Determination of the spatial orientation of arbitrarily arranged identical particles of unknown structure from their projections

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1. The problem formulated in the title of this paper is important for the theory of three-dimensional reconstruction, i.e., determination of the internal structure and external shape from their projections. Three-dimensional reconstruction methods have found extensive application in x-ray, NMR, and ultrasonic tomography of the human body and other objects, in electron microscopy of biomolecules, in radio astronomy, and in many other areas. The problem of three-dimensional reconstruction was formulated for the first time in 1917 by Radon.[1] In the 1970s, a number of authors found new ideas and algorithms for three-dimensional reconstruction.[2]

Let us consider a three-dimensional function $\rho(x, y, z)$ that describes the density distribution inside a body and the shape of the body. The two-dimensional (p) and one-dimensional (q) projections of this function in Cartesian coordinates are determined by the relations

$$\int \rho(x, y, z)\,dz = p(x, y), \quad \int p(x, y)\,dy = q(x) = \int \rho(x, y, z)\,dy\,dz. \tag{1}$$

In general, for the projection of the function $\rho(\mathbf{r})$ along an arbitrary unit vector τ in the plane $\mathbf{X}(x_1, x_2)$, $\mathbf{X} \perp \tau$ (Fig. 1) we have

$$\int \rho(\mathbf{r})\,d\tau = p_\tau(X) \tag{2}$$

Similarly, in the $\mathbf{X}$ plane we can project p in any one-dimensional projection q, prescribing the projection angle ψ (Fig. 1),

$$\int p(X)\,dx_{\parallel\psi} = q(x_{\perp\psi}). \tag{3}$$

we note that

$$\int \rho(\mathbf{r})\,d^3\mathbf{r} = \int p(x)\,d^2X = \int q(x)\,dx = V = \text{const}. \tag{4}$$

The algorithms of three-dimensional reconstruction allow the three-dimensional structure of a body ρ to be determined from a set of various projections p_{τ_i} (i = 1, 2, ..., n). It is understood here, however, that the mutual orientations of the projection directions τ_i are known, e.g., the body is rotated about an axis through particular intervals of angle.

However, there are problems in which the orientation of the vectors τ_i is not known in advance. Typical in this respect is the problem of investigating the structure of ribosome particles by means of electron microscopy. These identical asymmetric particles are deposited onto a substrate; in general, these particles take very different, arbitrary directions on the substrate. The electron-microscope photograph is a set of various projections p_{τ_i} of these particles, i.e., in essence is a set of projections of one body in unknown orientations. These orientations must be known in order to effect a three-dimensional reconstruction. Some approaches to problems of this kind have been considered in Ref. 3.

2. We consider the relationship between ρ, p, and q for arbitrary orientations and their corresponding Fourier transforms

$$\mathcal{F}\rho = \int \rho(\mathbf{r}) \exp 2\pi i(\mathbf{r}\cdot\mathbf{S})\,d^3\mathbf{r} = \Phi(\mathbf{S}), \tag{5}$$

where $\mathcal{F}$ is the Fourier operator, and $\mathbf{S}$ (X, Y, Z) is the vector of Fourier space (reciprocal space),

$$\mathcal{F}p_\tau = \int p(X_{\perp\tau}) \exp 2\pi i(X\cdot S_{\perp\tau})\,d^2x = P[\mathbf{S}(X_1, X_2, 0)]. \tag{6}$$

Here $\mathbf{X}_1$ and $\mathbf{X}_2$ are the coordinates of the reciprocal space in the zero plane which is perpendicular to τ. Relation (6) is well known as the theorem of projections: the Fourier integral $\mathbf{P}(\mathbf{X}_1, \mathbf{X}_2)$ of the projection $p(x_1, x_2)$ (along τ) is the planar central (passing through $\mathbf{S} = 0$) cross section $\mathbf{P}(\mathbf{X}_1, \mathbf{X}_2, 0)$ of the three-dimensional distribution $\Phi(\mathbf{S})$ (3), perpendicular to τ.

Similarly, in accordance with (3), if in the plane $\mathbf{X}(\mathbf{X}_1, \mathbf{X}_2)$ and in the plane $\mathbf{S}(\mathbf{X}_1, \mathbf{X}_2)$ parallel to it we fix the rotation angle ψ that prescribes the direction of projection of a two-dimensional projection into a one-dimensional

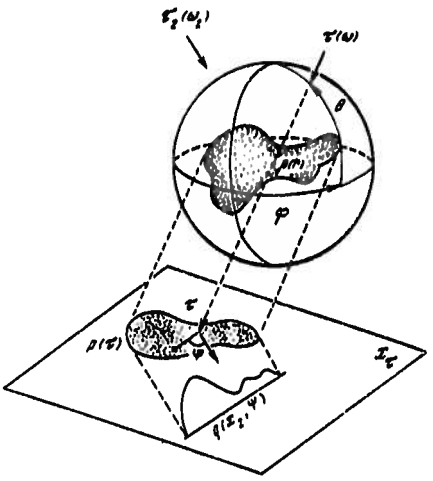

FIG. 1. A three-dimensional body ρ in the sphere of unit projection vectors τ, its two-dimensional projection $p(\tau)$ onto the plane X_τ, and the one-dimensional projection $q(\psi)$ of the function p onto the plane X.

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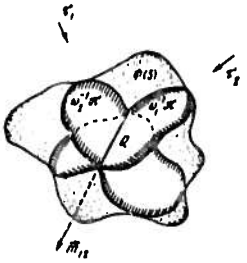

FIG. 2. The two-dimensional cross sections P_1 and P_2 of the three-dimensional Fourier transform Φ (S) have a straight intersection Q, the general one-dimensional transform m_{12}.

projection (Fig. 2), we would have

$$\mathcal{F}q = \int q(X_\psi)\exp 2\pi i(x_\psi X_\psi)\,dx_\psi = Q(X_\psi) = \Phi(X_\psi, 0, 0); \qquad (7)$$

i.e., the Fourier transform Q of the one-dimensional projection q is the one-dimensional central cross section of the transform Φ(5), which also lies in the plane of the two-dimensional transform P (6).

The method of determining the mutual orientations of the particles ρ from the projections p_l follows from Eqs. (2)–(7), and it can be implemented both in real space directly from the projections p and q and also in reciprocal space from their Fourier transforms P and Q.

Figure 1 shows the projection of a particle for one direction of projection τ, but by analogy one can construct the projections for any other directions τ_w.

The projection is prescribed by the Euler angles $\omega(\theta, \varphi, \psi)$, where θ and φ determine the direction of the unit projection vector τ and ψ determines the angular orientation of the projection p relative to ρ.

We denote in terms of π the plane Z = 0. We can then state that:

a) the two-dimensional Fourier transforms $\omega_1^{-1}\pi$ and $\omega_2^{-1}\pi$ intersect along the straight line $m_{12} = [\tau_1, \tau_2]$, in which lies the one-dimensional transform Q common to both of them;

b) accordingly, the projections p_1 and p_2 can be projected at different (proper) angles ψ_{1l} and ψ_{1j} into the one-dimensional projections $q_1(\psi_l)$ and $q_2(\psi_j)$ and have one common projection, viz., the projection onto the straight line of intersection of the planes $\omega_1^{-1}\alpha$ and $\omega_2^{-1}\alpha$, where α is the plane Z = 0, onto which our particle is projected (Fig. 3, see Figs. 1 and 2).

From a and b follows a simple prescription for finding the mutual orientations of arbitrarily arranged particles (i.e., transforms $\omega_1^{-1}\omega_k$, $2 \le k \le n$), either directly in real space or from their Fourier transforms P.

3. Reciprocal space. From the two-dimensional Fourier transforms P_{k_1} and P_{k_2} (projections p_{k_1}, p_{k_2}) we find in each of them, in some angular interval, a series of one-dimensional central cross sections $Q_{k_1,\psi_l}(x)$, $Q_{k_2,\psi_j}(x)$, $1 \le i, j \le n$, where ψ_l and ψ_j are the angles of rotation in the planes P_{k_1} and P_{k_2} (although these planes are canonically identified with the plane π, it is more convenient for us to represent them as being different). The equality of a pair $Q_{k_1,\psi_l}(x) = Q_{k_2,\psi_j}(x)$ determines two straight lines $l_{k_1k_2}$ in the plane P_{k_1} and $l_{k_2k_1}$ in the plane P_{k_2}, as well as the method of identifying these straight lines, so that the functions prescribed on them coincide. In practice, the common cross section can be found or chosen by minimization of the integral $\int |Q_{k_1,\psi_l}(x) - Q_{k_2,\psi_j}(x)]^2|dx$ [in the case of an asymmetric particle, one would naturally expect to find exactly one pair of coinciding crystal cross sections and also to find that $Q_{k_1,\psi_l}(x) \ne Q_{k_1,\psi_l}(-x)$].

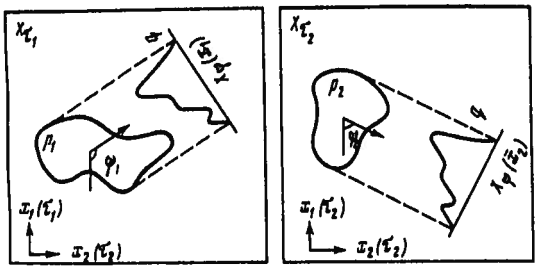

FIG. 3. Any two-dimensional projections p_1 and p_2 of an unknown three-dimensional function ρ have (each in its own plane) an identical (common) one-dimensional projection q at some angles ψ_1 and ψ_2.

Lemma. The arrangement of three (or more) planes (nonintersecting) can be determined unique to within the motion or mirror symmetry in space if:

1) on each plane are known straight lines along which other planes should interest, and;

2) a method is given for identifying the respective straight lines on different planes ($l_{k_1k_2}$ on P_{k_1} and $l_{k_2k_1}$ on P_{k_2}).

It can be assumed that ω_1 is an identify transformation and we must find $\omega_2, \ldots, \omega_n$. According to the lemma, we can find the planes $\pi, \omega_2^{-1}\pi, \ldots, \omega_n^{-1}\pi$ to within the mirror symmetry relative to π. The transformation ω_k^{-1} is now determined from the condition that it takes the plane π and the straight line l_{k_1} on it into the plane $\omega_k^{-1}\pi$ with the given straight line $l_{1k} = \pi \cap \omega_k^{-1}\pi$ on it (the functions on the straight lines l_{k1} and l_{1k} are identified in this case).

We note that the vectors τ_l are easily found if we proceed from the vectors $m_{j_1j_2}$ (on which the straight lines are drawn; see point *a*) since the vector τ_l is proportional to $[m_{1j}, m_{1k}]$.

4. Real space. On each of the projections p_1, p_2 we fix a proper polar system of coordinates (Fig. 3). In each of them we find on some angular interval a set of one-dimensional projects q_1,ψ_l, q_2,ψ_j. The equality of a pair, $q_1,\psi_l = q_2, \psi_m = q_{12}$, determines on each of the projections the straight lines, n_{12} and n_{21}, which are prescribed on them by their proper angles $\psi_l = \psi_{12}$ and $\psi_m = \psi_{21}$. By selecting and finding the common projection q_{12}, we can minimize the integral $\int |q_{1l} - q_{2j}|^2 dx$. Upon adding a third projection, in the same way we can find a straight line n_{13} with its proper angle ψ_{13} on p_1, a straight line n_{23} with its angle ψ_{23} on p_2, and on the third projection in its coordinate system we can find the straight lines n_{31} with the angle ψ_{31} and n_{32} with the angle ψ_{32}.

The polar coordinates with variable angles ψ in each of the projections were chosen arbitrarily, but despite this circumstance, the differences

$$\psi_{12} - \psi_{13}, \quad \psi_{21} - \psi_{23}, \quad \psi_{31} - \psi_{32} \qquad (8)$$

are determined invariantly and are the angles between the straight lines of intersection of each plane by the other two planes.

As in Sec. 3, we need only use the lemma.

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Recovery of profiles of damaged regions of discontinuity in thin subsurface layers from x-ray diffraction data

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X-ray diffraction methods, originating from the investigations carried out by Burgeat and Taupin et al.,[1-4] are used extensively in studying damaged regions of a crystal structure close to the surface which occur by ion implantation, by a process of diffusion, and by other destructive effects. This leads to a change in interplanar distances and to partial amorphization. For the analysis of the x-ray diffraction curves, Burgeat and Taupin[1] used the Tokagi–Topen equations, whereby employing the dynamic approximation, the dependence of interplanar distances on the nonuniform distribution of the impurities near to the surface was calculated. In the diffraction from thin layers, the weak scattering is described by a simple kinematic approximation which was studied in Refs. 5-7. This circumstance made it possible not only to find such integral quantities as the depth of the affected layer, the average levels of amorphization, and changes in interplanar distances[5] but also to reconstruct in detail the structure of the layer directly contiguous to the damaged region.[7]

Opportunities for investigated damaged regions in crystal structures have recently increased greatly due to the use of triple crystal x-ray diffraction (TCD).[8-11] In the TCD method, because of the ability to resolve the diffuse scattering, precise measurements of rocking curves are possible at very large angular deviations from the Bragg position. Here the extent of spatial resolution increases considerably and in investigations of Refs. 12-13 damaged layers, which were only a few monolayers thick, were studied by TCD; here the deviation from the Bragg angle exceeded the width of the rocking curve almost 1000 times. Diffraction at such large angular deviations, which was studied in Refs. 11-13, was given the name "asymptotic Bragg diffraction" (ABD).

The kinematic approximation can be used for the analysis of the diffraction from thin layers. However, since in x-ray diffraction experiments only the intensities are measured and all the phase information is lost, the process of recovering the scattering characteristics of the crystal structure from the rocking curve leads to more than one solution. The fact of this ambiguity of solution is well established but the matter of the degree of ambiguity and how to find the equivalent solutions have been virtually unexplored. Afanas'ev et al.[13] have shown that in several cases there exist at least two different, but equivalent from the point of view of diffraction intensity, solutions. For a damaged layer N monolayers thick, in the absence of surface relaxation, the two equivalent sets of Debye–Waller layer factors V_n, $\tilde{V}_n$, $n = 1, \ldots, N$ are related by the equation

$$\tilde{V}_n = 1 - V_{N-n+1}, \quad n = 1, \ldots, N. \tag{1}$$

In the present study we solve the problem of reconstituting all the equivalent solutions for the scattering characteristics of damaged layers of crystals under conditions of asymptotic Bragg diffraction.

The amplitude of the diffraction from a damaged layer N monolayers thick for the case of a symmetric reflection can be expressed as the sum of the amplitudes from individual monolayers:

$$A_N(\theta) = \frac{\pi f_h(\theta)}{\sin\theta_B} \sum_{n=1}^{N} \exp(-W_n + i\varphi_n + iqn),$$
$$q = 2\pi \operatorname{ctg}\theta_B \Delta\theta, \quad \Delta\theta = \theta - \theta_B, \quad \varphi_n = 2\pi \sum_{m=n+1}^{N+1} \frac{\Delta d_m}{d_0}, \quad n = 1, \ldots, N, \tag{2}$$

where θ is the angle of incidence, θ_B is the Bragg angle, $\Delta\theta$ is the angular deviation from the Bragg angle, $\exp(-W_n)$ is the Debye–Waller factor for the n-th layer, Δd_n is the difference between the n-th interplanar distance and the first, d_0 is the interplanar distance in the ideal crystal, $f_h(\theta)$ is the h-Fourier component of the polarizable portion of the unit cell which includes the scattering structure factor.

We restrict the analysis to the case where $\Delta\theta \gg \theta_0$, where θ_0 is the Darwin "plateau." We can then write amplitude of the diffraction from the undamaged crystal in the kinematic approximation

$$A_0(\theta) = \frac{\pi f_h(\theta)}{\sin\theta_B} \frac{\exp(iq(N+1))}{1 - \exp(iq)}.$$

We also restrict the discussion to the case in which $\Delta\theta$ is small, i.e., $\Delta\theta \ll \theta_B$ [this condition has already been taken into account in Eq. (2) by disregarding the angular dependences of the Debye–Waller factors and phase dis-

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