

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

2.5.6.5. The method of back-projection

This method is also called the synthesis of projection functions. Let us consider a two-dimensional case and stretch along τ_{ψ_i} each one-dimensional projection L^i (Fig. 2.5.6.5) by a certain length b ; thus, we obtain the projection function

$$L^i(\mathbf{x}) = \frac{1}{b} L^i(x_i) \cdot 1(\tau_i). \quad (2.5.6.13)$$

Let us now superimpose h functions L^i

$$\sum_{i=1}^h L^i(\mathbf{x}) = \Sigma_2(\mathbf{x}). \quad (2.5.6.14)$$

The continuous sum over the angles of projection synthesis is

$$\begin{aligned} \Sigma_2(\mathbf{x}) &= \int_0^\pi L(\psi, \mathbf{x}) \, d\psi = \rho_2(\mathbf{x}) * |\mathbf{x}|^{-1} \\ &\simeq \sum_{i=1}^h L^i = \rho_2(\mathbf{x}) + B(1); \end{aligned} \quad (2.5.6.15)$$

this is the convolution of the initial function with a rapidly falling function $|\mathbf{x}|^{-1}$ (Vainshtein, 1971*b*). In (2.5.6.15), the approximation for a discrete set of h projections is also written. Since the function $|\mathbf{x}|^{-1}$ approaches infinity at $x = 0$, the convolution with it will reproduce the initial function $\rho(\mathbf{x})$, but with some background B decreasing around each point according to the law $|\mathbf{x}|^{-1}$. At orthoaxial projection the superposition of cross sections $\varphi_2(\mathbf{x}, z_k)$ arranged in a pile gives the three-dimensional structure φ_3 .

Radon operator. Radon (1917; see also Deans, 1983) gave the exact solution of the problem of reconstruction. However, his mathematical work was for a long time unknown to investigators engaged in reconstruction of a structure from images; only in the early 1970s did some authors obtain results analogous to Radon's (Ramachandran & Lakshminarayanan, 1971; Vainshtein & Orlov, 1972, 1974; Gilbert, 1972*a*).

The convolution in (2.5.6.15) may be eliminated using the Radon integral operator, which modifies projections by introducing around each point the negative values which annihilate on superposition the positive background values. The one-dimensional projection modified with the aid of the Radon operator has the form

$$\tilde{L}(x_\psi) = \frac{1}{2\pi^2} \int_0^\infty \frac{2L(x_\psi) - L(x_\psi + x'_\psi) - L(x_\psi - x'_\psi)}{x'^2_\psi} \, dx'_\psi. \quad (2.5.6.16)$$

Now $\varphi_2(\mathbf{x})$ is calculated analogously to (2.5.6.14), not from the initial projections L but from the modified projection \tilde{L} :

$$\varphi_2(\mathbf{x}) = \int_0^\pi \tilde{L}(\psi, \mathbf{x}) \, d\psi \simeq \sum_{i=1}^k \tilde{L}_i(\psi_i, \mathbf{x}). \quad (2.5.6.17)$$

The reconstruction of high-symmetry structures, in particular helical ones, by the direct method is carried out from one projection making use of its equivalence to many projections. The Radon formula in discrete form can be obtained using the double Fourier transformation and convolution (Ramachandran & Lakshminarayanan, 1971).

2.5.6.6. The algebraic and iteration methods

These methods have been derived for the two-dimensional case; consequently, they can also be applied to three-dimensional reconstruction in the case of orthoaxial projection.

Let us discretize $\varphi_2(\mathbf{x})$ by a net m^2 of points φ_{jk} ; then we can construct the system of equations (2.5.6.10).

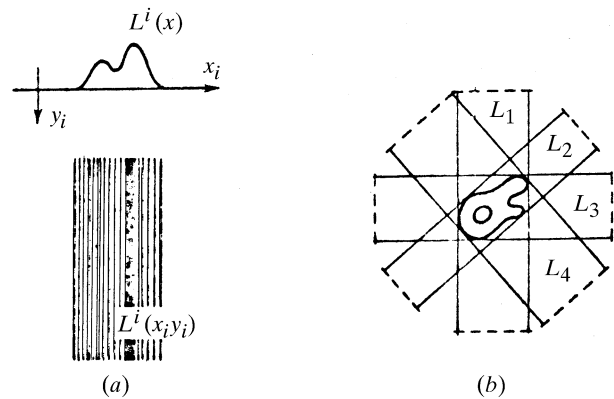


Fig. 2.5.6.5. (a) Formation of a projection function; (b) superposition of these functions.

When h projections are available the condition of unambiguous solution of system (2.5.6.10) is: $h \geq m$. At $m \simeq (3-5)h$ we can, in practice, obtain sufficiently good results (Vainshtein, 1978).

Methods of reconstruction by iteration have also been derived that cause some initial distribution to approach one $\varphi_2(\mathbf{x})$ satisfying the condition that its projection will resemble the set L^i . Let us assign on a discrete net φ_{jk} as a zero-order approximation the uniform distribution of mean values (2.5.6.7)

$$\varphi_{jk}^0 = \langle \varphi \rangle = \Omega/m^2. \quad (2.5.6.18)$$

The projection of the q th approximation φ_{jk}^q at the angle φ_i (used to account for discreteness) is L_n^{iq} .

The next approximation φ_{jk}^{q+1} for each point jk is given in the method of 'summation' by the formula

$$\varphi_{jk}^{q+1} = \max[\varphi_{jk}^q + (L_n^i - L_n^{i,q})/N_{L_n}^i; 0], \quad (2.5.6.19)$$

where $N_{L_n}^i$ is the number of points in a strip of the projection L_n^i . One cycle of iterations involves running φ_{jk}^q around all of the angles ψ_j (Gordon *et al.*, 1970).

When carrying out iterations, we may take into account the contribution not only of the given projection, but also of all others. In this method the process of convergence improves. Some other iteration methods have been elaborated (Gordon & Herman, 1971; Gilbert, 1972*b*; Crowther & Klug, 1974; Gordon, 1974).

2.5.6.7. Reconstruction using Fourier transformation

This method is based on the Fourier projection theorem [(2.5.6.3)–(2.5.6.5)]. The reconstruction is carried out according to scheme (2.5.6.6) (DeRosier & Klug, 1968; Crowther, DeRosier & Klug, 1970; Crowther, Amos *et al.* 1970; DeRosier & Moore, 1970; Orlov, 1975). The three-dimensional Fourier transform $\mathcal{F}_3(\mathbf{u})$ is found from a set of two-dimensional cross sections $\mathcal{F}_2(\mathbf{u})$ on the basis of the Whittaker–Shannon interpolation. If the object has helical symmetry (which often occurs in electron microscopy of biological objects, *e.g.* on investigating bacteriophage tails, muscle proteins) cylindrical coordinates are used. Diffraction from such structures with c periodicity and scattering density $\varphi(r, \psi, z)$ is defined by the Fourier–Bessel transform:

$$\begin{aligned} \Phi(R, \Psi, Z) &= \sum_{n=-\infty}^{+\infty} \exp\left[in\left(\Psi + \frac{\pi}{2}\right)\right] \int_0^\infty \int_0^{2\pi} \int_0^l \varphi(r, \psi, z) \\ &\quad \times J_n(2\pi r R) \exp[-i(n\psi + 2\pi z Z)] r \, dr \, d\psi \, dz \\ &= \sum_n G_n(R, Z) \exp\left[in\left(\Psi + \frac{\pi}{2}\right)\right]. \end{aligned} \quad (2.5.6.20)$$