Chapter 5
Calculation of Images of Thin Specimens

Abstract This chapter presents approximate methods of calculating transmission electron microscope images of thin specimens. The thickness of the specimen is ignored, which may be appropriate for very thin specimens. Multiple scattering is also generally ignored. This approach is intermediate between the transfer function (in previous chapters) and the multislice and Bloch wave methods (discussed in later chapters) and has the advantage of requiring much less computer time.

This chapter discusses the calculation of an electron microscope image neglecting the geometrical thickness of the specimen (i.e., very thin specimens). Many practical specimens are too thick for this type of calculation to be quantitatively correct. However, this approach can provide a qualitative insight into the structure in the image and it requires much less computer time. This type of image simulation is sometimes referred to as a phase grating approximation or a kinematical image approximation because it does not properly include the effects of multiple or plural scattering within the specimen. Calculation of the transmission function of thin specimens is also a necessary part of more advanced calculations including a realistic specimen thickness that will be considered in later chapters. In particular the calculation presented in this chapter will form a single slice of the multislice algorithm.

The kinetic energy of the imaging electrons in the electron microscope approaches their rest mass energy. A detailed quantum mechanical calculation of the motion of these electrons should properly be calculated using relativistic quantum mechanics (the Dirac equation with spin). As discussed in Sect. 2.3 the relativistic effects can be approximated by using the nonrelativistic Schrödinger equation (neglecting electron spin) with the relativistically correct wavelength and mass of the electron. This approximation is probably accurate enough at 100 keV but may be less accurate at 1 MeV. Nonrelativistic quantum mechanics is however dramatically easier to work with, and this approximation will be used here.
5.1 The Weak Phase Object

The primary interaction between the specimen and the imaging electrons is between the electrostatic potential of the specimen and the charge on the electron. The electrons traveling down the column of the microscope (before hitting the specimen) are a superposition of one or more plane waves. In the CTEM the incident electrons are primarily in a single plane wave and the STEM probe is a superposition of many plane waves (i.e., a spherically convergent probe). It suffices to consider the effect of the specimen on one plane wave. The wave function $\psi$ for one plane wave traveling along the optic axis in the $z$ direction is:

$$\psi(x) = \exp(2\pi i k_z z) = \exp\left(\frac{2\pi iz}{\lambda}\right),$$  \hspace{1cm} (5.1)

where $\lambda$ is the wavelength of the electron and $k_z = 1/\lambda$ is the propagation wave vector. The relativistic expression for the reciprocal of the electron wavelength in vacuum [see (2.5)] is:

$$k_z = \frac{1}{\lambda} = \frac{\sqrt{eV(2m_0c^2+eV)}}{hc},$$  \hspace{1cm} (5.2)

where $m_0$ is the rest mass of the electron, $c$ the speed of light in vacuum, $h$ Planck’s constant, and $eV$ is the kinetic energy of the electron in vacuum.

**Fig. 5.1** An incident (high energy) electron plane wave passing through the electrostatic potential $V_s$ of the specimen. The wave function is drawn as lines of constant phase, and the specimen is assumed to have a uniform constant potential. The electron wavelength is reduced by the positive potential inside the specimen. This drawing is not to scale.

The imaging electrons typically have a much higher energy than the electrons in the specimen. If the specimen is thin the imaging electrons pass through the specimen with only a small deviation in their path. This deviation can be approximated as a small change in wavelength of the electrons as they pass through the specimen (see Fig. 5.1). The specimen has a small electrostatic potential which influences the electron wavelength. If the potential inside the specimen is positive then the imaging electrons are accelerated inside the specimen giving them a smaller wavelength. If $eV_s$ is the additional electrostatic potential energy of the imaging