

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

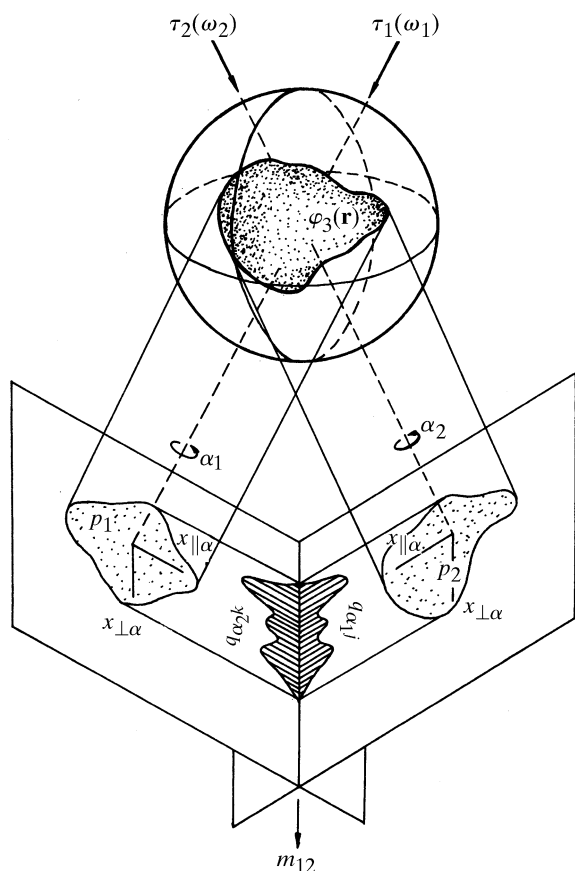


Fig. 2.5.6.6. Relative position of the particle and planes of projection.

accordance with Lemma 1, there exists a one-dimensional projection, common for both p_1 and p_2 , which determines angles α_{1j} and α_{2k} along which p_1 and p_2 should be projected for obtaining the identical projection q_{12} (Fig. 2.5.6.5). Comparing $q_{1, \alpha_{1j}}$ and $q_{2, \alpha_{2k}}$ and using the minimizing function

$$D(1,2) = |q_{1, \alpha_{1j}} - q_{2, \alpha_{2k}}|^2 \quad (2.5.6.30)$$

it is possible to find such a common projection q_{12} . (A similar consideration in Fourier space yields Q_{12} .)

The mutual spatial orientations of any three non-coplanar projection vectors τ_1, τ_2, τ_3 can be found from three different two-dimensional projections p_1, p_2 and p_3 by comparing the following pairs of projections: p_1 and p_2, p_1 and p_3 , and p_2 and

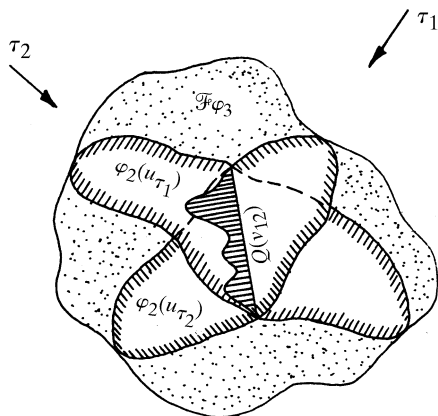


Fig. 2.5.6.7. Section of a three-dimensional Fourier transform of the density of the particles, corresponding to plane projections of this density.

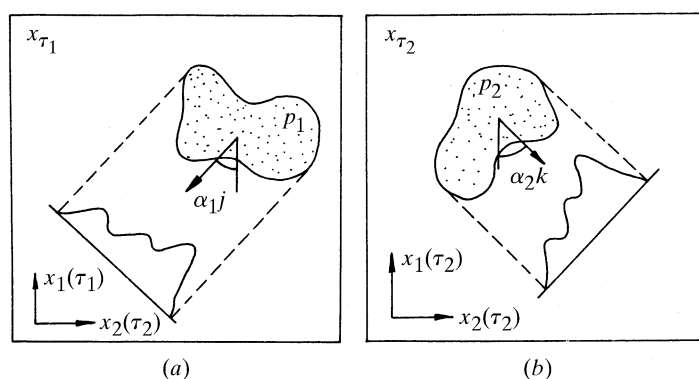


Fig. 2.5.6.8. Plane projections of a three-dimensional body. The systems of coordinates in planes (a) and (b) are chosen independently of one another.

p_3 , and by determining the corresponding q_{12}, q_{13} and q_{23} . The determination of angles ω_1, ω_2 and ω_3 reduces to the construction of a trihedral angle formed by planes h_{12}, h_{13} and h_{23} . Then the projections $p_i(\omega_i)$ with the known ω_i ($i = 1, 2, 3$) can be complemented with other projections ($i = 4, 5, \dots$) and the corresponding values of ω can be determined. Having a sufficient number of projections and knowing the orientations ω_i , it is possible to carry out the 3D reconstruction of the object [see (2.5.6.27); Orlov, 1975; Vainshtein & Goncharov, 1986a; Goncharov *et al.*, 1987].

2.5.7. Direct phase determination in electron crystallography (D. L. DORSET)

2.5.7.1. Problems with 'traditional' phasing techniques

The concept of using experimental electron-diffraction intensities for quantitative crystal structure analyses has already been presented in Section 2.5.4. Another aspect of quantitative structure analysis, employing high-resolution images, has been presented in Sections 2.5.5 and 2.5.6. That is to say, electron micrographs can be regarded as an independent source of crystallographic phases.

Before direct methods (Chapter 2.2) were developed as the standard technique for structure determination in small-molecule X-ray crystallography, there were two principal approaches to solving the crystallographic phase problem. First, 'trial and error' was used, finding some means to construct a reasonable model for the crystal structure *a priori*, e.g. by matching symmetry properties shared by the point group of the molecule or atomic cluster and the unit-cell space group. Secondly, the autocorrelation function of the crystal, known as the Patterson function (Chapter 2.3), was calculated (by the direct Fourier transform of the available intensity data) to locate salient interatomic vectors within the unit cell.

The same techniques had been used for electron-diffraction structure analysis (nowadays known as *electron crystallography*). In fact, advocacy of the first method persists. Because of the perturbations of diffracted intensities by multiple-beam dynamical scattering (Chapter 5.2), it has often been suggested that trial and error be used to construct the scattering model for the unit crystal in order to test its convergence to observed data after simulation of the scattering events through the crystal. This indirect approach assumes that no information about the crystal structure can be obtained directly from observed intensity data. Under more favourable scattering conditions nearer to the kinematical approximation, *i.e.* for experimental data from thin crystals made up of light atoms, trial and error modelling, simultaneously minimizing an atom-atom nonbonded potential function with the crystal-