13

Diffracted Beams

CHAPTER PREVIEW

In Chapter 11 we discussed why diffraction occurs; in this chapter we give a more detailed mathematical treatment. It may be more detailed than you need at this stage. Diffraction is one of those phenomena that lends itself directly to a detailed mathematical modeling, but there is a danger: *don't become so engrossed in the math that you miss the principles involved; conversely, don't ignore the subject because it is mathematically daunting!* The topic of this chapter is one which causes major problems for many microscopists. The treatment we will follow is known as the 'dynamical theory.' Later we will make some gross simplifications, partly because this is instructive and partly because these simplifications do apply to some important special cases; the kinematical approximation is one such simplification. Many other texts begin with the so-called 'kinematical' treatment and then advance to the more realistic, more general dynamical case. We will not do this but we will introduce the words and assumptions in Chapter 27.

The main principle of dynamical scattering was discussed in Chapter 11: an electron beam can be strongly scattered by a set of planes of atoms. When these planes are suitably oriented with respect to the beam, they produce a diffracted beam. This diffracted beam can then be rediffracted by a second set of planes in the same specimen, and so on. The physical reason for this repeated, or dynamical, diffraction, is that the electron beam and the atoms in the crystal interact strongly due to Coulomb forces. (X-rays are much less strongly affected by atoms and are thus more likely to be only scattered once, i.e., kinematical scattering.) This repeated scattering between the diffracted beams and the direct beam is the persistent topic of this chapter.

If you have a strong background in physics, you may find the simplifications used in this treatment somewhat unsatisfactory because we should be considering Bloch waves in a periodic object (our crystalline sample). We will discuss the analysis of Bloch waves in Chapter 14. Remember that *experimentally* we will associate arrays of spots in DPs with Bragg beams. Then we will relate these beams to images. We see both images and 'beams' on the screen of the TEM.

In future chapters, we will always discuss the thickness of the specimen in terms of the *extinction distance*. This is a term which we introduce here as a *characteristic length* for a *particular diffracted beam*. So, even in a rigorous Bloch-wave analysis, it is still important to understand the origin of the terminology introduced here (Table 13.1). Remember that the reason for looking at these equations is that they are directly useful to you when you are using the microscope, because they *describe* both the intensity of the electron beam in DPs and the contrast seen in TEM images of crystalline materials.

13.1 WHY CALCULATE INTENSITIES?

In this chapter, we will consider only scattering from perfect, defect-free, crystalline materials.

Ultimately we want to understand the images we see in the microscope. The detail we see in these images is determined by the intensity of the electron beam or beams and this varies for different positions in the image. Our motivation for calculating the intensity of diffracted beams is, therefore, to understand contrast features in TEM images.

In general, the analysis of the intensity of diffracted beams in the TEM is not simple because a beam which is diffracted once will easily be rediffracted. We call this repeated diffraction 'dynamical diffraction.' In a perfect crystal, imagine dividing the crystal into two halves, one

TABLE 13.1 Terminology and Notation

Ψ^T at P	The *total* wave function of the electron beam as measured at a point P at the bottom of the specimen. This wave function is a solution to the Schrödinger equation both inside and outside the specimen. What interests us is not Ψ^T but $\phi_{\mathbf{g}}$ and $\phi_{\mathbf{0}}$
$\phi_{\mathbf{g}}$	The amplitude of the *diffracted* beam for reflection G. The intensity is $\lvert\phi_{\mathbf{g}}\rvert^2$
$\phi_{\mathbf{0}}$	The amplitude of the *direct* beam. Don't use the term 'transmitted' beam; all the beams we are studying are transmitted. Don't call it the 'forward-scattered' beam; diffracted beams can also be forward scattered. $\phi_{\mathbf{0}}$ is a special value of $\phi_{\mathbf{g}}$ for the case where $\mathbf{g} = \mathbf{0}$
θ	The angle between a particular set of lattice planes and the direction of the beam scattered constructively by those planes
θ_B	The Bragg angle; a specific value of θ when $\mathbf{s} = \mathbf{0}$
dz	The thickness of a diffracting slice. This thickness can be as small as we wish to make it; it is not limited to atomic planes
$\xi_{\mathbf{g}}$	A characteristic length for reflection **g**; it is called the *extinction distance*
D, G	D is a diffracted beam; G is a special D and indicates that it is a Bragg-diffracted beam (neither is bold) (see Section 11.5)
χ	The electron wave vector in a vacuum
k	The electron wave vector in the specimen

above the other. The upper half diffracts the direct beam. The lower half further diffracts the direct beam but also rediffracts the diffracted beam. Don't confuse this rediffraction with the term 'double diffraction,' which has a special meaning, described in Chapter 23. If instead of cutting the specimen into two, you cut the specimen into many thin slices, you have multiple, instead of just double, diffraction. We call this effect dynamical diffraction.

Because of dynamical diffraction, we cannot use the intensities of spots in electron DPs (except under very special conditions such as CBED) for structure determination, in the way that we use intensities in X-ray patterns. Actually, a more important practical consideration is that the intensity of the electron beam varies strongly as the thickness of the specimen changes; the thickness may change across distances which are much smaller (as small as 1.5 nm or less) than the lateral dimensions of the electron beam (typically >1 μm in the TEM imaging mode). As we will see in Chapters 24–27 when we discuss images, the beam intensity also changes when lattice defects are present which is why we can 'see' defects in the TEM.

13.2 THE APPROACH

The approach we take here is to develop the basic equations describing the diffraction process and to identify parameters which will be important in understanding the contrast in the image. The different images will then be discussed in Part 3.

Inside a crystalline material, we should think in terms of Bloch waves because only certain wave-propagation vectors are allowed in infinite periodic structures: fortunately you don't need to have a thorough understanding of Bloch waves to understand contrast features in the microscope. However, we will consider them in Chapter 14, because a full understanding of the fundamental principles of diffraction from crystals will require this knowledge. What we 'see' in a DP relates directly to 'beams' because the DP, whether in the microscope or on a print, is *outside* the crystal. In this chapter, we will follow the analysis of Chapter 11, considering the amplitudes of beams simply because this gives a good intuitive understanding of the images—what we *see* in the TEM is the intensity, which is directly related to the amplitude ($I \propto |\phi|^2$).

A NOTE ON TERMINOLOGY

In Figure 13.1 we have labeled both the diffracted beams and the spot in the DP, G_i ($i = 1, 2$, etc.). When discussing images we will often refer to $\mathbf{g}_1$, the diffraction vector for the beam G_1. Then colloquially we will call **g** the 'reflection **g**'; the origin for this terminology goes back to the diagram for Bragg diffraction: geometrically it looks like 'reflection.'

So, what do we need to calculate? We need to calculate the intensity of the beam at the exit surface of the specimen, e.g., at all points, such as P in Figure 13.1, because this becomes the 'image' after suitable magnification.

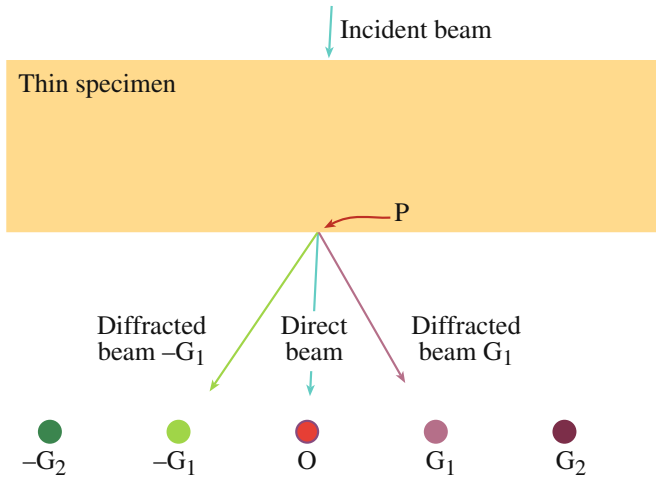

FIGURE 13.1. Defining the point P. The incident beam is scattered inside the thin sample. We want to know the intensities of the direct beam (O) and the diffracted (G_i) beams for each point P at the bottom surface of the specimen (the exit surface).

Before concluding this topic, we will briefly discuss the approximations we are making. One of the most important of these is the column approximation, which is introduced almost without being noticed. It is not a necessary assumption but it simplifies calculations and again aids intuitive understanding. You will also recognize many similarities to visible-light microscopy, but be wary, there are also many differences.

13.3 THE AMPLITUDE OF A DIFFRACTED BEAM

In the analysis of diffracted beams we will consider only crystalline materials. Since any crystal can be constructed by stacking unit cells, we begin by remembering the amplitude scattered by a single unit cell. We can rewrite equation 3.18 so that the amplitude of the electron beam scattered from a unit cell is

$$A_{\text{cell}} = \frac{e^{2\pi ikr}}{r} \sum_i f_i(\theta) e^{2\pi i \mathbf{K}.\mathbf{r}} \qquad (13.1)$$

where the summation is over all i atoms in the unit cell and θ is the angle at which the diffracted beam is traveling relative to the incident beam. We have included the term outside the summation because of how the wave propagates; the r^{-1} term is present because we have a constant flux of electrons traveling through an expanding spherical surface, radius r. The quantities **k**, **K,** and **r** were defined in Chapter 11 and $f(\theta)$ is the atomic-scattering factor. You will often see the sign of the exponent after $f(\theta)$ reversed. Unfortunately, there are two conventions! These conventions are discussed in Section 13.12; we will use the positive convention to be consistent with most materials-science texts.

Figure 13.2 reminds us that $\mathbf{K} = \mathbf{k}_D - \mathbf{k}_I$. The vectors **r** and $\mathbf{r}_i$ are different: **r** is the distance from a point P on the bottom of the specimen to the scattering center and $\mathbf{r}_i$ defines the position of an atom in the unit cell. Remember that $f_i(\theta)$ is the *scattering strength* for the 'i' atom ($f_i(\theta)$ is greater for Au than for Al, etc., as we saw in Figure 3.5). Since we are summing over all the atoms in the unit cell, we can rename this sum as $F(\theta)$, the *structure factor* of the unit cell. (It's just the scattering factor of the unit cell.) Notice that $F(\theta)$ depends on the nature of all the atoms in the unit cell, their positions, and the direction in which the beam is propagating (related to **K** and hence θ). Go back and check Section 3.9.

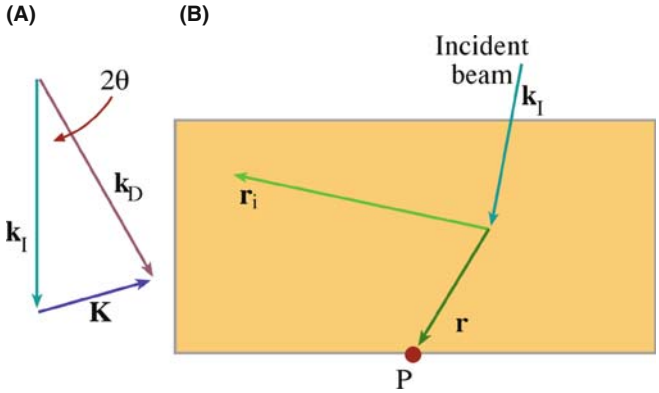

FIGURE 13.2. (A) A reminder that $\mathbf{K} = \mathbf{k}_D - \mathbf{k}_I$. The vector $\mathbf{k}_D$ represents the propagation vector for *any* wave. It does not have to be a diffracted beam but it will only give a spot in the DP when it does correspond to a diffracted beam. (B) shows the relation between the radius of the spherical wavefront, r, the position vector of the i^{th} atom, $\mathbf{r}_i$, and the point where the intensity is calculated, P.

Therefore, expression 13.1 can be rewritten as

$$A_{\text{cell}} = \frac{e^{2\pi i \mathbf{k}.\mathbf{r}}}{r} F(\theta) \qquad (13.2)$$

To find the intensity at some point P, we then sum over all the unit cells in the specimen. For simplicity, we will not solve this problem mathematically here but simply quote the result and discuss its meaning. Let's say we have n unit cells per unit area on a plane parallel to the crystal surface and a is the distance between these planes. The volume of a unit cell, V_c, is simply a/n. The amplitude in a *diffracted beam* (in the direction identified by θ) is denoted as $\phi_{\mathbf{g}}$ and is given by

$$\phi_{\mathbf{g}} = \frac{\pi a i}{\xi_{\mathbf{g}}} \sum_n e^{-2\pi i \mathbf{K}.\mathbf{r}_n} e^{-2\pi i \mathbf{k}_D.\mathbf{r}} \qquad (13.3)$$

Here $\mathbf{r}_n$ denotes the position of each unit cell. (Think about the signs in this equation.) In this analysis, the quantities $f(\theta)$ and $F(\theta)$ both have dimensions of length. We'll now explain what the length $\xi_{\mathbf{g}}$ means in equation 13.3; it is a length because $\phi_{\mathbf{g}}$, the scattering amplitude, is dimensionless (ξ is pronounced 'ksi,' rhyming with 'sigh').

The derivation of these equations involves some tricky manipulation which we will return to later. Some analyses actually make the unrealistic assumption that the intensity of the direct beam, $|\phi_{\mathbf{0}}|^2$, remains unchanged. This assumption is usually not justified, especially when the specimen has a finite thickness! If $|\phi_{\mathbf{g}}|^2$ is not zero then $|\phi_{\mathbf{0}}|^2$ cannot still be 1.

13.4 THE CHARACTERISTIC LENGTH $\xi_{\mathbf{g}}$

At this stage in our analysis it is best to think of the quantity $\xi_{\mathbf{g}}$ as a 'characteristic length' for the diffraction vector **g** so as not to have any preconceived ideas of what it represents. A detailed analysis shows that the magnitude of $\xi_{\mathbf{g}}$ can be expressed as

$$\xi_{\mathbf{g}} = \frac{\pi V_c \cos\theta_B}{\lambda F_{\mathbf{g}}} \qquad (13.4)$$

where $F_{\mathbf{g}}$ is the $F(\theta)$ for reflection **g** (i.e., $F_{\mathbf{g}}$ is a special value of $F(\theta)$ when θ is the Bragg angle).

The quantity ξ_g is an extremely important one; it gives us a way of thinking about nearly all diffraction-contrast phenomena. It is measured in nanometers (or Å) and is known as the 'extinction distance' for reasons that will become obvious.

From equation 13.4, you can see that the magnitude of ξ_g is related to F_g (and through V_c to the lattice parameter) and the wavelength of the electrons, λ. If the structure factor (F_g) is large, ξ_g will be small. Therefore, ξ_g will be small for Au but large for Si. F_g is large when the atomic number is large, because the Coulomb interactions are larger and $f(\theta)$ is large. Similarly, as the accelerating voltage is increased, ξ_g, for a particular material, will increase because the wavelength of the electrons decreases. Table 13.2 lists some useful extinction distances (all for 100-keV electrons).

SUMMARIZE ξ_g

ξ_g is the characteristic length for the diffraction vector **g.** We call it the **extinction distance** because of a property we'll discover later.

Note that ξ_g is a scalar quantity. ξ_g depends on the lattice parameters (through V_c), the atomic number (through F_g), and the kV used (through λ).

The effect of the lattice parameter on ξ_g is illustrated nicely by comparing values of ξ_{111} for diamond, Si, and Ge: the value for Si is larger than for Ge, as expected, because of the smaller atomic number but note that ξ_g for Si is also larger than that for diamond, which has a lower atomic number! Diamond has a particularly small lattice parameter, hence there are more atoms in a given volume.

13.5 THE HOWIE-WHELAN EQUATIONS

The direct and diffracted beams are detected outside the crystal and we see them on the viewing screen. Now we can think of the wave function inside the crystal as being the sum of the beams passing through the crystal. The direct beam has amplitude ϕ_0 (bold **0** to emphasize that the diffraction vector has zero length) and the amplitudes of the diffracted beams can be written as ϕ_{g_1}, ϕ_{g_2}, etc. Each beam has an appropriate phase factor. We write ψ^T, the total wave function, as a series

$$\psi^T = \phi_0 e^{2\pi i \chi_o \cdot \mathbf{r}} + \phi_{g_1} e^{2\pi i \chi_{G_1} \cdot \mathbf{r}} + \phi_{g_2} e^{2\pi i \chi_{G_2} \cdot \mathbf{r}} + \ldots\ldots \quad (13.5)$$

where the wave vectors are χ_O and χ_D (χ (chi) is pronounced 'kai' and rhymes with sky); χ_O is often written simply as χ. We use χ_O here to emphasize that it is a vector which terminates on the point O in reciprocal space; χ_{G_1} terminates on the 'point' G_1, etc. At this stage, we are using wave vectors χ_O and χ_D which describe the wave in the vacuum rather than in the crystal. We will change to being inside the crystal shortly. Most of the time, you could write χ as **k**, but there are occasions when the difference is important so we start with χ and then change over.

First, we simplify equation 13.5 by considering only one diffracted beam G, i.e., we make a 'two-beam approximation' (O is the other beam). This is a very important approximation, which we'll use often. Two-beam conditions mean that we tilt the crystal so there is only one strong diffracted beam (with $\mathbf{s} = 0$). All other diffracted beams are weak ($\mathbf{s} >> $ or $<< 0$), and we ignore their contribution to ϕ_g. Then if the amplitude ϕ_g changes by a small increment as the beam passes through a thin slice of material which is *dz* thick we can write down expressions for the *changes* in ϕ_g and ϕ_0 by using the concept introduced in equation 13.3 but replacing *a* by the short distance *dz*

$$d\phi_g = \left\{ \frac{\pi i}{\xi_g} \phi_0 e^{2\pi i (\chi_O - \chi_D) \cdot \mathbf{r}} + \frac{\pi i}{\xi_0} \phi_g \right\} dz \quad (13.6)$$

$$d\phi_0 = \left\{ \frac{\pi i}{\xi_0} \phi_0 + \frac{\pi i}{\xi_g} \phi_g e^{2\pi i (\chi_D - \chi_O) \cdot \mathbf{r}} \right\} dz \quad (13.7)$$

Here $\chi_O - \chi_D$ is the change in wave vector as the ϕ_g beam scatters into the ϕ_0 beam. Similarly $\chi_D - \chi_O$ is the change in wave vector as the ϕ_0 beam scatters into the ϕ_g beam. Now the *difference* $\chi_O - \chi_D$ is identical to $\mathbf{k}_O - \mathbf{k}_D$ although the individual terms are not equal. Then remember that $\mathbf{k}_D - \mathbf{k}_O$ ($= \mathbf{K}$) is $\mathbf{g} + \mathbf{s}$ for the perfect crystal.

You might wonder why we have introduced the wave vector χ when it appears to be the same as the **k** we used in equation 13.1. The reason is that equation 13.1 is a very general equation describing scattering from any group of atoms, but we are now going to consider two special cases, namely, an electron in the vacuum (wave vector χ) and one in a crystal (wave vector **k**). Incidentally, the excitation error, **s**, should really be written as $\mathbf{s}_g$, since it refers to a particular **g** vector. You can think

TABLE 13.2 Examples of Extinction Distances (in nm)*

Material					
hkl =	110	111	200	220	400
Al	–	56.3	68.5	114.4	202.4
Cu	–	28.6	32.6	47.3	76.4
Au	–	18.3	20.2	27.8	43.5
MgO	–	272.6	46.1	66.2	103.3
Fe	28.6	–	41.2	65.8	116.2
W	18.0	–	24.5	35.5	55.6
Diamond		47.6	–	66.5	121.5
Si		60.2	–	75.7	126.8
Ge		43.0	–	45.2	65.9

*For two-beam condition at 100 kV.

of the parameter $\xi_{\mathbf{0}}$ as the characteristic length for forward scattering, i.e., scattering from any beam into itself, whereas $\xi_{\mathbf{g}}$ corresponds to scattering through an angle corresponding to a diffraction vector **g**.

The change in $\phi_{\mathbf{g}}$ depends on the magnitude of **both** $\phi_{\mathbf{g}}$ and $\phi_{\mathbf{0}}$.

These two equations (13.6 and 13.7) can then be rearranged to give a pair of coupled differential equations. We say that $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$ are 'dynamically coupled.' The term *dynamical diffraction* thus means that the amplitudes (and therefore the intensities) of the direct and diffracted beams are constantly changing, i.e., they are dynamic

$$\frac{d\phi_{\mathbf{g}}}{dz} = \frac{\pi i}{\xi_{\mathbf{g}}}\phi_{\mathbf{0}}e^{-2\pi isz} + \frac{\pi i}{\xi_{\mathbf{0}}}\phi_{\mathbf{g}} \tag{13.8}$$

and

$$\frac{d\phi_{\mathbf{0}}}{dz} = \frac{\pi i}{\xi_{\mathbf{0}}}\phi_{\mathbf{0}} + \frac{\pi i}{\xi_{\mathbf{g}}}\phi_{\mathbf{g}}e^{2\pi isz} \tag{13.9}$$

Microscopists usually refer to this pair of equations as the '*Howie-Whelan*' equations after Howie and Whelan (1961), who laid the foundations for understanding diffraction contrast in the TEM; you may also see them referred to as the 'Darwin-Howie-Whelan equations' since Darwin (1914) developed the dynamical theory for X-rays! Note that we are further simplifying the expression by writing

$$e^{-2\pi i\mathbf{s}\cdot\mathbf{r}} = e^{-2\pi isz} \tag{13.10}$$

In doing so, we are making the approximation that **s** and **r** are both parallel to z, i.e., at this time, we ignore components of **s** that are not parallel to the electron beam. The approximation may be written as

$$|\mathbf{s_g}| = s_z \tag{13.11}$$

We then drop the z subscript; just remember it is still there. There are situations where the difference can become important.

Although this approach is totally phenomenological (i.e., we haven't really given any physical justification for the assumptions we have made and actually we know we should use Bloch waves), you will see that it provides enormous insight into the interpretation of your images and DPs. In Chapter 25, we will use these ideas to understand why we see defects in the TEM.

The fundamental idea is that, at any given position in the specimen, the change in the amplitudes of *both* the direct beam and the diffracted beam depends on the amplitude of *both* beams. The fact that part of the change in ϕ_0 is due to the magnitude of ϕ_0 itself, gives rise to the term *forward scattering*; remember the origin of scattering from Section 2.2. Note that scattering from $\phi_{\mathbf{g}}$ to $\phi_{\mathbf{g}}$ is also forward scattering, although it takes place in a different forward direction (i.e., $\theta = \theta_B$ and scattering is parallel to $\mathbf{k}_D$ rather than $\mathbf{k}_O$). So forward scattering does occur but it does not change the direction of the beam. However, it does have a characteristic length, $\xi_{\mathbf{0}}$; this length is another way of saying we have a refractive-index effect for electrons which we'll address later in Section 14.4.

DIRECT

Remember: don't refer to the direct beam as the unscattered or the transmitted beam!

13.6 REFORMULATING THE HOWIE-WHELAN EQUATIONS

From here on, the math is quite straightforward. What we are going to do may seem like a lot of work to derive one equation (13.48) but the result will allow you to picture more clearly what is happening. If you don't want to bother with the math, you can skip to equations 13.47 and 13.48 but you must not miss those two equations; they are essential for understanding images of crystalline materials.

The pair of equations, 13.8 and 13.9, can be simplified by making the substitutions (i.e., a transformation of variables)

$$\phi_{\mathbf{0}(\mathrm{sub})} = \phi_{\mathbf{0}}e^{\frac{-\pi iz}{\xi_{\mathbf{0}}}} \tag{13.12}$$

and

$$\phi_{\mathbf{g}(\mathrm{sub})} = \phi_{\mathbf{g}}e^{2\pi isz - \frac{\pi iz}{\xi_{\mathbf{0}}}} \tag{13.13}$$

Then equations 13.8 and 13.9 become

$$\frac{d\phi_{\mathbf{g}(\mathrm{sub})}}{dz} = \frac{\pi i}{\xi_{\mathbf{g}}}\phi_{\mathbf{0}(\mathrm{sub})} + 2\pi is\phi_{\mathbf{g}(\mathrm{sub})} \tag{13.14}$$

and

$$\frac{d\phi_{\mathbf{0}(\mathrm{sub})}}{dz} = \frac{\pi i}{\xi_{\mathbf{g}}}\phi_{\mathbf{g}(\mathrm{sub})} \tag{13.15}$$

Since $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{0}(\mathrm{sub})}$ only differ by a phase factor, we will ignore the difference in calculating intensities since only the amplitude is then important; similarly for $\phi_{\mathbf{g}}$ and $\phi_{\mathbf{g}(\mathrm{sub})}$. The result of our substitution is that we have removed the phase factor involving $\xi_{\mathbf{0}}$, i.e., we've removed the refractive-index effect. Equations 13.14 and 13.15 can be combined to give the second-order differential equation for $\phi_{\mathbf{0}}$

$$\frac{d^2\phi_0}{dz^2} - 2\pi i s\frac{d\phi_0}{dz} + \frac{\pi^2}{\xi_g^2}\phi_0 = 0 \qquad (13.16)$$

We can obtain a similar equation for ϕ_g and then obtain solutions for these reformulated expressions.

Note that the only other quantities appearing in this equation for ϕ_0 are z, s, and ξ_g: z and s are geometric parameters; the nature of the material only enters through ξ_g.

13.7 SOLVING THE HOWIE-WHELAN EQUATIONS

If we can solve the Howie-Whelan equations, then we can predict the intensities in the direct and diffracted beams (i.e., $|\phi_0|^2$ and $|\phi_g|^2$ in the two-beam case). If we take it step by step, then we know that solutions to equation 13.16 (a second-order differential equation in one variable, ϕ_0) must have the form

$$\phi_0 = C_0 e^{2\pi i\gamma z} \qquad (13.17a)$$

So we can write that

$$\frac{d\phi_0}{dz} = 2\pi i\gamma C_0 e^{2\pi i\gamma z} \qquad (13.17b)$$

and

$$\frac{d^2\phi_0}{dz^2} = -4\pi^2\gamma^2 C_0 e^{2\pi i\gamma z} \qquad (13.17c)$$

What we need to determine is the phase γ and the amplitude C_0. Note that since z is a distance in real space, then γ must be a distance in reciprocal space. Substituting this expression into equation 13.16 shows that γ must be a solution to the algebraic equation

$$\gamma^2 - s\gamma - \frac{\xi_g^{-2}}{4} = 0 \qquad (13.18)$$

Now ϕ_g is related to ϕ_0 through equation 13.15. By substituting equation 13.17a into equation 13.15 we find that for each ϕ_0, we also have a ϕ_g given by

$$\phi_g = 2\xi_g\gamma C_0 e^{2\pi i\gamma z} \qquad (13.19)$$

To emphasize the similarity to equation 13.17a we can define

$$\phi_g = C_g e^{2\pi i\gamma z} \qquad (13.20)$$

Then we can see directly that

$$\frac{C_g}{C_0} = 2\xi_g\gamma \qquad (13.21)$$

We've actually got this far without solving any equation! There are two solutions to the quadratic equation (13.18), using the standard formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad (13.22)$$

to give

$$\gamma^{(1)} = \frac{\left(s - \sqrt{s^2 + \frac{1}{\xi_g^2}}\right)}{2} \qquad (13.23a)$$

and

$$\gamma^{(2)} = \frac{\left(s + \sqrt{s^2 + \frac{1}{\xi_g^2}}\right)}{2} \qquad (13.23b)$$

We have now found two solutions to the Howie-Whelan equations.

There are two different values for ϕ_0 and two corresponding values for ϕ_g.

Now we need to understand what these solutions mean physically. Specifically, what can we learn about $\gamma^{(1)}$ and $\gamma^{(2)}$? Note that they are always real but may be positive or negative depending on the sign and size of s and that they are *independent* of z.

13.8 THE IMPORTANCE OF $\gamma^{(1)}$ AND $\gamma^{(2)}$

Since $\gamma^{(1)}$ and $\gamma^{(2)}$ are solutions of equation 13.18 from the properties of quadratic equations or by combining equations 13.23a and b, we know that

$$\gamma^{(1)} + \gamma^{(2)} = s \qquad (13.24)$$

which is a purely geometric quantity, and

$$\gamma^{(1)} \times \gamma^{(2)} = -\frac{1}{4\xi_g^2} \qquad (13.25)$$

which is a property of the material. Remember that γ is a length in reciprocal space.

In order to make the equations easier to work with, it is useful to define another quantity, w, which is *dimensionless* but has the same sign as s.

$$w = s\xi_g \qquad (13.26)$$

In practical situations w may vary from 0 to ± 10. We can then express the two forms of equation 13.21 (because there are *two* values of γ) in terms of γ or, more conveniently, in terms of w

$$\frac{C_g^{(1)}}{C_0^{(1)}} = 2\xi_g\gamma^{(1)} = w - \sqrt{w^2 + 1} \qquad (13.27)$$

and

$$\frac{C_{\mathbf{g}}^{(2)}}{C_{\mathbf{0}}^{(2)}} = 2\xi_{\mathbf{g}}\gamma^{(2)} = w + \sqrt{w^2+1} \qquad (13.28)$$

(the superscripts on $C_{\mathbf{g}}^{(1)}$, etc., correspond to the superscripts on $\gamma^{(1)}$ and $\gamma^{(2)}$, i.e., the two solutions to the original quadratic equation). Now it is useful to make another substitution (or transformation) to simplify these relationships. We define β by

$$w = \cot\beta \qquad (13.29)$$

Now we can impose a restriction on the absolute magnitudes of $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$ so that they satisfy the relations

$$C_{\mathbf{0}}^{(1)2} + C_{\mathbf{g}}^{(1)2} = 1 = C_{\mathbf{0}}^{(2)2} + C_{\mathbf{g}}^{(2)2} \qquad (13.30)$$

By normalizing these values for C separately for each value of γ, we are restricting the intensity of the beam to values between 0 and 1 (see below). Then if we substitute equation 13.29 into equation 13.27 and then into equation 13.28 we find (using $1-\cos\beta = 2\sin^2(\beta/2)$ and $\sin\beta = 2\sin(\beta/2)\cos(\beta/2)$) that the C values have the following simple forms

$$\begin{aligned} C_{\mathbf{0}}^{(1)} &= \cos\tfrac{\beta}{2} \quad & C_{\mathbf{g}}^{(1)} &= -\sin\tfrac{\beta}{2} \\ C_{\mathbf{0}}^{(2)} &= \sin\tfrac{\beta}{2} \quad & C_{\mathbf{g}}^{(2)} &= \cos\tfrac{\beta}{2} \end{aligned} \qquad (13.31)$$

Now you can understand why we introduced β in equation 13.29. The two independent solutions to the reformulated Howie-Whelan equation for $\phi_{\mathbf{0}}$ (13.16) are then $\phi_{\mathbf{0}} = C_{\mathbf{0}}^{(1)}\exp(2\pi i\gamma^{(1)}z)$ and $\phi_{\mathbf{0}} = C_{\mathbf{0}}^{(2)}\exp(2\pi i\gamma^{(2)}z)$ and *each value* has a corresponding value for $\phi_{\mathbf{g}}$.

We can already see that the ratio of the amplitudes of the diffracted and direct beams, $C_{\mathbf{g}}$ to $C_{\mathbf{0}}$ (and therefore the intensities), in equation 13.21 depends on γ, the phase of the wave, and hence on s, the excitation error. Hence the ratios in equations 13.27 and 13.28 depend on how close the specimen is to the Bragg orientation. We are particularly concerned about *the* Bragg condition because we have chosen a two-beam situation.

THE SUBSTITUTION

Because of this simple substitution you can easily confirm that, for this two-beam situation, the probability of finding the electron in one beam or the other remains unity ($|\psi^{\mathrm{T}}|^2 = 1$). Hence the reason we use a normalized intensity in equation 13.30.

In the two-beam approximation, equation 13.5 is expressed in terms of $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$, both of which depend on γ (equation 13.17), so equation 13.5 can then be written in terms of both values of γ (and hence $C_{\mathbf{0}}^{(1)}$, $C_{\mathbf{0}}^{(2)}$, etc.), giving two independent quantities $b^{(1)}$ and $b^{(2)}$. Either of these two functions could be ψ^{T}, the total wave function. Alternatively, the total wave function could be some combination of them, i.e., part $b^{(1)}$ plus part $b^{(2)}$. Both of these wave functions are dependent on $\mathbf{r}$ and have their own values of $\mathbf{k}$ that we identify as $\mathbf{k}^{(j)}$.

Each value of γ gives a different value of $\mathbf{k}$ that we call $\mathbf{k}^{(j)}$.

Thus we can write expressions for $b^{(1)}$ and $b^{(2)}$.

$$b^{(1)}\left(\mathbf{k}^{(1)},\mathbf{r}\right) = C_{\mathbf{0}}^{(1)}e^{2\pi i\,\mathbf{k}^{(1)}.\mathbf{r}} + C_{\mathbf{g}}^{(1)}e^{2\pi i(\mathbf{k}^{(1)}+\mathbf{g}).\mathbf{r}} \qquad (13.32)$$

and

$$b^{(2)}\left(\mathbf{k}^{(2)},\mathbf{r}\right) = C_{\mathbf{0}}^{(2)}e^{2\pi i\,\mathbf{k}^{(2)}.\mathbf{r}} + C_{\mathbf{g}}^{(2)}e^{2\pi i(\mathbf{k}^{(2)}+\mathbf{g}).\mathbf{r}} \qquad (13.33)$$

Remember: each of these Bloch-wave functions could be a wave in the crystal—each one depends on only one of the $\mathbf{k}$ values. In general, the total wave function will be a combination of these two waves. We'll return to the important relationship between $\mathbf{k}$ and γ in Section 13.9. We use the letter 'b' here because we've actually obtained expressions for the Bloch waves mentioned in Section 13.2, which we'll discuss in the next chapter.

13.9 THE TOTAL WAVE AMPLITUDE

We have now found two different wave functions which can both propagate in the crystal. We still have to determine what $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$ are. The total wave vector, ψ^{T}, is a combination of the two (Bloch) waves, $b^{(1)}$ and $b^{(2)}$

$$\psi^{\mathrm{T}} = \mathcal{A}^{(1)}b^{(1)} + \mathcal{A}^{(2)}b^{(2)} \qquad (13.34)$$

where the constants $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$ determine the relative contribution of each (Bloch) wave. We can now combine the last few equations (13.31–13.33 and 13.34) to give

$$\begin{aligned} \psi^{\mathrm{T}} = \mathcal{A}^{(1)}\{&\cos\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(1)}.\mathbf{r}} - \sin\tfrac{\beta}{2}e^{2\pi i(\mathbf{k}^{(1)}+\mathbf{g}).\mathbf{r}}\} \\ +\mathcal{A}^{(2)}\{&\sin\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(2)}.\mathbf{r}} - \cos\tfrac{\beta}{2}e^{2\pi i(\mathbf{k}^{(2)}+\mathbf{g}).\mathbf{r}}\} \end{aligned} \qquad (13.35)$$

All that now remains is to determine the magnitudes of $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$ which we can do by remembering that we have a thin TEM specimen. In mathematical terminology the constants $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$ must now be determined using the boundary conditions.

It is helpful to rearrange equation 13.35 first

$$\psi^{T}=\{\mathcal{A}^{(2)}\sin\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(2)}.\mathbf{r}}-\mathcal{A}^{(1)}\cos\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(1)}.\mathbf{r}}\}+\{\mathcal{A}^{(2)}\cos\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(2)}.\mathbf{r}}-\mathcal{A}^{(1)}\sin\tfrac{\beta}{2}e^{2\pi i\mathbf{k}^{(1)}.\mathbf{r}}\}e^{2\pi i\mathbf{g}.\mathbf{r}} \quad (13.36)$$

Only the second term depends on **g**, so this must be the $\phi_{\mathbf{g}}$ term. We know that at the top of the specimen ($\mathbf{r} = 0$), $\phi_{\mathbf{0}}$ is unity and $\phi_{\mathbf{g}}$ is zero (independent of γ)—the amplitude of the diffracted beam is zero before it's diffracted! It follows directly that

$$\mathcal{A}^{(1)} = \cos\frac{\beta}{2} \quad (13.37)$$

$$\mathcal{A}^{(2)} = \sin\frac{\beta}{2} \quad (13.38)$$

These equations (13.37 and 13.38) tell us that $\mathcal{A}$ in equation 13.34 is just determined by the value of **s**, i.e., the deviation from the Bragg condition. So you can adjust the values of $\mathcal{A}$ by changing **s**, which we now know just involves tilting the specimen.

Now, finally, we can write down the general expressions for $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$, each as a function of z. First we need to modify equation 13.5 by using the substitution of equations 13.12 and 13.13, so it becomes

$$\psi^{T} = \phi_{\mathbf{0}}e^{2\pi i\,\mathbf{k}.\mathbf{r}} + \phi_{\mathbf{g}}e^{2\pi i(\mathbf{k}+\mathbf{g}).\mathbf{r}} \quad (13.39)$$

(Remember that $\chi_D = \chi_O + \mathbf{g} + \mathbf{s}$ (or $\mathbf{k}_D = \mathbf{k}_O + \mathbf{g} + \mathbf{s}$), where $\mathbf{k}_O$ is written as **k** and D is G_1 in equation 13.5; then you'll see that the term containing **s** in equation 13.13 drops out.) The $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$ components in equation 13.36 are easily recognized by the presence of $\exp(2\pi i\mathbf{g}\cdot\mathbf{r})$. Comparing equations 13.36 and 13.39 (having replaced $\mathcal{A}$ using equations 13.37 and 13.38) we see that

$$\phi_{\mathbf{g}} = \sin\frac{\beta}{2}\cos\frac{\beta}{2}\left\{e^{2\pi i(\mathbf{k}^{(2)}-\mathbf{K}).\mathbf{r}} - e^{2\pi i(\mathbf{k}^{(1)}-\mathbf{K}).\mathbf{r}}\right\} \quad (13.40)$$

Since we are only considering the z component, we know, from equations 13.17 and 13.19, that the exponential term must have the phase $2\pi i\gamma z$, i.e.,

$$(\mathbf{k}^{(2)} - \mathbf{K})_z = \gamma^{(2)} \text{ and } (\mathbf{k}^{(1)} - \mathbf{K})_z = \gamma^{(1)} \quad (13.41)$$

What we are interested in is the magnitude of $\gamma^{(1)}$ and $\gamma^{(2)}$.

We can now manipulate equation 13.40 using equation 13.41 and the expression $e^{i\theta} = \cos\theta + i\sin\theta$ to give

$$\phi_0 = \{\cos(\pi z\Delta\mathbf{k}) - i\cos\beta.\sin(\pi z\Delta\mathbf{k})\}e^{\pi isz} \quad (13.42)$$

and

$$\phi_{\mathbf{g}} = +i\sin\beta.\sin(\pi z\Delta\mathbf{k}).e^{\pi isz} \quad (13.43)$$

In these equations Δk is simply $|\mathbf{k}^{(2)} - \mathbf{k}^{(1)}|$. Leaving the term $e^{\pi isz}$ in these equations does not affect the amplitudes of $\phi_{\mathbf{0}}$ and $\phi_{\mathbf{g}}$ or the beam intensities but it will make it easier for you to check that these expressions satisfy, for example, equation 13.16.

A KEY RESULT

We have shown directly that $\phi_{\mathbf{0}}$ in equation 13.39 is a mixture of terms containing $\mathbf{k}^{(1)}$ and $\mathbf{k}^{(2)}$. This is why $\phi_{\mathbf{g}}$ depends on Δk.

13.10 THE EFFECTIVE EXCITATION ERROR

We can now write down the intensity at the bottom (exit surface) of the specimen ($z = t$) and manipulate the equations by substituting for Δk and w. The term Δk in equations 13.42 and 13.43 is the same as $\Delta\gamma$, i.e., $\gamma^{(2)} - \gamma^{(1)}$ (see equation 13.41). We can therefore write down Δk by considering equations 13.27 and 13.28

$$\Delta k = \frac{\sqrt{w^2+1}}{\xi_{\mathbf{g}}} \quad (13.44)$$

The intensity in the diffracted beam, $|\phi_{\mathbf{g}}|^2 = \phi_{\mathbf{g}}\phi_{\mathbf{g}}^*$, is obtained from equation 13.43

$$I_{\mathbf{g}} = \left|\phi_{\mathbf{g}}\right|^2 = \sin^2\beta.\sin^2(\pi t\Delta k) \quad (13.45)$$

$$I_{\mathbf{g}} = \left|\phi_{\mathbf{g}}\right|^2 = \frac{1}{w^2+1}\sin^2\frac{\pi t\sqrt{w^2+1}}{\xi_{\mathbf{g}}} \quad (13.46)$$

We can make this equation look more familiar by defining an effective excitation error, s_{eff}

$$s_{\text{eff}} = \sqrt{s^2 + \frac{1}{\xi_{\mathbf{g}}^2}} = \frac{\sqrt{w^2+1}}{\xi_{\mathbf{g}}} \quad (13.47)$$

Now the equation becomes

$$\left|\phi_{\mathbf{g}}\right|^2 = \left(\frac{\pi t}{\xi_{\mathbf{g}}}\right)^2.\frac{\sin^2(\pi t s_{\text{eff}})}{(\pi t s_{\text{eff}})^2} \quad (13.48)$$

This equation gives us the intensity in the Bragg-diffracted beam. In writing down equation 13.47, we have defined another important new quantity s_{eff}, so labeled because it's the *effective* excitation error.

THE REALLY IMPORTANT EQUATION

It's so important, we'll repeat it

$$\left|\phi_{\mathbf{g}}\right|^2 = \left(\frac{\pi t}{\xi_{\mathbf{g}}}\right)^2.\frac{\sin^2(\pi t s_{\text{eff}})}{(\pi t s_{\text{eff}})^2}$$

One important result shown directly by equation 13.45 is that the intensity, I_g, in the diffracted beam emerging from the specimen is proportional to $\sin^2(\pi t \Delta k)$ and thus I_0 is proportional to $\cos^2(\pi t \Delta k)$. I_g and I_0 are both periodic in both t and s_{eff}. As ϕ_g increases and decreases, ϕ_0 behaves in a complementary manner so that

$$I_0 = 1 - I_g \tag{13.49}$$

Remember when testing this formula that $I = \phi\phi^*$ (ϕ^* is the complex conjugate of ϕ).

The effective excitation error, s_{eff}, is a very important quantity. We can summarize some important properties

- The quantity s_{eff} is never zero.
- When s is zero, s_{eff} is ξ_g^{-1}.
- When s is very large, then s_{eff} becomes essentially the same as s.

13.11 THE COLUMN APPROXIMATION

When we form an image, we try to focus the objective lens on a plane in or below the specimen (remember that here, below means underfocus). One special plane we can choose is the plane which corresponds to the bottom of the specimen, assuming that this plane is perpendicular to the direction of the propagating beam. Whatever plane we choose, what we see depends on the beams that finally leave the bottom of the specimen, so let's concentrate on this one plane. Look at Figure 13.3A; P is the point at the bottom of the specimen, and we are calculating the values of ϕ_0 and ϕ_g at this point to construct our image. Where do the electrons come from in order to contribute to ϕ_0 and ϕ_g? The answer is the cone APB where the angle APB is $\sim 2\theta_B$. In other words, we don't just have a diffracted beam which propagates through the specimen from the top to point P. There is actually a cone of material which contributes to the intensity at point P. The shape of the cone can be calculated using the Fresnel-zone construction, which was actually developed nearly 200 years ago for visible-light optics. Figure 13.3B, which is how the cone is usually drawn, summarizes the relevant parameters; don't forget that a cone, not a triangle, of material contributes to the intensity at P. A clear derivation is given by Hecht. Why is it a Fresnel diffraction? The answer is that we form an image, i.e., look at a plane, which is very close to where the diffraction 'event' occurred, we are in the near-field, or Fresnel, regime (see Section 2.9).

FOCUSING

As usual, we should focus only by moving the specimen up and down, but we don't.

Let's consider some actual numbers: At 100 kV, $\lambda = 3.7$ pm, $\theta_B \sim 0.01$ radians or $\sim 0.5^\circ$. So if the thickness of the specimen is 100 nm, then AB is $\sim$ 2 nm. If we increase the t, then the width of the column will also increase. However, if we increase the accelerating voltage so as to increase the thickness we can penetrate, the wavelength decreases causing the Bragg angle also to decrease. This allows us to make the approximation shown in Figure 13.4A and B when calculating ϕ_0 and ϕ_g. This model is known as the column approximation.

The great advantage of this approximation is that it allows us to calculate the scattering from slices which have a constant width as we pass down the column, which itself lies in a well-defined direction (generally parallel to $\mathbf{k}_D$). We might anticipate problems with very small defects on a very

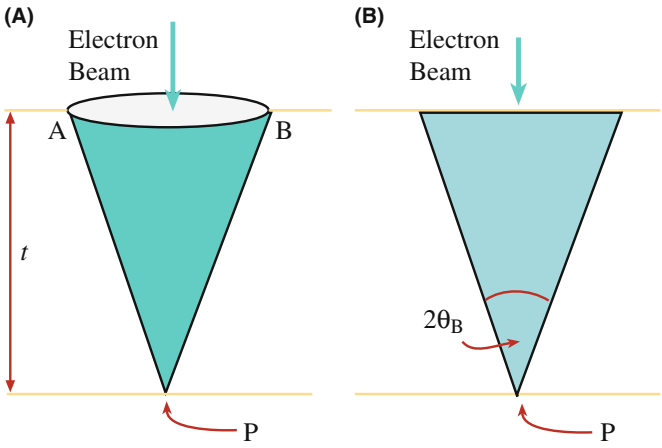

FIGURE 13.3. (A) The intensity of the beams at point P at the bottom of the specimen is influenced by all the scattering within a cone of material. The solid angle of the cone is determined by the diameter of the Fresnel zones which, in turn, are principally determined by λ. The cross section (B) is the more typical view of the cone.

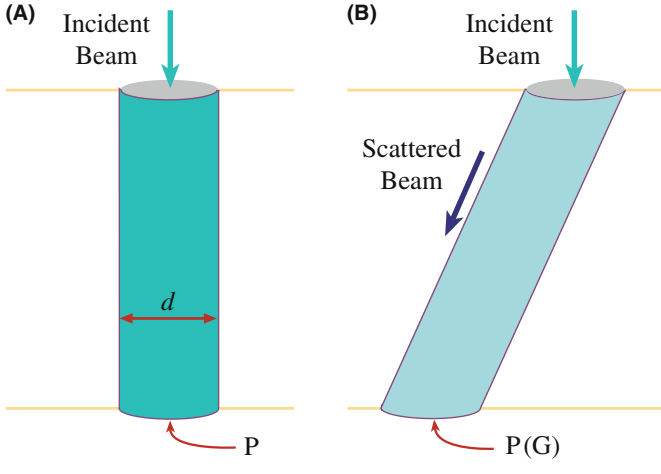

FIGURE 13.4. The column approximation for (A) the direct beam and (B) a diffracted beam. A column replaces the cone. The diameter of the column (d) should be the *average* diameter of the cone it replaces (AB/2 in Figure 13.3). (B) This value will depend on the thickness of the sample. In practice it is usually taken to be ~2 nm.

fine detail, especially when these features can vary their positions in the foil. The more correct, non-column treatment was introduced by Takagi; the analysis by Howie and Basinski is what we use in computer programs.

COLUMN APPROXIMATION

The column approximation often hides itself very well, but it is actually used in many calculations of images.

13.12 THE APPROXIMATIONS AND SIMPLIFICATIONS

In order to minimize the mathematics and to emphasize the underlying physical principles involved in the analysis of diffracted beams, we have made a number of assumptions, simplifications, and approximations. Although we are not going to cover all of these points, you should be aware of some of them

- We have completely neglected any effects due to backscattering of the electrons. This approximation is reasonable since we are dealing with electrons which have very high energies. However, if you are familiar with SEM, you will have encountered backscattered electron (BSE) imaging and possibly, rocking-beam channeling patterns (RCPs) or electron backscattered diffraction (EBSD) patterns. So some electrons must be backscattered.
- In some parts of the discussion, it is an implicit assumption that the crystal has a center of symmetry. This assumption is hidden in our use of $\xi_{\mathbf{g}}$. If the material is non-centrosymmetric, then the BF image and images formed using only a systematic row of reflections will not be affected. Differences will occur in some DF images or when non-systematic reflections contribute to the image. In these cases, you will need to use a computer program to predict or interpret the contrast.

TWO OPPOSITE CONVENTIONS

Two conventions are used to describe the exponential dependence on **k** and **r**; both are commonly used.

$$e^{2\pi i\mathbf{k}.\mathbf{r}} \quad \text{or} \quad e^{-2\pi i\mathbf{k}.\mathbf{r}}$$

These conventions have been discussed by Spence. In our analysis, we have chosen to use $e^{2\pi i\mathbf{k}.\mathbf{r}}$ which Spence has termed the 'quantum-mechanical' convention.
Note that Spence uses the alternative 'crystallographic' convention, except when he discusses Bloch waves.

- From Chapter 11, you know that it is impossible to set up a true two-beam condition for a thin TEM specimen. There will always be more than one diffracted spot visible. So how do we measure $\xi_{\mathbf{g}}$ exactly? The answer is that we don't, but we can make a very good estimate.
- Remember the use of z and t. When we consider the diffracted beam, then z and t are measured along the direction of the diffracted beam. In general, this distance will be different for each beam. The saving feature is that we are usually concerned with small Bragg angles. As a thought exercise, you might consider the effect of having a steeply inclined wedge or a specimen which, although parallel sided, is steeply inclined to the electron beam.
- The full analysis of scattering includes a term in r^{-1} which says that the intensity falls off as r^{-2}. This is just the standard flux relation—the number of electrons passing through a spherical surface around the scattering point is constant. (The surface area of a sphere is proportional to r^2.) This term has been omitted throughout our discussion since it only affects the absolute intensity. A practical lesson from this is that you should use the lowest magnification that will give you the desired resolution; remember that the highest useful magnification in a TEM image is about 10^6 (see Section 6.6.B).

In the quantum mechanical convention, the time-dependent Schrödinger equation is written as

$$\frac{h^2}{8\pi^2 m}\nabla^2\psi = -i\frac{h}{2\pi}\frac{d\psi}{dt} \tag{13.51}$$

with the full solution being

$$\psi(\mathbf{r}, t) = Ae^{+i(\mathbf{k}.\mathbf{r}-\omega t)} \tag{13.52}$$

- The concept of a refractive-index effect for electron waves is directly analogous to that for visible-light waves, or any other electromagnetic radiation, in that the potential of the crystal causes a change in the kinetic energy of the electrons (because their total energy is unchanged) and therefore, their velocity is changed. Normally, of course, we think of this as a change in the wavelength of the electrons. The magnitude of **k** will always be larger than that of χ.
- We have not mentioned the absorption of Bragg beams, yet we know that this must occur since we can only examine thin specimens in the TEM. Absorption of beams is considered in Section 14.6 and Section 23.8.

13.13 THE COUPLED HARMONIC OSCILLATOR ANALOG

The expression for the intensity of the diffracted beam is particularly simple when $s = 0$. Then from equation 13.48 we can write

$$|\phi_{\mathbf{g}}|^2 = \sin^2\left(\frac{\pi t}{\xi_{\mathbf{g}}}\right) \tag{13.53}$$

and similarly

$$|\phi_{\mathbf{0}}|^2 = 1 - \sin^2\left(\frac{\pi t}{\xi_{\mathbf{g}}}\right) \tag{13.54}$$

Both equations now only have one variable, the thickness of the specimen. We will refer to these equations when we discuss images in Chapter 23, but we can note immediately that $I_{\mathbf{g}}$ is zero at $t = 0$ and again at $t = \xi_{\mathbf{g}}$ (or in general at $t = n\xi_{\mathbf{g}}$, where n is an integer). This is the reason we call $\xi_{\mathbf{g}}$ the extinction distance. This situation corresponds to two coupled simple-harmonic oscillators with energy (i.e., intensity, $I_{\mathbf{0}}$ and $I_{\mathbf{g}}$) being continuously transferred from one to the other and back again. Notice that $I_{\mathbf{g}}$ can only increase to unity when $\mathbf{s} = 0$.

CHAPTER SUMMARY

In this chapter, we have derived equations and introduced terminology that will form the basis for our discussion of diffraction-contrast images. It is not necessary for you to be able to reproduce the mathematical derivations but equations 13.47 and 13.48 are crucial and must be understood. Our analysis was quickly limited to two beams, the direct beam and one Bragg-diffracted beam. In deriving the Howie-Whelan equations, we must consider both forward scattering and Bragg diffraction. We introduced a new parameter, the critical length $\xi_{\mathbf{g}}$, and explained why this parameter is called the extinction distance. This length was defined in equation 13.4 which shows that $\xi_{\mathbf{g}}$ depends on the *material*, the *reflection,* and the *wavelength of the electrons*. Two particular points you need to remember are

- If the voltage increases then λ decreases and $\xi_{\mathbf{g}}$ increases.
- The contribution of each Bloch wave is determined by **s**.

In Section 24.3, we'll show how the two-beam analysis can be extended using the concept of the scattering matrix.

REFERENCES

This treatment of diffracted beams follows that given by Hirsch and Whelan and the textbook by Hirsch et al. that built on Darwin's treatment of X-ray diffraction.

HISTORY

Darwin, CG 1914 *Röntgen-Ray Reflection I;II* Phil, Mag. **27** 315–333 and 675-690. Charles Galton Darwin was a grandson of Charles Robert Darwin and, like (*the*) Darwin (and Hirsch), became a Fellow of Christ's College.

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THE COLUMN APPROXIMATION

Howie, A and Basinski, ZS 1968 *Approximations of the Dynamical Theory of Diffraction Contrast* Phil. Mag. **17** 1039–1063.

Takagi, S. 1962 *Dynamical Theory of Diffraction Applicable to Crystals with Any Kind of Small Distortion* Acta Cryst. **15** 1311–1312.

NOTATION

Spence, JCH 2003 *Experimental High-Resolution Electron Microscopy* 3rd Ed. Oxford University Press New York. Uses the quantum-mechanical convention rather than the crystallographic one.

THE COMPANION TEXT

The H-W equations are the basis of many home-written programs including those available in the text by Head et al. If you are taking the time to simulate diffraction-contrast images, you might as well use a package which will allow you at least to assess the influence of beams in the systematic row and then see how such multi-beam images compare to those predicted by this analytical treatment. A complete chapter is devoted to this topic in the companion text.

SELF-ASSESSMENT QUESTIONS

Q13.1 What does $\xi_{\mathbf{g}}$, the characteristic length, depend on?
Q13.2 How is the structure factor related to the characteristic length, $\xi_{\mathbf{g}}$?
Q13.3 What do we mean by the phrase *two-beam condition* and when is it satisfied?
Q13.4 Can forward scattering change the direction of the beam?
Q13.5 What does dynamical diffraction mean in the two-beam case?
Q13.6 What is the difference relationship between the constant $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$ and $\mathbf{s}$?
Q13.7 How can we change the value of the constants $\mathcal{A}$?
Q13.8 Explain in words how changing the accelerating voltage affects the characteristic length, $\xi_{\mathbf{g}}$?
Q13.9 Why do we use the column approximation?
Q13.10 What will happen to the width of the column if the thickness of the specimen increases. How can we change the width of the column?
Q13.11 How does dynamical diffraction affect the interpretation of DPs?
Q13.12 What is the structure factor and what does it depend on?
Q13.13 Why is $\xi_{\mathbf{g}}$, the characteristic length, better known as the extinction distance?
Q13.14 What is the total wave function and why should we really be talking about Bloch waves?
Q13.15 What is the relationship between the intensity of the incident beam and the intensity of the diffracted beam? Give the equations and the name they go by.
Q13.16 Write down an expression for the effective excitation error.
Q13.17 Give an equation for the intensity in the Bragg-diffracted beam using the effective excitation error s_{eff} for a specimen thickness t.
Q13.18 What happens to the effective excitation error when $s = 0$? Can the effective excitation error ever equal zero? (Explain your reasoning.)
Q13.19 What value does the effective excitation error approach as the excitation error, s, becomes large?
Q13.20 Define what $\phi_{\mathbf{g}}$ and $\phi_{\mathbf{0}}$ mean in the context of this chapter and how they relate to the beam intensities $I_{\mathbf{g}}$ and $I_{\mathbf{0}}$?
Q13.21 In principle, could the intensities predicted by the Howie-Whelan equations affect what you see in DPs? Is this likely to occur in practice?

TEXT-SPECIFIC QUESTIONS

T13.1 Examine Table 13.2. (a) Discuss why MgO, 111 looks odd. (b) Explain why ξ_{220} for diamond is less than ξ_{220} for Si and why this appears unexpected at first.
T13.2 Taking reasonable values for the different parameters: V_c, θ_B, λ, and F, deduce ξ_{111} for Cu and W using equation 13.4.
T13.3 Starting with equations 13.6 and 13.7, deduce equations 13.8 and 13.9 showing where we make the approximations.
T13.4 We state that we know we should use Bloch waves. Why is this so? Would this be true if the specimen were amorphous? If not, what would you recommend (assuming that you have to work with amorphous materials)?
T13.5 Derive equation 13.18.
T13.6 We show that there are two solutions to the Howie-Whelan equations. Explain in words why this is so. What is the physical significance of this result?
T13.7 Show that equations 13.42 and 13.43 do satisfy equation 13.16.
T13.8 Consider the Cu_{220} reflection in a 200-kV TEM. Increase s in six equal increments to a value of 2×10^{-3} Å^{-1} (six values excluding 0 but including 2×10^{-3} Å^{-1}). Construct a table to show how s_{eff} varies. Give your results in Å^{-1} and nm^{-1}.

T13.9 In Figure 13.4 d is said to be ~2 nm. Consider five samples of Si with thickness 20, 50, 100, 200 nm, and 1 μm in a 200-eV TEM with 220 excited. What value should we use for d in each case?

T13.10 Repeat question 13.9 for Cu and 111.

T13.11 We state that the highest useful magnification in a TEM is about 10^6. How is this changed if we add a CCD camera? What is the lowest useful magnification with and without a CCD camera (excluding the DP)? How is this changed if you use a FEGTEM?

T13.12 For the perfect crystal situation, what is the ratio of $|\phi_{\mathbf{g}}|^2$ to $|\phi_{\mathbf{0}}|^2$ when s is 10^{-1} Å^{-1} and 10^{-2} Å^{-1} for the 220 reflection in Cu and Si at 100 kV. Explain any assumptions you make.

T13.13 Do you think Darwin's papers are really relevant to the Howie-Whelan equations?

T13.14 Using reasonable values for f, deduce values for $\xi_{\mathbf{g}}$ for

a) Cu with 220 and 100 keV
b) Si with 111 and 200 keV
c) W with 100 and 300 keV.

What assumptions have been made in applying this formula?

T13.15 Are the values given in Table 13.2 for Al, Fe, and Ge consistent?

T13.16 We differentiate between χ and $\mathbf{k}$. Do you expect there is a significant difference? Discuss the magnitude of this difference, how it varies with kV and how you might assess this magnitude.

T13.17 Using earlier equations, deduce equations 13.8 and 13.9.

T13.18 How will dynamical scattering of X-rays compare to that for electrons?

T13.19 After equation 13.16 we state that the nature of the material only enters through $\xi_{\mathbf{g}}$. Argue against this statement.

T13.20 Consider Figure 12.6A for Cu G = 220 and 100-keV electrons. Deduce w in equation 13.26. Hence, determine β in equation 13.2.

T13.21 Use the results of the previous question to deduce $C_0^{(1)}$, etc., in equation 13.31.