the recorder, through different angles θ (Fig. 1). As shown in the figure, each shadowgraph may be considered to be made up of linear strips, each strip corresponding to a different section perpendicular to the z -axis. For such a strip, corresponding to the section at z , the logarithm of the ratio of the intensity at a point $P(z, l)$ to the incident intensity is a measure of the integral of the (optical) density of the object along a line through the point parallel to the direction of incidence of the beam [2]. We shall call this function $g(l; \theta; z)$ * for the shadowgraph of the section at the setting θ . The density distribution in the section at z [namely $f(x, y; z)$ or $f(r, \varphi; z)$] can be expressed in terms of $g(l; \theta; z)$ by the following Fourier transform (F.T.) relationships:

$$F(R; \theta) = \int_{-\infty}^{+\infty} g(l; \theta) \exp(2\pi i R l) dl \quad (1)$$

$$f(r, \varphi) = \int_0^{2\pi} \int_0^{+\infty} F(R, \theta) \exp[-2\pi i R r \cos(\varphi - \theta)] R dR d\theta \quad (2)$$

for each section z . We thus obtain the data $f(r, \varphi; z)$ using all the linear strips at z in the different shadowgraphs taken at various angles θ . The *three-dimensional* density distribution $f(r, \varphi, z)$ in the object is then obtained in cylindrical polar coordinates by putting the above sections together. Thus, the problem reduces to the reconstruction of a series of two-dimensional (*planar*) sections from a set of one-dimensional (*linear*) shadowgraphs. For this reason, we shall hereafter restrict our discussion essentially to one section of the object at right angles to the rotation axis.

* The semicolons are used to indicate that g is measured as a function of l only, but depends also on the parameters θ , describing the angular setting, and z , defining the section perpendicular to the rotation axis. When the parameters are considered explicitly as variables, the semicolons are replaced by commas.

We shall now show that the basic Eq. (1) and (2) can be rewritten in a form not involving Fourier transforms, but containing only integrals of functions defined in the real space of observation. Eq(2) can be recast into the form,

$$f(\varphi) = \int_0^\pi \int_{-\infty}^{+\infty} |R| F(R, \theta) \exp[-2\pi i R r \cos(\varphi - \theta)] dR d\theta \tag{3}$$

Suppose we define

$$g'(l; \theta) = \int_{-\infty}^{+\infty} |R| F(R; \theta) \exp(-2\pi i R l) dR \tag{4}$$

Then Eq. (3) for $f(r, \varphi)$ becomes

$$f(r, \varphi) = \int_0^\pi g'[r \cos(\varphi - \theta), \theta] d\theta \tag{5}$$

Eqs. (4) and (5) are the essential basis of our new formulation, in which $g'(l; \theta)$ can be expressed in terms of the shadowgraph data $g(l; \theta)$ by the following procedure: Fourier-inverting Eq. (1),

$$g(l; \theta) = \int_{-\infty}^{+\infty} F(R, \theta) \exp(-2\pi i R l) dR \tag{6}$$

Comparing Eq. (4) and Eq. (6), we see that the F.T. of $g(l; \theta)$ is $F(R; \theta)$, while the F.T. of $g'(l; \theta)$ is $|R| F(R; \theta)$, so that

$$\text{F.T. of } g'(l; \theta) = [\text{F.T. of } g(l; \theta)] \times [\text{F.T. of } q(l)] \tag{7}$$

where $|R|$ is the F.T. of the function $q(l)$, or

$$|R| = \int_{-\infty}^{+\infty} q(l) \exp(2\pi i R l) dl \tag{8}$$

Using the well-known convolution theorem for the inverse of the product of Fourier transforms, it follows from Eq. (7) that $g'(l; \theta)$ is the convolution of $g(l; \theta)$ and $q(l)$, or, explicitly,

$$g'(l; \theta) = \int_{-\infty}^{+\infty} g(l_1; \theta) q(l - l_1) dl_1 \tag{9}$$

Thus, to evaluate the modified function $g'(l; \theta)$, we require the function $q(l)$ explicitly. Inverting Eq. (8), we have, formally,

$$q(l) = \int_{-\infty}^{+\infty} |R| \exp(-2\pi i R l) dR \tag{10}$$

This integral cannot, however, be evaluated as the integrand diverges. To overcome this difficulty, we may replace the limits $-\infty$ and $+\infty$ in Eq. (10) by $-A/2$ and $+A/2$, where A is some (large) finite number, when the integral exists for all values of l . Thus, define

$$q_A(l) = \int_{-A/2}^{+A/2} |R| \exp(-2\pi i R l) dR \tag{11}$$

Disregarding the difference between $q_A(na)$ and $q(na)$ when A is large enough, we have, evaluating the integral in Eq. (11),

$$\begin{aligned} q(na) &= 1/4a^2 \quad \text{for } n = 0 \\ &= -1/\pi^2 n^2 a^2 \quad \text{for } n \text{ odd} \\ &= 0 \quad \text{for } n \text{ even} \end{aligned} \tag{12}$$

Hence, if we have data for $g(l; \theta)$ at a set of equally spaced

points $l = ma$ (where m is a positive or negative integer), then Eq. (9) can be expressed in the form of an infinite sum as

$$g'(na; \theta) = a \sum_{m=-\infty}^{+\infty} g(ma; \theta) q[(m - n)a], \tag{13}$$

or, using Eq. (12),

$$g'(na; \theta) = g(na; \theta)/4a - (1/\pi^2) \sum_{p \text{ odd}} g[(n + p)a; \theta]/p^2 \tag{14}$$

We have assumed here that $g(l; \theta)$ is given at a set of points separated by the interval a . This is, in fact, a great advantage, since measurements on shadowgraphs are most conveniently made by scanning the data at regular intervals along a line on a photograph using a densitometer, or by using some suitable device for direct measurement of intensity. This interval becomes an important parameter in the application of the method. Summarizing the above arguments, we may describe the convolution method as follows:

For a two-dimensional object (or section), linear shadowgraphs at different angles θ are scanned at intervals a and these data are then convoluted with $q(na)$ to obtain $g'(na; \theta)$ [using Eq. (14)], also at intervals a . These are then used for calculating $f(r, \varphi)$ using Eq. (5), which may also be written in the form of a sum;

$$f(r, \varphi) = f(jr_0, k\varphi_0) = \sum_{t=1}^N g'[jr_0 \cos(k\varphi_0 - t\theta_0), t\theta_0] \tag{15}$$

where j, k, t, N are integers and r_0 and φ_0 are intervals of r and φ . The interval for θ is $\theta_0 = \pi/N$, where N is the number of shadowgraphs recorded at regular intervals over the range $-\pi/2$ to $+\pi/2$. In Eq. (15), the value of $jr_0 \cos(k\varphi_0 - t\theta_0)$ will not in general be a multiple of a ; therefore we have to interpolate between the calculated values of $g'(na; \theta)$, so that the resolution of the final data obtained for $f(r, \varphi)$ will depend on the fineness of the interval at which the shadowgraph data are available and the consequent accuracy of the interpolation.

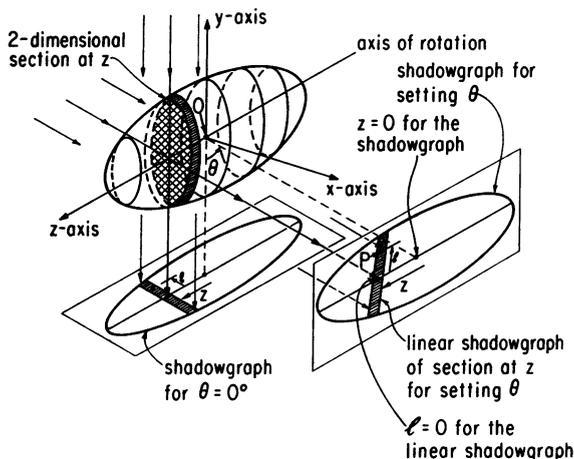


FIG. 1. Diagram illustrating the formation of shadowgraphs with incident beam at angle θ to the zero setting normal to the xz plane. The section at right angles to the axis of rotation at z (shown shaded) yields the linear strip in the oval shadowgraph on the right. Measurement of the intensity at the point P gives the values of $g(l; \theta; z)$.

TEST OF THE CONVOLUTION METHOD

The convolution method has been applied to a number of simple, as well as more complicated, hypothetical-object density distributions. In each example, the density function $f(x, y)$, or $f(r, \varphi)$, was assumed, and the corresponding simulated shadowgraph function $g(l; \theta)$ was evaluated at suitable steps a for l and θ_0 for the angle θ varying from -90° to $+90^\circ$ (on a computer) by integration of $f(x, y)$ along appropriate lines. The shadowgraphs thus obtained were used for the computer reconstruction of the objects, using Eq. (14) and (15). The data are presented as $f(x, y)$ on a square grid of suitable spacing b , and the results are denoted by the symbol CON (standing for the 'convolution' method). From a detailed comparison of the original and the reconstructed objects for different values of a and θ_0 , the validity, accuracy, and other features of the new method have been examined. For comparison, the F.T. method was also used in some cases, either by using Eq. (1) and (2), or by obtaining $F(X, Y)$ at points on a square grid in Fourier space from $F(R, \theta)$ by interpolation and reconstructing $f(x, y)$ from $F(X, Y)$ using standard formulae. The two methods are denoted by the symbols FTP (Fourier transform using polar coordinates) and FTC (Fourier transform using Cartesian coordinates).

Circular disk of uniform density

The three methods, CON, FTP, and FTC, were applied to the reconstruction of a disk having uniform density $f(r, \varphi) = 1$ for $r \leq 1$ and zero for $r > 1$. The results are given in Fig. 2, in which the density variations along a radius are shown. Reconstruction was made with 12 shadowgraphs ($\theta_0 = 15^\circ$) scanned at intervals of $a = 0.1$. Correspondingly, the F.T. of $g(l; \theta)$ was calculated for $-A/2 \leq R \leq A/2$ with $A = 1/a = 10$, at intervals of $R_0 = 0.25$ for R . For the FTC method, X and Y were also varied over the same range as R , at intervals of R_0 . It will be seen from Fig. 2 that the reconstruction from the CON method is much closer to the true density distribution than that from either the FTP or the FTC method, particularly in the region of uniform density for $r < 0.8$. The accuracy of reconstruction may be quantitatively represented by the value of the mean relative error, \mathcal{R} , defined by

$$\mathcal{R} = [\Sigma |f(\text{reconstructed}) - f(\text{true})|] / \Sigma |f(\text{true})| \quad (16)$$

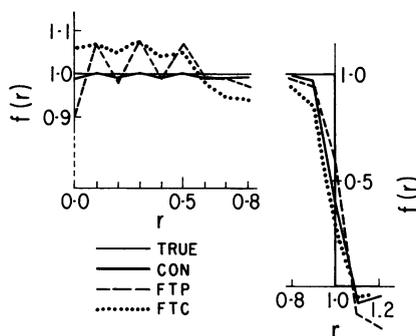


FIG. 2. Original and reconstructed density distribution along a radius for circular disk of uniform density of radius of 1. The calculated values are at intervals $b = 0.1$ for r . The region near the boundary, namely between $r = 0.8$ and 1.2, where the density rapidly falls from 1.0 to 0.0, is shown separately to the right on a different scale for f . Note the very small deviations from the true value of the CON data in the uniform region inside the disk for $r \leq 0.8$.

(The term \mathcal{R} -value is adopted from x-ray crystallography; a curly \mathcal{R} is used to distinguish this from the polar coordinate R in Fourier space). The \mathcal{R} -values for the three different methods, corresponding to $\theta_0 = 30^\circ$ and 15° and $a = 0.2$ and 0.1 are given in Table 1. [The values of $f(jb, kb)$ were obtained in all cases with $b = 0.1$]. It can be seen from this table that the error is least for the CON method in all cases. However, in the region beyond $r = 0.8$, errors are quite large for all three methods. This is to be expected, since it is well known that the Fourier sum always leads to values larger than the true value by about 10% at a sharp discontinuity, and that the sharp discontinuity is blurred because of termination errors in the sum. One may, therefore, conclude that in regions of nearly uniform density, the CON method is capable of an accuracy 5- to 10-times better than that attainable using the F.T. method.

Disk with nondiscontinuous boundary and an off-center hump

In order to study the efficiency of the method without the complication of a sharp boundary with discontinuous changes in density, and also to test if the method is capable of revealing a fairly localized, small density change in a flat region, the object represented in Fig. 3(a) and (b) was chosen, which has a uniform density from the center up to $r = 0.8$, except for an off-center hump, beyond which it trails off smoothly to zero at $r = 1.2$. Fig. 3(c) shows the results of applying the convolution method using $a = 0.1$, and $\theta_0 = 30^\circ$. The reconstruction is seen to be quite good, even with six shadowgraphs, although there is an error of more than 2% near the peak of the hump H, and somewhat larger errors in the varying region, V. When the same shadowgraphs are scanned at a finer interval, with $a = 0.05$, the errors become much smaller, as is shown by Fig. 4, for the region around H.

In order to obtain a comparison with the F.T. methods of reconstruction, the \mathcal{R} -values for the different regions of the object are collected together in Table 2 for densities reconstructed at $b = 0.1$ in all cases. It will be seen that the CON method is distinctly superior when the density does not vary rapidly, and even when it does, scanning at $\theta_0 = 15^\circ$ and $a = 0.1$ improves the accuracy of this method much more than for the F.T. methods with $R_0 = 0.25$. However, the accuracy of the FTP method is influenced by the fact that, in obtaining f from $F(R, \theta)$ by Eq. (3), the integral is approximated by a sum using data at intervals $R_0 = 0.25$. Since the accuracy of the integration can be improved by reducing R_0 , other conditions remaining the same, a new calculation was made using $R_0 = 0.125$ for $\theta = 15^\circ$ and $a = 0.1$. As is seen from Table 2, the accuracy of both the FTP and FTC methods improved

TABLE 1. Values of the mean relative errors (\mathcal{R}) for the circular disk for $r < 0.8$ using the CON, FTP, and FTC methods

θ_0 ($^\circ$)	a	\mathcal{R} (in %) for		
		CON	FTP	FTC
30	0.2	1.5	9.4	7.7
30	0.1	0.6	7.6	5.3
15	0.2	1.2	8.0	7.6
15	0.1	0.3	5.3	5.2
15	0.1	0.3	2.9*	3.9*

* $R_0 = 0.125$; for other values, $R_0 = 0.25$.

appreciably and became comparable with that of the CON method, particularly in the regions H and V of varying density. The data in Fourier space for the FTC method were, however, taken only at intervals of 0.25 for X and Y, since this corresponds to the reconstruction of a unit cell with edge equal to 4 units in real space, definitely larger than the size of 2.4 units of the object studied. Nevertheless, the accuracy of FTC improves because the data for $F(X, Y)$ are now obtained by interpolation from values of $F(R, \theta)$ given on a finer grid of points. In the uniform region U also, the accuracy of reconstruction of the F.T. methods increases appreciably when R_0 is reduced from 0.25 to 0.125 (see Table 2), but the CON method is still more accurate. This effect, namely that CON is superior in accuracy to both FTP and FTC, is also observed for the uniform region ($r < 0.8$) of the circular disk (last line of Table 1). It should be mentioned, however, that halving the interval for R doubles the computation time for FTP (see Table 3, next section).

In view of the advantages of the CON method, the effect of changing the intervals a and θ_0 over a wide range ($\theta_0 = 3^\circ, 6^\circ, 15^\circ, 30^\circ, 60^\circ$; $a = 0.05, 0.1, 0.2$) was studied using this method alone. The general conclusion was that, although the accuracy

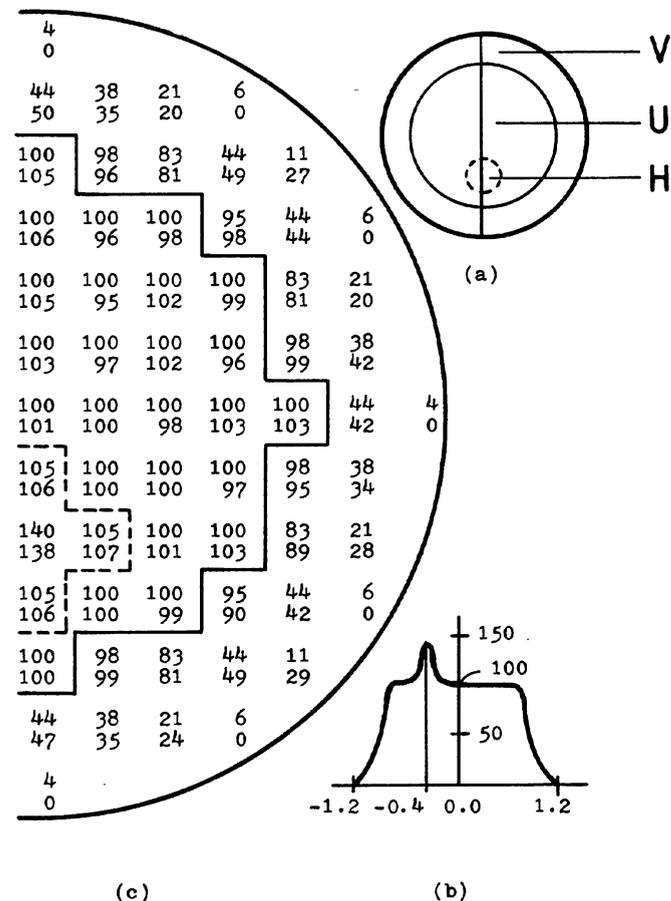


FIG. 3. (a) Schematic diagram of three regions of density variations in reconstructed object: V—"varying" portion, with f increasing from 0 at $r = 1.2$ to 100 at $r = 0.8$; U = "uniform" region for $r < 0.8$, except for the small region H (enclosed by broken lines), which has a "hump" of higher density than U, with a maximum of 140. (b) Profile of the density variation along the marked vertical line, passing through all three regions. (c) True (above) and reconstructed density (below) obtained using the CON method, for $\theta_0 = 30^\circ, a = 0.1$. Values are given at intervals of $b = 0.2$ for x and y , for $x = 0.0$ to 1.2 and $y = -1.2$ to +1.2.

TABLE 2. \mathcal{R} -values for a disk with varying density and non-discontinuous boundary for the three regions, H, U, and V shown in Fig. 3.

$\theta_0(^\circ)$	a	\mathcal{R} (in %) for		
		CON	FTP	FTC
<i>Region H</i>				
30	0.2	2.9	5.5	4.8
30	0.1	0.9	3.7	3.3
15	0.2	3.5	4.0	5.0
15	0.1	0.9	3.7	3.0
15	0.1	0.9	1.1*	1.3*
<i>Region U</i>				
30	0.2	2.0	4.9	5.3
30	0.1	1.8	4.2	4.2
15	0.2	1.4	4.3	5.3
15	0.1	0.4	4.1	4.1
15	0.1	0.4	1.3*	1.8*
<i>Region V</i>				
30	0.2	10.0	12.9	10.7
30	0.1	9.2	11.5	9.7
15	0.2	7.0	6.4	10.7
15	0.1	3.0	6.8	9.7
15	0.1	3.0	3.2*	3.2*

* $R_0 = 0.125$ for these values; $R_0 = 0.25$ for others.

improved with making either interval smaller, there was no appreciable gain in accuracy by taking a larger number of shadowgraphs (i.e. decreasing θ_0) beyond the range at which $\langle r \rangle \theta_0 \sim a$ (where $\langle r \rangle$ is the mean r for the object, and θ_0 is in radians). Thus, taking region U of the object in Table 2, $\langle r \rangle \theta_0$ is about 0.2 for 30° and 0.1 for 15° , and there is only a small reduction in \mathcal{R} -values, from 2.0 to 1.4% for $a = 0.2$, on going from $\theta_0 = 30$ to 15° , while it drops from 1.8 to 0.4 for $a = 0.1$. Conversely, for a given number of shadowgraphs, no great gain in overall accuracy is obtained by scanning at an interval finer than $\langle r \rangle \theta_0$. For example, if a is changed from 0.2 to 0.1, \mathcal{R} drops only from 2.0 to 1.8 for $\theta_0 = 30^\circ$, while it decreases from 1.4 to 0.4 for $\theta_0 = 15^\circ$.

Reconstruction using only three shadowgraphs

In order to show how a reasonable idea of the gross density variations in the interior of an object may be obtained using just three shadowgraph data, the elliptical object with varying density shown in Fig. 5(a) was reconstructed using shadowgraphs at $\theta = -60^\circ, 0^\circ$, and $+60^\circ$, the value $\theta = 0^\circ$

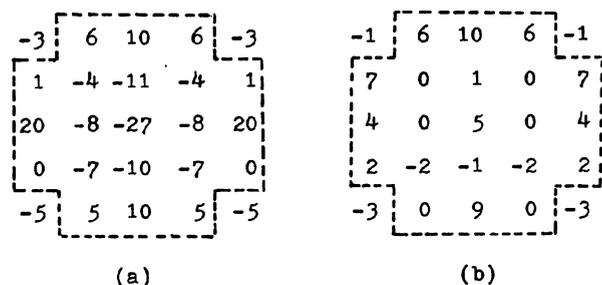


FIG. 4. The values of $[f(\text{reconstructed}) - f(\text{true})] \times 10$, at intervals of $b = 0.1$ for x and y , around the region H of the object shown in Fig. 3, for $\theta_0 = 30^\circ$ (a) $a = 0.1$ and (b) $a = 0.05$. The location of the hump is shown by the dashed lines.

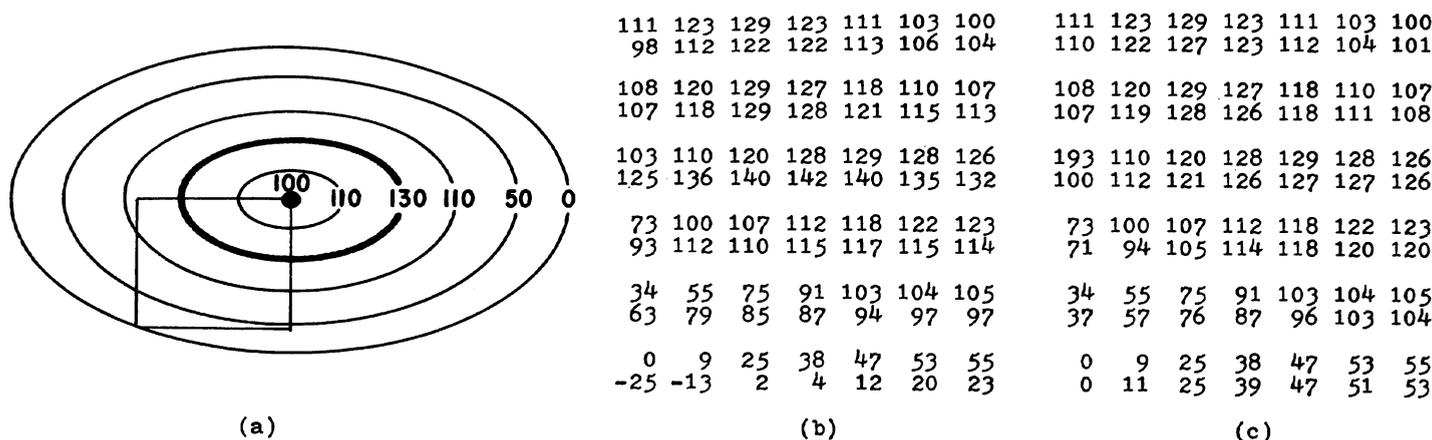


FIG. 5. (a) Contours indicating the shape and density variation of the reconstructed object. (b) True (above) and reconstructed (below) densities in the region marked by the rectangle in (a), obtained with just three shadowgraphs. (c) Same as (b), but using data from 12 shadowgraphs at 15° intervals.

corresponding to the projection on the major axis. The scanning interval was $a = 0.1$. The reconstructed density distribution showed a reasonable approximation to the original, as shown in Fig. 5(b). Fig. 5(c) shows how good the reproduction becomes when 12 shadowgraphs are used, scanned at $a = 0.1$; the error, in general, does not exceed 2%.

ADVANTAGES OVER THE FOURIER METHOD

The above examples clearly show that the convolution method has great potentialities for reconstruction of the density distribution of objects from transmission photographs, such as electron micrographs or x-radiographs. Apart from the increased accuracy of the CON method over the F.T. methods, perhaps its most important merit is the speed of computation. This speed arises principally because the computations are all one-dimensional summations in this method, and no double summations are needed as in the F.T. technique. With increasing resolution leading to more numbers of terms in each sum, the relative advantage of the convolution process would even be larger. This is shown clearly in Table 3, where FTP is seen to be 30-times slower than CON for $\theta_0 = 15^\circ$ and $a \sim 0.1$ for approximately equivalent accuracy. FTC is comparatively very slow, but gives slightly better reconstructions than FTP with a smaller number of shadowgraphs, although the FTC method is still less accurate than CON; the FTC method appears to have no advantage over FTP for small enough θ_0 and a . The very large computing times for FTC could be reduced by using fast algorithms such as those due to Cooley and Tukey [3], but the CON method is also capable of being

made much faster, for instance, by storing values of $1/p^2$ and a table of cosines.

In general, the CON method seems to be the best, both from the point of view of speed and of accuracy. Since the computing times in standard FORTRAN are only a few seconds for the two-dimensional section in the CON method described here ($a \sim 0.1$), much larger resolution could be obtained for three-dimensional objects with reasonable computing times by improved programming methods.

APPLICATION TO ELECTRON MICROGRAPHS

An important feature of the CON method is that it is completely operative in real space, and there is no problem analogous to the so-called "phase problem" in crystallography. In view of this, various ways of treating the data obtained from shadowgraphs of helical structures can be worked out using techniques analogous to those described in this paper. Thus, if we have a single shadowgraph (say electron micrograph) at right angles to the helical axis, over a complete repeat c along the helical axis with N repeating units, each of height $h = c/N$, then we have effectively N shadowgraphs at angles $j\theta_0$ ($\theta_0 = 2\pi/N, j = 1$ to N) of the unit lying between the sections $z = 0$ and $z = h$. If sections are taken at right angles to the axis at suitable intervals z_0 ($h = Mz_0, M = \text{an integer}$), each such section can be reconstructed from the corresponding data in the N shadowgraphs, and thus the full three-dimensional picture of the repeating unit of the helical structure can be obtained by the technique described above.

As we have recently shown (unpublished data), it seems to be possible to reconstruct objects of arbitrary size and shape when only partial data over a restricted range of angles is available. This possibility is of great importance to the problem of three-dimensional reconstruction from electron micrographs when it is not possible to rotate the stage by a full 180° without obstructing the beam, or in radiography where, for some reason, shadowgraphs cannot be obtained for certain orientations of the object.

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TABLE 3. Computing times (t) required using the different methods for a typical object used in the study

θ_0 (°)	a	t in seconds		
		CON	FTP	FTC
30	0.2	2.0	30.2	130
30	0.1	2.6	48.6	480
15	0.2	3.6	41.5	130
15	0.1	4.8	83.0	480
15	0.1	4.8	158.5*	487*

* $R_0 = 0.125$ for these values; $R_0 = 0.25$ for others.