THE PRINCIPLES OF TRANSMISSION ELECTRON MICROSCOPY
IMAGE FORMATION

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ABSTRACT

The knowledge of the theoretical principles of image formation is crucial for understanding what we observe in transmission electron microscope. Two processes mainly determine the image contrast: the electron interaction with specimen and the electron-optical imaging process including the microscope aberrations. Multislice calculation and contrast transfer function are main tools used for interpretation of high-resolution transmission electron microscopy images.

1. INTRODUCTION

To obtain an enlarged image it is necessary to have object, probing beam, and converging lenses. Probably, Zaccharias Janssen and his son Hans [1], in about 1590, discovered that it is possible to observe enlarged (20 times in this case) images of small opaque objects with several glass lenses in a tube. Further improvement introduced by Antony van Leeuwenhoek [2] and Robert Hooke [3] provided resolution of optical microscopes to 1 micron.

2. HISTORICAL BACKGROUND

In 1873, Ernst Abbe published his famous work on the theory of the microscope. He made clear the difference between magnification and resolution. In conclusion, he gave the sine condition formula for determining resolving power of microscope. This formula telling that the resolving power is proportional to the wavelength and inversely proportional to numerical aperture, which is a product of a refraction index and sinus of half-angle of the light cone used for image formation. According to this the physical resolution for light microscopes have been limited to 200 nm.

In 1927, Hans Bush showed that a coil, through which an electrical current flows, could focus an electron beam (see computer animation [4]). In 7th April 1931, Ernst Ruska and Max Knoll obtained first enlarged (17.4 times in this case) electron image with an instrument consisting of two magnetic lenses and with a use of electrons as a probing beam. In 1923 Prince Louis de Broglie postulated that ordinary matter has wave-like properties. Four years later, C. J. Davisson and L. H. Germer confirmed experimentally the wave nature of the electrons and proved that electron wavelength depends inversely proportional to the momentum. These facts opened a way for development of electron optic instruments with spatial resolution, according to sine condition, of several picometers, because a
wavelength for electron beam with energy of hundreds keV is of few picometers. Up to now this theoretical limit is far from the magnification power of the present days TEM. Mainly that situation is result of lenses aberrations and electron beam incoherency.

3. IMAGE FORMATION

Among aberrations a most important rule plays the spherical aberration, which is the inability of a lens to focus all incident beams from a point source to a point (see computer animation [5]). Electrons entering the lens at a larger angle are converged more strongly then the electrons close to the lens axis (paraxial electrons) and therefore electrons originating from a point are imaged at a disc instead to a point. The disc diameter increases with the half-angle cone of electron entering the lens resulting in lowering resolution. It was shown that in the case of single magnetic lenses spherical aberration has a value around 1 mm [6]. It means that electrons emitted in a cone with 1° half angle will be focused to a disc with 0.2 nm (2 Å) diameter. From other side, according to Abbe’s sine condition, resolution increases with increasing half-angle. In 1949, Scherzer found optimal values of resolution, focal length (Scherzer defocus), half angle for given spherical aberration and electron beam wavelength. For example in the case of spherical aberration 1 mm and 200 kV accelerating voltage, resolution is 0.23nm and half-angle is 0.62°. Unfortunately Scherzer in his calculation did not include incoherence of electron wave, which additionally destructs image quality in similar way like spherical aberration.

The focal length of a magnetic lens depends on the energy of electrons. The total dispersion of the energy of electrons (temporal coherence) is combined by several contributions: the initial energy dispersion ΔE when the electrons leave the cathode, variations of the accelerating voltage ΔV, fluctuation of the lens current ΔI and the energy loss resulting from the interactions of the electron with the specimen. This energy dispersion causes a difference in the focal length, and in consequence a point in the object plane is imaged as a disc of the radius proportional to coefficient of chromatic aberration. Finally, image of transparent object depends on convergence of illuminated wave (spatial coherence). In the ideal situation, all electrons entering a sample should have the same velocity (magnitude and direction) or in another words; a wave front of the incident beam should be planar. Any deviation from the ideal condition results in spread of image sharpens.

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To understood theory of image formation in TEM, it is necessary to introduce some elements of quantum mechanics. The first element is an electron wave function (EWF), which gives amplitude and phase of an electron wave in given point and time. The square of EWF represents the intensity of electron beam. The second element is an atomic form factor (AFF), which described interaction of electron with a single atom A. The AFF gives amplitude of electron wave emitted (scattered) at the angle θ in respect to the direction of incident wave. Electron is scattered on electric field of nucleus and electron “clouds” around it. The AFF strongly depend on atomic number Z (number of protons) of an atom. The interaction of electrons with specimen is a subject of solving Schrödinger equation for fast electrons and potential superposed from AFF of individual atoms. In 1959, J. M. Cowley and A. F. Moodie invented commonly used a multislice method of calculating EWF on exit surface of specimen [7]. In this method specimen is cut in the direction perpendicular to the incident electron beam into slices of the thickness of the order of one atomic layer (about 1-2 Å). For EWF entering “top” plane of each slice a phase shift proportional to slice potential is introduced. Next, the EWF is propagated in the “layers” of vacuum on very small distances and under very small angles (Fresnel approximation). The obtained EWF is used as the input EWF for the next slice. This procedure is repeated to reach exit surface of the specimen.
Next element is a contrast transfer function (CTF), which describes modification of EWF performed by microscope optical system. CTF can be treated as a black box, which in the input has EWF exited specimen and on the output gives EWF at a screen.

Fig. 1 Multislice computer simulated HRTEM image of Cd\textsubscript{1-x}Mn\textsubscript{x}Te quantum well in <110> projection, the sample thickness increases vertically, Scherzer defocus=-43 nm, 200kV acceleration voltage, aperture radius 5 nm\textsuperscript{-1}, C\textsubscript{s}=1.0 mm, $\alpha=1$ mrad, focus spread =10 nm)
CTF taking into account all parameters related with the instrument: accelerating voltage (wavelength), spread of focus (temporary coherence), electron beam convergence (spatial coherence), spherical aberration, diameter of objective lens aperture (half-angle).

The simulation of TEM image is important, because contrast distribution can’t be directly interpreted as position of atomic positions. For an example let’s take a look for Fig. 1, where is presented a mosaic of computer simulated images of Cd$_{1-x}$Mn$_x$Te quantum well with trapezoid profile of Mn concentration $x$ [8]. Calculations were done for sample with increasing thickness (in vertical direction) and Mn concentration changing in horizontal direction.

![Fig. 2. Deformation determined from the simulated HRTEM image of Cd$_{1-x}$Mn$_x$Te quantum well](image)

Fig. 2 shows the result of the lattice deformation determined from the images. It is seen that for sample thickness up to 5 nm the maximums of contrast intensity correspond to positions of atomic column, but in the 5-9 nm range this is not true. Next region where atomic columns position overlapped white dots on image are between 9 and 14 nm thickness. In conclusion only experimental images obtained for the sample with thickness between 9 and 14 nm can been taken for quantitative measurement of Mn concentration.

Lately, computer aid method, based on a pair of strong hexapoles separated by a round doublet transfer lens is used for correction spherical and other aberrations [9, 10]. Initial experiments with the aberration corrected microscopes confirmed that it is possible to achieve resolution below 0.1 nm. It also opens way for possibilities for scanning techniques, like 3D reconstruction of atoms position in a sample. The idea of such measurement is presented on Fig. 3 [11]. Aberration corrected electron optical system allows to focused electrons to the probing “point” of 0.1 nm in size, and determine what kind of atom occupied this volume from measurement of scattering power of illuminated volume element.
Fig. 3. Schematically showed depth sectioning in the STEM. The impurity atoms (lighter) may be identified from the image or by spectroscopy and the entire specimen reconstructed at atomic resolution in 3D

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