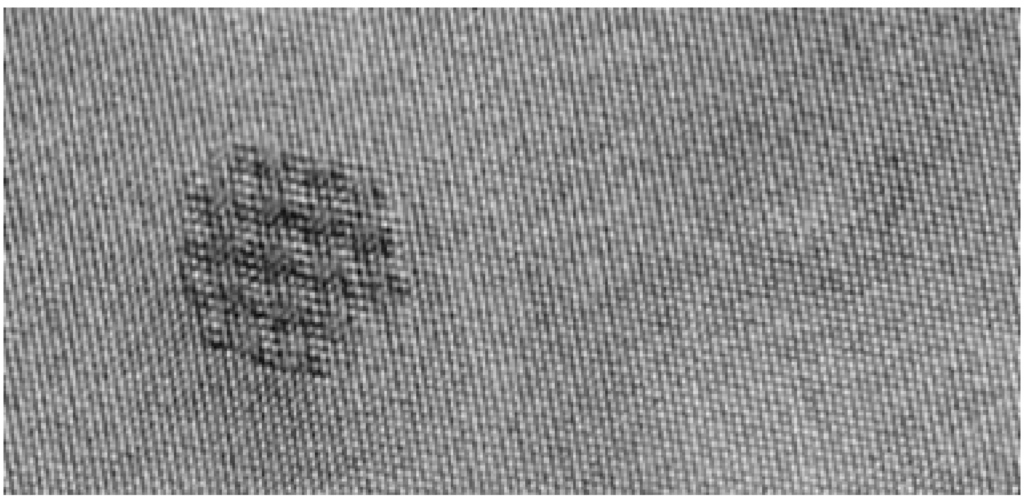
10. High-Resolution TEM Imaging



Spatial resolution is important for any microscopy. This chapter presents the theory, technique, and examples of achieving the ultimate resolution of a transmission electron microscope with the method of "high-resolution transmission electron microscopy." Recall (Sect. 2.3.3) that the HRTEM image is an interference pattern between the forward-scattered and diffracted electron waves from the specimen. Interference patterns require close attention to the phases of the waves. While the ray optics approach is useful for a few geometrical arguments, the most important issues in HRTEM are best understood in terms of the phase of the electron wavefront and how this phase is altered by the specimen and by the objective lens. The specimen itself is approximated as an object that provides phase shifts to the electron wavefront, sometimes in proportion to its scattering potential. The method of HRTEM also demands close attention to the performance of the objective lens and other characteristics of the microscope.

The physical optics theory presented in this chapter treats diffraction and microscopy in terms of phase shifts of wavefronts. Several elegant tools and models are provided. Unfortunately, simple and convenient models of lenses and especially the specimen are usually inadequate for interpreting real images from real specimens. For HRTEM to provide information on atom arrangements in a material, computer simulations of the image are usually required. Mature codes for the analysis of HRTEM images are available, and this chapter provides an overview of how they work and how they are used. Several examples are presented to show the reader what types of research problems are possible with high-resolution imaging. These were chosen in part to show how much trust can be placed in simple interpretations of HRTEM images.

Finally, the method of Z-contrast imaging is described in Sect. 10.6. Although Z-contrast imaging offers atomic resolution, it is fundamentally different from HRTEM because it is based on incoherent, rather than coherent scattering.

10.1 Huygen's Principle

10.1.1 Wavelets from Points in a Continuum

This chapter uses the "physical optics" approach to electron diffraction. It is based on Huygen's principle of physical optics, which was developed to understand the diffraction of light. It is much older than the electron wave mechanics of Chaps. 3–5. Up to now, most of our effort has been to understand electrons in periodic or heterogeneous media, for which we worked with electron wavelets scattered by individual atoms. The approach used in Sects. 9.4 and 9.5 was a departure from this emphasis on individual atoms. In these sections, the intensity of the scattering was calculated from heterogeneities in a density function (Sect. 9.5.4). Now we return to scattered wavelets, but we treat the medium as a continuum. The obvious way to do this is to set the potential $U(\boldsymbol{r}')$ equal to a constant, U, in the Schrödinger equation itself:

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi + U\,\Psi = E\,\Psi \ , \tag{10.1}$$

which has the plane wave solution, normalized to volume, V:

$$\Psi(x,y,z) = \frac{1}{\sqrt{V}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \ , \tag{10.2}$$

where:

$$\boldsymbol{k} = k_x\widehat{\boldsymbol{x}} + k_y\widehat{\boldsymbol{y}} + k_z\widehat{\boldsymbol{z}} \ , \tag{10.3}$$

$$\boldsymbol{r} = x\widehat{\boldsymbol{x}} + y\widehat{\boldsymbol{y}} + z\widehat{\boldsymbol{z}} \ , \tag{10.4}$$

$$k = |\boldsymbol{k}| = \sqrt{k_x^2+k_y^2+k_z^2} = \sqrt{\frac{2m\,(E-U)}{\hbar^2}} \ . \tag{10.5}$$