

2.5. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY IN STRUCTURE DETERMINATION

atomic positions to a greater accuracy, since practically the whole of reciprocal space with 1.0–0.4 Å resolution is used and the three-dimensional arrangement of atoms is calculated. At the same time, in electron microscopy, owing to the peculiarities of electron optics and the necessity for an objective aperture, the image of the atoms in a crystal $\psi'(\mathbf{x}) * A(\mathbf{x})$ is a convolution, with the aperture function blurring the image up to 1.5–2 Å resolution. In practice, in TEM one obtains only the images of the heaviest atoms of an object. However, the possibility of obtaining a direct image of a structure with all the defects in the atomic arrangement is the undoubted merit of TEM.

2.5.5. Image reconstruction³

BY B. K. VAINSHTEIN

2.5.5.1. Introduction

In many fields of physical measurements, instrumental and informative techniques, including electron microscopy and computational or analogue methods for processing and transforming signals from objects investigated, find a wide application in obtaining the most accurate structural data. The signal may be radiation from an object, or radiation transmitted through the object, or reflected by it, which is transformed and recorded by a detector.

The image is the two-dimensional signal $I(xy)$ on the observation plane recorded from the whole three-dimensional volume of the object, or from its surface, which provides information on its structure. In an object this information may change owing to transformation of the scattered wave inside an instrument. The real image $J(xy)$ is composed of $I(xy)$ and noise $N(xy)$ from signal disturbances:

$$J(xy) = I(xy) + N(xy). \quad (2.5.5.1)$$

Image-reconstruction methods are aimed at obtaining the most accurate information on the structure of the object; they are subdivided into two types (*Picture Processing and Digital Filtering*, 1975; Rozenfeld, 1969):

(a) Image restoration – separation of $I(xy)$ from the image by means of compensation of distortions introduced in it by an image-forming system as well as by an account of the available quantitative data reflecting its structure.

(b) Image enhancement – maximum exclusion from the observed image $J(xy)$ (2.5.5.1) of all its imperfections $N(xy)$ from both accidental distortions in objects and various ‘noise’ in signals and detector, and obtaining $I(xy)$ as the result.

These two methods may be used separately or in combination.

The image should be represented in the form convenient for perception and analysis, e.g. in digital form, in lines of equal density, in points of different density, in half-tones or colour form and using, if necessary, a change or reversal of contrast.

Reconstructed images may be used for the three-dimensional reconstruction of the spatial structure of an object, e.g. of the density distribution in it (see Section 2.5.6).

This section is connected with an application of the methods of image processing in transmission electron microscopy (TEM). In TEM (see Section 2.5.2), the source-emitted electrons are transmitted through an object and, with the aid of a system of lenses, form a two-dimensional image subject to processing.

Another possibility for obtaining information on the structure of an object is structural analysis with the aid of electron

diffraction – EDSA. This method makes use of information in reciprocal space – observation and measurement of electron-diffraction patterns and calculation from them of a two-dimensional projection or three-dimensional structure of an object using the Fourier synthesis. To do this, one has to find the relative phases of the scattered beams.

The wavefunction of an electron-microscopic image is written as

$$\psi_1 = \mathcal{F}^{-1} T \mathcal{F} q \psi_0. \quad (2.5.5.2)$$

Here ψ_0 is the incident plane wave. When the wave is transmitted through an object, it interacts with the electrostatic potential $\varphi(\mathbf{r})$ [$\mathbf{r}(xyz)$ is the three-dimensional vector in the space of the object]; this process is described by the Schrödinger equation (Section 2.5.2.1). As a result, on the exit surface of an object the wave takes the form $q\psi_0(\mathbf{x})$ where q is the transmission function and \mathbf{x} is the two-dimensional vector $\mathbf{x}(xy)$. The diffraction of the wave $q\psi_0$ is described by the two-dimensional Fourier operator:

$$\mathcal{F} q = Q(\mathbf{u}) = \int q(\mathbf{x}) \exp[2\pi i(\mathbf{x}\mathbf{u})] d\mathbf{x}. \quad (2.5.5.3)$$

Here, we assume the initial wave amplitude to be equal to unity and the initial phase to be zero, so that $q\psi_0 = q$, which defines, in this case, the wavefunction in the back focal plane of an objective lens with the reciprocal-space coordinates $\mathbf{u}(u, v)$. The function Q is modified in reciprocal space by the lens transfer function $T(\mathbf{u})$. The scattered wave transformation into an image is described by the inverse Fourier operator $\mathcal{F}^{-1} T Q$.

The process of the diffraction $\mathcal{F} q \psi_0 = Q$, as seen from (2.5.5.1), is the same in both TEM and EDSA. Thus, in TEM under the lens actions $\mathcal{F}^{-1} T Q$ the image formation from a diffraction pattern takes place with an account of the phases, but these phases are modified by the objective-lens transfer function. In EDSA, on the other hand, there is no distorting action of the transfer function and the ‘image’ is obtained by computing the operation $\mathcal{F}^{-1} Q$.

The computation of projections, images and Fourier transformation is made by discretization of two-dimensional functions on a two-dimensional network of points – pixels in real space $\mathbf{x}(x_j, y_k)$ and in reciprocal space $\mathbf{u}(u_m, v_n)$.

2.5.5.2. Thin weak phase objects at optimal defocus

The intensity distribution $I(xy) \sim |\psi_1|^2$ of an electron wave in the image plane depends not only on the coherent and inelastic scattering, but also on the instrumental functions. The electron wave transmitted through an object interacts with the electrostatic potential $\varphi(\mathbf{r})$ which is produced by the nuclei charges and the electronic shells of the atoms. The scattering and absorption of electrons depend on the structure and thickness of a specimen, and the atomic numbers of the atoms of which it is composed. If an object with the three-dimensional distribution of potential $\varphi(\mathbf{r})$ is sufficiently thin, then the interaction of a plane electron wave ψ_0 with it can be described as the interaction with a two-dimensional distribution of potential projection $\varphi(\mathbf{x})$,

$$\varphi(\mathbf{x}) = \int_0^b \varphi(\mathbf{r}) dz, \quad (2.5.5.4)$$

where b is the specimen thickness. It should be noted that, unlike the three-dimensional function of potential $\varphi(\mathbf{r})$ with dimension $[M^{1/2} L^{3/2} T^{-1}]$, the two-dimensional function of potential projection $\varphi(\mathbf{x})$ has the potential-length dimension $[M^{1/2} L^{1/2} T^{-1}]$ which, formally, coincides with the charge dimension. The transmission function, in the general case, has the form

³ Questions related to this section may be addressed to Dr P. A. Penczek (see list of contributing authors).