Thinking in Reciprocal Space

12

CHAPTER PREVIEW

In the previous chapter, you've already encountered vectors **k** and **g** and seen that they have lengths with units Å^{-1} or nm^{-1}. These vectors are referred to as reciprocal lattice vectors. Now we are going to discuss what this reciprocal lattice is. The reciprocal lattice is simply a lattice in reciprocal space. Note that this lattice is just as real as the "real lattice" in "real" space. It's like a new world in *Gulliver's Travels* but the relationship to "our" world is not a linear scaling factor but a reciprocal one. If something (an object or a length) is large in real space, then it's small in reciprocal space.

> When you see an object in real space you need to think, "What would it look like in reciprocal space?"

The reciprocal lattice is a purely geometrical construction. We'll separate the discussion into two parts: (i) the math and (ii) the properties of this lattice. The first is the same as you will meet in any text on solid-state physics; the second relates to how we use this construction in TEM. What we will find is that the lattice gives us a method for picturing the geometry of diffraction; it gives us a "pictorial representation" of diffraction. It helps us visualize how diffraction patterns will vary as the orientation and physical characteristics of the specimen vary.

D. B. Williams et al., *Transmission Electron Microscopy*

Thinking in Reciprocal Space

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12.1. WHY INTRODUCE ANOTHER LATTICE?

If you're new to the field of diffraction, the concept of reciprocal space may seem a daunting theoretical proposal. You must persevere. This model gives a physical picture of diffraction geometries that is extremely helpful to you, the experimentalist. The best approach is to think of any crystal as having two lattices. The first describes the arrangement of the unit cells of atoms in the crystal (your specimen). The second is an array of points which is uniquely defined for any given crystal but does not correspond to arrays of atoms; instead, each point is associated with a particular set of planes in the crystal. Of course, the reciprocal lattice is just as real as the "real" lattice; both are simply geometrical constructions. We'll use the reciprocal lattice to give you a physical picture of what happens when a crystal diffracts.

> Think of any crystal as having two lattices, one real and the other reciprocal.

Historical Note: The reciprocal lattice was rediscovered independently by Ewald and Laue in 1911–14, but it had been described by Gibbs in 1881 and by Bravais (in a somewhat less useful form) in 1850! The discussion of Ewald's contribution to the subject is recommended reading (Ewald 1962).

In Chapter 11 we showed that Bragg diffraction of electrons by crystals occurs when **K** is equal to **g**. The reciprocal lattice concept allows us to define a lattice where all the lattice points correspond to the possible **g** vectors.

> In the reciprocal lattice, sets of parallel ($hk\ell$) atomic planes are represented by a single point located a distance $1/d_{hk\ell}$ from the lattice origin.

To understand why we use the reciprocal lattice, remember that we can always write Bragg's Law (equations 11.2 and 11.3) as

$$\frac{2\sin\theta_B}{\lambda} = \frac{n}{d} = |\mathbf{K}| \qquad [12.1]$$

Thus the vector **K** is reciprocally related to d, and vice versa. Before using this new lattice, however, we must work through its formal definition.

12.2. MATHEMATICAL DEFINITION OF THE RECIPROCAL LATTICE

In this section we will go through the definition of the reciprocal lattice as a mathematical construction and prove some of the special mathematical properties of the vector, **g**. You don't need to learn the proofs but you will need to know these equations.

> The mathematics of the reciprocal lattice construction is simple vector algebra.

In real space, we can define any lattice vector, $\mathbf{r}_n$, by the equation

$$\mathbf{r}_n = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c} \qquad [12.2]$$

where the vectors **a**, **b**, and **c** are the unit-cell translations in real space while n_1, n_2, and n_3 are all integers.

Any reciprocal lattice vector, $\mathbf{r}^*$, can be defined in a similar manner

$$\mathbf{r}^* = m_1\,\mathbf{a}^* + m_2\,\mathbf{b}^* + m_3\,\mathbf{c}^* \qquad [12.3]$$

where **a** *, **b***, and **c*** are the unit-cell translations in reciprocal space while m_1, m_2, and m_3 are all integers. These new vectors are defined by the relations

$$\mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0 \qquad [12.4]$$

In words, **a*** is normal to both **b** and **c**, etc. We also define that

$$\mathbf{a}^*\cdot\mathbf{a} = 1;\ \mathbf{b}^*\cdot\mathbf{b} = 1;\ \mathbf{c}^*\cdot\mathbf{c} = 1 \qquad [12.5]$$

Be careful; this result does not mean that **a*** is parallel to **a** (think about this!). The direction of **a*** is actually completely defined by equation 12.4. It is perpendicular to both **b** and **c** and must therefore be the normal to the plane containing **b** and **c**.

> The vector **a*** is always perpendicular to the plane (100) even when **a** is not.

Equation 12.5 then uniquely defines the length of the vector **a*** in terms of the length of the vector **a**. Therefore, this equation gives the scale or dimension of the reciprocal lattice. The product of the projection of **a*** on the vector **a** multiplied by the length of **a** is unity. We can see that if **a**, **b**, and **c** are large, then the corresponding reciprocal lattice vectors will be small if we choose conventionally shaped unit cells.

Since V_c, the volume of the unit cell, is given by $\mathbf{a}\cdot\mathbf{b}\wedge\mathbf{c}$, then from equation 12.5 we can write **a*** as

$$\mathbf{a}^* = \frac{\mathbf{b}\wedge\mathbf{c}}{V_c} \qquad [12.6]$$

This definition emphasizes that the vector **a*** is orthogonal to the vectors **b** and **c**. However, just as **a**, **b**, and **c** need not be normal to one another, **a***, **b***, and **c*** are also not necessarily normal to one another. We use the usual clockwise convention in defining the vector product in equation 12.6.

12.3. THE VECTOR g

We can generalize our definition of **g** a little more. Any vector in reciprocal space can be defined as a combination of the vectors **a***, **b***, and **c***. In particular, we can write **K** in this form for use later

$$\mathbf{K} = \xi\,\mathbf{a}^* + \eta\,\mathbf{b}^* + \zeta\,\mathbf{c}^* \qquad [12.7]$$

A particularly important reciprocal lattice vector is the vector $\mathbf{g}_{hk\ell}$, which is defined as

$$\mathbf{g}_{hk\ell} = h\,\mathbf{a}^* + k\,\mathbf{b}^* + \ell\,\mathbf{c}^* \qquad [12.8]$$

where *h*, *k*, and *ℓ* are all integers and together define the plane $(hk\ell)$.

The definition of the plane $(hk\ell)$ is that it cuts the *a*, *b*, and *c* axes at $1/h$, $1/k$, and $1/\ell$, respectively. If you look at Figure 12.1, you'll see that the vector **AB** can be written as $\mathbf{b}/k - \mathbf{a}/h$. This vector, and all vectors in the $(hk\ell)$ plane, are normal to the vector $\mathbf{g}_{hk\ell}$ defined in equation 12.8. You can prove this by taking the dot product of **AB** and **g** and using equations 12.4 and 12.5. Therefore, the vector $\mathbf{g}_{hk\ell}$ must be *normal* to the plane $(hk\ell)$.

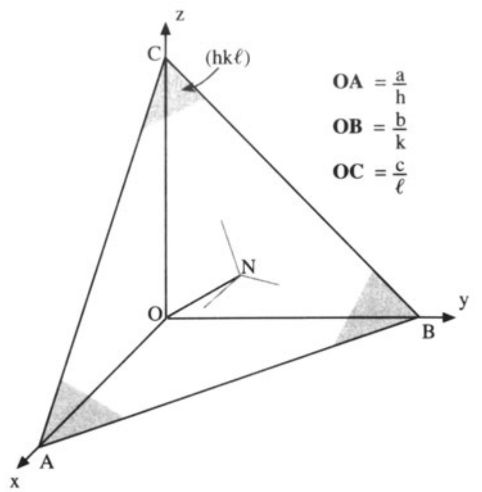

Figure 12.1. The plane ABC has Miller indices $(hk\ell)$. The vectors **OA**, **OB**, and **OC** have lengths a/h, b/k, and c/ℓ. The vector **ON**, which may be written as **n**, is normal to the plane $(hk\ell)$. In the text we see that the reflection, **g**, which is associated with diffraction from the $(hk\ell)$ planes, is parallel to **n** and normal to all vectors in $(hk\ell)$.

$$\left(\frac{\mathbf{b}}{k} - \frac{\mathbf{a}}{h}\right)\cdot\left(h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*\right) = 0 \qquad [12.9]$$

The vectors **AB**, **BC**, and **CA** all lie in the plane $(hk\ell)$ and each is normal to $\mathbf{g}_{hk\ell}$. All that we now have to prove is that the length of the vector $|\mathbf{g}_{hk\ell}|$ is given by $(d_{hk\ell})^{-1}$. To show this relationship, consider a unit vector, **n**, normal to the plane (i.e., parallel to $\mathbf{g}_{hk\ell}$) and take the dot product with any unit vector inclined to this plane (e.g., $\mathbf{a}/h$ or $\mathbf{b}/k$).

The unit vector, **n**, parallel to **g** is simply $\mathbf{g}/|\mathbf{g}|$. Therefore, the shortest distance from the origin O to the plane is the dot product of **n** with vector **OB** (or **OC**, etc.)

$$\mathbf{n}\cdot\frac{\mathbf{a}}{h} = \frac{\mathbf{g}}{|\mathbf{g}|}\cdot\frac{\mathbf{a}}{h} = \frac{\left(h\mathbf{a}^* + k\mathbf{b}^* + \ell\mathbf{c}^*\right)}{|\mathbf{g}|}\cdot\frac{\mathbf{a}}{h} = \frac{1}{|\mathbf{g}|} \qquad [12.10]$$

where we again used equations 12.4 and 12.5. Since the origin, O, by definition lies on a plane in this family of planes, equation 12.10 gives the distance between parallel $(hk\ell)$ planes, so that

$$d_{hk\ell} = \frac{1}{|\mathbf{g}|} \qquad [12.11]$$

as we required.

- The definition of the *hkℓ* indices is OA = *a*/*h*; OB = *b*/*k*; OC = *c*/*ℓ*.
- The plane ABC can then be represented as (*hkℓ*).

We should emphasize a few points before moving on:

- Remember: the reciprocal lattice is so called because all lengths are in reciprocal units.
- If you are familiar with the derivation of band-gap concepts in elementary solid-state physics, you will have already used these ideas. The difference is that the energies of the electrons being produced in the microscope are ≥100 keV, whereas those in solids are ~1 eV. This will affect the magnitudes of **k** but the **a***, etc., will not change with kV.
- Reciprocal-space notation. We introduced the use of brackets in Section 11.7. Now we'll extend this notation to the reciprocal lattice: (*hkℓ*) is shorthand notation for a particular vector in reciprocal space because it is normal to the (*hkℓ*) plane in real space; {*hkℓ*} is then the general form for these reciprocal lattice vectors. [*UVW*] is a particular plane in reciprocal space, e.g., it may contain many {*hkℓ*} points so that in real space it would be a direction—the zone axis for the {*hkℓ*} real-space planes (see Table 12.1). When indexing diffraction spots, you will often find that the brackets have been entirely omitted; this is a sort of convention. You should use brackets if there is any ambiguity, or for emphasis.
- *Warning:* the real-lattice vectors and the reciprocal-lattice vectors with the same indices (e.g., [123] and the normal to the plane (123)) are *parallel only* in the case of cubic materials. In other material, some special vectors may be parallel to one another, but most pairs will not be parallel. This difference can surprise even the experienced microscopist, particularly if you're used to studying cubic metals. For example, if you orient the electron beam to be along the [123] zone axis in an orthorhombic crystal such as olivine, the beam will *not* be normal to the (123) plane.

TABLE 12.1. Notation for Planes, Directions, and Reflections

Real space	Reciprocal space	Indices
Particular direction	Particular plane	[*UVW*]
General direction	General plane	<*UVW*>
Particular plane	Particular direction	(*hkℓ*)
General plane	General direction	{*hkℓ*}
Diffracting plane	Indexed reflection	*hkℓ*

12.4. THE LAUE EQUATIONS AND THEIR RELATION TO BRAGG'S LAW

To understand the value of the reciprocal lattice, we will now reconsider some of the terms we discussed previously. We use Bragg's Law (Section 11.7) because it is so useful. It gives us a physical picture of the constructive interference phenomenon, but it does not really correspond to the actual situation in TEM. Our justification in using Bragg's Law is that we can derive it as a special form of the Laue equations, which really do describe diffraction in the TEM.

So we'll now derive Bragg's Law from the Laue equations using simple vector algebra. For much of our discussion we assume that the crystal is infinitely large; we can always take the reciprocal lattice to be infinite. We can then use intuition to see that constructive interference will only occur when

$$\mathbf{K} = \mathbf{g} \tag{12.12}$$

From Figure 12.2 we can see that the magnitude of **K** is always 2 sin θ/λ. At the Bragg condition it is also equal to the magnitude of **g**, i.e., 1/*d*. Therefore, at the Bragg condition we can write

$$\frac{2\sin\theta}{\lambda} = \frac{1}{d_{hk\ell}} \tag{12.13}$$

i.e.

$$\lambda = 2d\sin\theta \tag{12.14}$$

which is Bragg's Law.

Equation 12.12 represents the Laue conditions for constructive interference; so we will refer to this as the condition for Laue, or Bragg, diffraction. Prove for yourself that $\mathbf{g}\cdot\mathbf{r}_n$ is always an integer, *N*. Then we can use equation 12.2 to write the Laue conditions

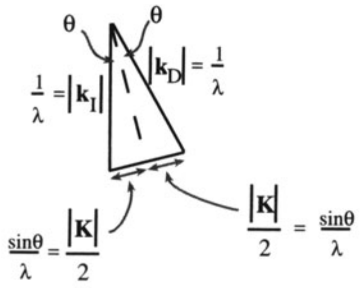

Figure 12.2. The geometric relationship between $\mathbf{k}_I$, $\mathbf{k}_D$, **K**, θ, and λ.

$$\mathbf{K}\cdot\mathbf{r}_n = N \qquad [12.15]$$

This equation tells us that we must satisfy certain conditions on **K** in order to have Bragg (or Laue) diffraction.

Using equation 12.7 and multiplying out this dot product we can see that this equation only holds when $\{n_1\xi + n_2\eta + n_3\zeta\}$ is an *integer*

$\mathbf{K}\cdot\mathbf{r}_n = N$ when ξ, η, and ζ are the integers h, k, and ℓ.

Note: this is a very special case. By setting $\mathbf{r}_n$ equal to the three unit vectors in turn, equation 12.15 gives three relationships

$$\mathbf{K}\cdot\mathbf{a} = h \qquad [12.16]$$

$$\mathbf{K}\cdot\mathbf{b} = k \qquad [12.17]$$

$$\mathbf{K}\cdot\mathbf{c} = \ell \qquad [12.18]$$

Of course, these equations are the same Laue diffraction conditions which we introduced back in Section 3.9.B, as given in equation 12.15. In Section 11.5 we quoted Bragg's Law, with an "*n*," as

$$n\lambda = 2d\sin\theta \qquad [12.19]$$

We also discussed the physical reason for *n*. We can now treat the same situation mathematically. If the integers *h*, *k*, and ℓ have a common factor then we can write

$$n\,d_{nh,nk,n\ell} = d_{hk\ell} \qquad [12.20]$$

So the *n* is implicit in the *d* used in equation 12.14. You will find that there are many other methods for treating this problem. We have chosen this approach to emphasize the underlying geometric principles.

12.5. THE EWALD SPHERE OF REFLECTION

The reciprocal lattice is a 3D array of points, each of which we will now associate with a reciprocal-lattice rod, or relrod for short, which is centered on the point. Furthermore, we will arrange each rod to be normal to the thin foil, but to have a finite thickness parallel to this foil normal. This geometry of the relrods holds even when we tilt the specimen. The fact that we have rods is the result of the shape of our TEM specimen. At this stage this is purely an empirical construction to allow us to explain why we see spots in the diffraction pattern even when the Bragg condition is not exactly satisfied. We will examine the shape of these rods and their origin in Chapter 16.

We now construct a sphere of radius $1/\lambda$. The sphere is known as the sphere of reflection or generally, and more simply, the "Ewald sphere," in honor of its inventor P.P. Ewald. Due to Ewald's German origins, Ewald is pronounced "A. Valt" rather than "E. Walled." Ewald's paper which first described the sphere was published in 1913 and was entitled "Contributions to the theory of interferences of X-rays in crystals." It appears, in translation, in the monograph edited by Cruickshank *et al.* (1992), along with several of his other papers; the articles collected in this review give a wonderful insight into the whole development of the theory of diffraction.

The sphere is usually represented in two dimensions by a circle and in most figures is drawn together with a two-dimensional section through the reciprocal lattice, as shown in Figure 12.3.

The key point is that when the sphere cuts through the reciprocal lattice point the Bragg condition is satisfied. When it cuts through a rod you still see a diffraction spot, even though the Bragg condition is not satisfied.

We combine the concept of the reciprocal lattice, the relrods, and the Ewald sphere construction to picture how the intensity of each diffracted beam varies as we tilt the specimen or the electron beam. You may see the position of a spot in the diffraction pattern move when the Ewald sphere is moved relative to the reciprocal lattice.

We can draw a sphere of radius $1/\lambda$ in reciprocal space so that it passes through the origin of the reciprocal

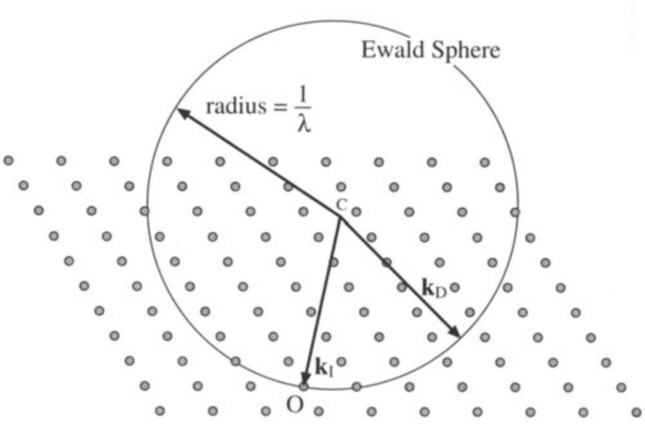

Figure 12.3. The Ewald sphere of reflection is shown intersecting a noncubic array of reciprocal-lattice points. The vector **CO** represents $\mathbf{k}_I$, the wave vector of the incident wave, and O is the origin of the reciprocal lattice. $\mathbf{k}_D$ is any radius vector. When the radius of the sphere is similar to the spacing between the points in the reciprocal lattice, as is the case for X-rays, the sphere can only intersect a few points, as shown. When λ is much smaller, as for 100-keV electrons, the radius is much larger, the sphere is flatter, and it intersects many more points.

lattice, point O, as defined in Chapter 11. If any point in the reciprocal lattice intersects the surface of the sphere, the set of planes corresponding to that point must satisfy the Bragg equation and hence the planes will diffract strongly. Equation 12.11 suggests that we define a vector **g** which can represent the quantity d^{-1}. The vector has a length and a direction. We choose the obvious length for **g** to be d^{-1} and make **g** the only unique vector for the plane ($hk\ell$), i.e., parallel to the normal to this plane.

We can associate an "intensity" with any position in reciprocal space, and in particular with any position along one of these rods.

The value for this intensity is such that if the Ewald sphere cuts through that point in reciprocal space, then the diffracted beam, **g**, will have that intensity.

In general, if the Ewald sphere moves, the intensity will change. The important idea to keep in mind is that the reciprocal lattice is just a construction we use to give us a pictorial way of looking at diffraction.

Of course, the diagram drawn in Figure 12.3 shows a cut through the Ewald sphere. We usually draw such a diagram to include the vector describing the incident beam CO, but this is not a requirement; in fact it is the exception, since our diagram is a two-dimensional cut through a 3D sphere. When we draw such a diagram we usually choose the plane of the diagram to contain the point O, since this point represents the direct beam. A common point of confusion concerns the location of the center of the Ewald sphere, C. The point C is not the origin; the origin is the point O. In fact C will probably not coincide with a reciprocal-lattice point.

The vector **CO** is $\mathbf{k}_I$ and has length $1/\lambda$; this defines where C is located, i.e., we start with O and measure back to C.

Now you can appreciate that it is only when the incident beam lies in our chosen plane that the vector **CO** will lie in that plane. For example, we may choose the plane to be parallel to the optic axis of the microscope but tilt the incident beam off this axis; in such cases we will still often be interested in the plane containing both the optic axis and the incident beam. Also notice that $\mathbf{k}_D$ could be any vector which begins at C and ends on the sphere.

Consider the relative dimensions of $d_{hk\ell}$ and λ. We can see that for X-rays where λ is ~0.2 nm and $1/\lambda$ is ~5 nm^{-1}, the Ewald sphere can only intersect a small number of relrods because $1/d$ is only ~3 nm^{-1}. This explains why it is necessary in X-ray diffraction to use white radiation (giving a wide range of λ) or to oscillate, rotate, or powder the specimen (thus producing many variations of d and θ) in order to produce enough diffraction spots to analyze the structure. For 100-keV electrons, however, λ is 0.0037 nm and $1/\lambda$ is 270 nm^{-1}. So the surface of the Ewald sphere is almost planar (but fortunately, as we will see in Section 12.6, not quite) in comparison with the array of reciprocal lattice spots. Therefore, in a TEM, the Bragg condition is nearly satisfied for many planes, and, as we saw in Figure 11.1, many diffraction spots are observed from a thin specimen corresponding to a section through the reciprocal lattice.

Rather than carry out the exercise of identifying arrays of spots for every orientation of the specimen, it is common practice to orient the specimen such that the beam is incident almost parallel to a low-index zone (U, V, and W are all small numbers), and then to compare the observed pattern with standard ones. We'll show you some standard patterns in Chapter 18. This approach is fine if you already know the crystal structure of your material. However, you'll need to know the full procedure if you have a material whose structure you don't know or if you are not able to rotate it to a low-index zone axis. This situation might arise, for example, when you are characterizing a grain boundary.

12.6. THE EXCITATION ERROR

We'll now introduce a new quantity, **s**, known as the excitation error or the deviation parameter. Always use these terms carefully! If the beam is exactly parallel to any zone axis then, according to the Laue conditions, there should be no spots in the diffraction pattern. Clearly there are many spots, so there is intensity in the diffracted beams even when the Bragg condition is not exactly satisfied. The actual intensity will depend on how far we are away from the Bragg condition. This distance is measured by a vector, **s**, in reciprocal space such that

$$\mathbf{K} = \mathbf{g} + \mathbf{s} \qquad [12.21]$$

This vector, **s**, is a measure of how far we deviate from the exact Bragg condition.

The Ewald sphere intersects the reciprocal lattice point at the center of a relrod when **s** = 0. Equation 12.21 is very imprecise! Although **g** is well defined, **K** is not, because it depends on $\mathbf{k}_D$, which could be any vector terminating on the Ewald sphere. In Figure 12.4, we show two special values of **s** by choosing two special values of $\mathbf{k}_D$. In one, $\mathbf{k}_D$ lies along the vector **CG** so $\mathbf{s}_c$ is also parallel to **CG**; in the second, $\mathbf{s}_z$ is chosen to be parallel to vector **CO**, the incident wave vector. A third special situation would be

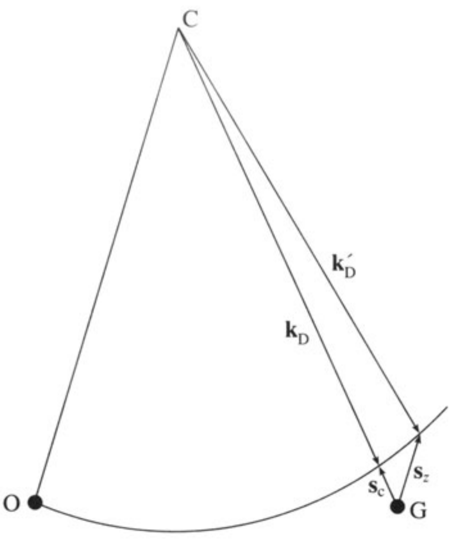

Figure 12.4. Two special values of **s** are illustrated. When $\mathbf{k}_D$ lies along **CG** then $\mathbf{s}_c$ is parallel to **CG**. Alternatively, we can choose **s** to be parallel to the incident beam direction **CO**; then $\mathbf{s} = \mathbf{s}_z$ and $\mathbf{k}_D$ becomes $\mathbf{k}'_D$. In each case, $\mathbf{k}_D$ ends on the Ewald sphere.

to define $\mathbf{s}_m$ as being perpendicular to the surface of the specimen, but we don't know where that is. Actually, we will often assume that $\mathbf{s}_m$ is perpendicular to **OG**, but this need not be the case. We will refer to **s** in several ways: $\mathbf{s}_\mathbf{g}$ will emphasize that **s** is defined for a particular **g** while $\mathbf{s}_z$ will emphasize that **s** lies along the *z*-axis, which often corresponds to the incident beam direction and the foil normal. We write **s** when we are not being specific.

When we drew Figure 12.4, you noticed that we placed the point G outside the Ewald sphere. By convention, we define the sign of **s** in this case to be negative, while **s** is positive when G is inside the Ewald sphere; note that we are using G to emphasize that we are referring to the point, not the vector, **g**, from the origin to the point. In Figure 12.4, the row of reciprocal lattice points (only G is shown) is essentially at 90° to the incident beam. If we take all such rows, we define a plane of points which are all at 90° to the incident beam. This plane of points is called the zero-order Laue zone (ZOLZ). We can now number all the planes of points which are parallel to the ZOLZ but do not contain the point O, and call these the higher-order Laue zones, or HOLZ. The first of these (going toward C) is the FOLZ, the second is the SOLZ, and the rest are just HOLZ.

If we now draw the Ewald sphere as shown in Figure 12.5, you can see that it will intersect points in the FOLZ and other HOLZ. We'll see examples of these kinds of diffraction patterns in Chapters 20 and 21.

We can change the value of **s** in two ways:

- First, if we tilt the specimen, the row of spots moves but the Ewald sphere does not.

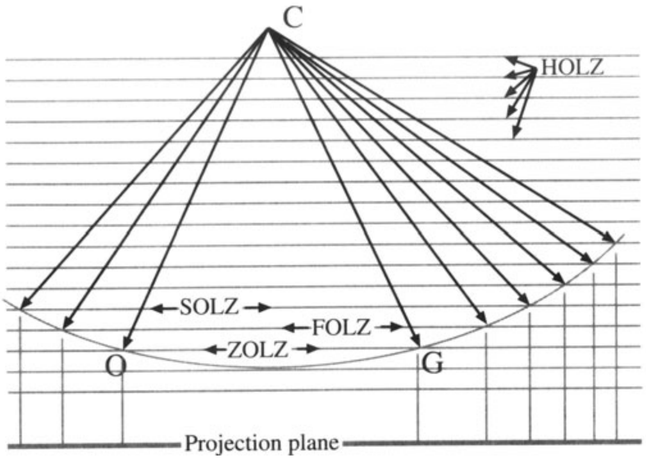

Figure 12.5. The Ewald sphere intercepts points in higher-order Laue zones (HOLZ) at large angles to the incident-beam direction. If the radius of the sphere increases (higher kV beam) then the sphere flattens and the HOLZ interception is at still larger angles.

- Second, if we tilt the beam above the specimen, the Ewald sphere moves, because $\mathbf{k}_I$ tilts, because C moves!

Convince yourself of this. The diffraction patterns with different values of **s** may appear identical, but be cautious (more about this in next chapter). The difference between these two processes is shown in Figure 12.6.

We'll conclude this section by giving you an experimental diffraction pattern to think about. Figure 12.7 shows a DP from a slightly misoriented twin boundary: all you need to know is that different grains are diffracting to give two different DPs. You can identify a ring of bright spots from each crystal. The question is: why are the rings displaced from one another? Yes, you're right, there is much more to this pattern that first meets the eye, as we'll see in Chapter 19.

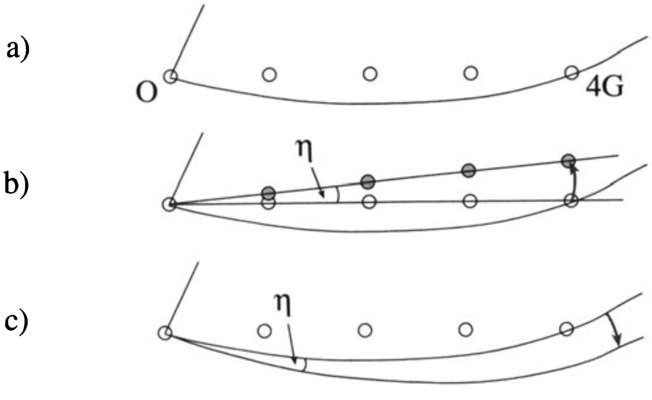

Figure 12.6. In (a) $s_z = 0$ for 4G. We can change s_z in two ways: (b) if we tilt the specimen through angle η, the row of spots moves inside the sphere; (c) if we tilt the beam through η above the specimen, in the opposite direction, the sphere moves outside the row of spots.

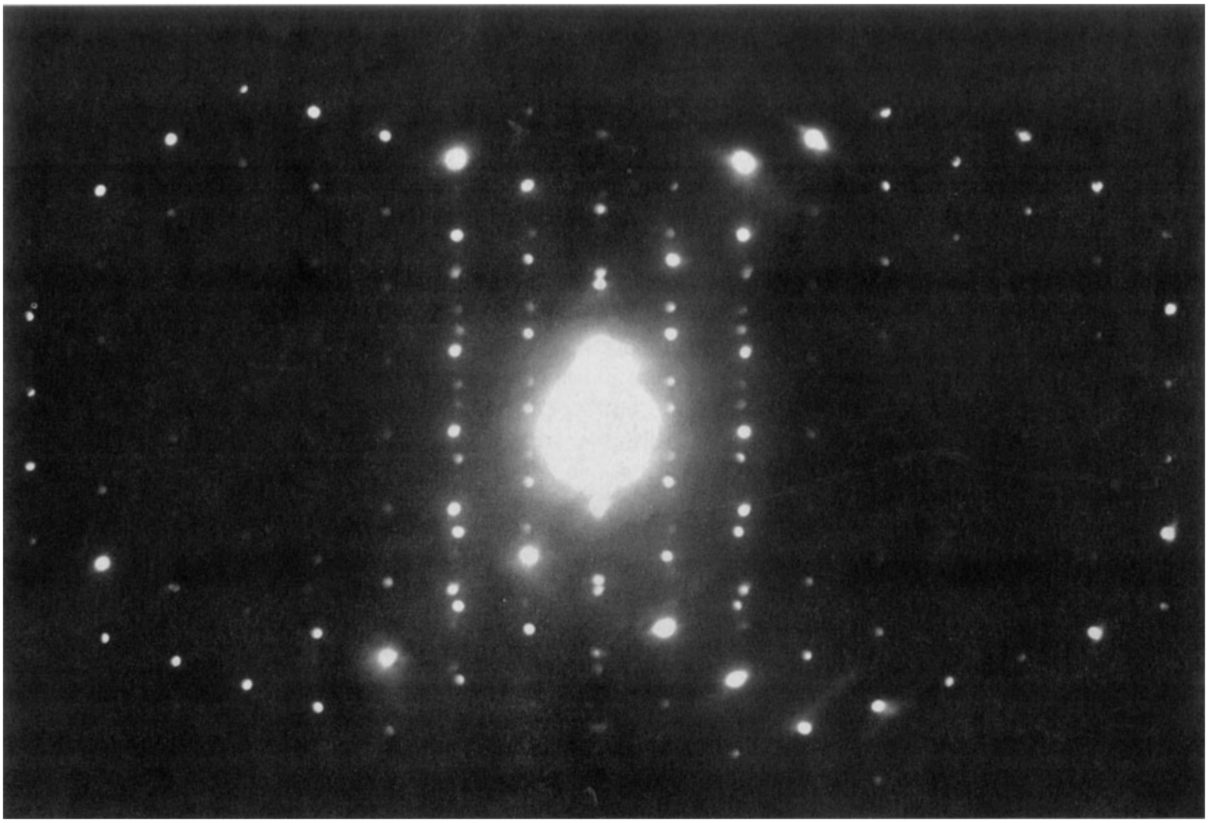

Figure 12.7. Diffraction pattern taken across a twin boundary in $MgAl_2O_4$ spinel. The rings of bright spots show where the Ewald sphere intercepts the reciprocal lattice of the crystals either side of the twin boundary.

12.7. THIN-FOIL EFFECT AND THE EFFECT OF ACCELERATING VOLTAGE

We will return to this topic in detail in Chapter 17 after we've examined a little more of the underlying theory. Here, we will briefly remind you that the radius of the Ewald sphere changes as we change kV. As the kV increases, the surface of the sphere becomes flatter. In a way, we were lucky with the initial choice of 100-keV electrons for TEMs since the sphere for 100-keV electrons has a very useful curvature. How does this curvature affect the diffraction pattern? Well, we know that $\mathbf{k}_I - \mathbf{k}_D = \mathbf{K} = \mathbf{g}$ where $|\mathbf{g}|$ is d^{-1}. Therefore, **g** does not change as we change λ. Since d does not change but λ does, then Bragg's Law tells us that θ must decrease as the kV increases. Therefore, if you keep the camera length constant, it will appear that the length of **g** in the diffraction pattern decreases as λ decreases. Notice that the key word here is "appear." If you look back at Section 9.6.B, you'll realize that the problem is that you must recalibrate the camera length for the new accelerating voltage.

The specimen is unchanged so the reciprocal lattice is the same. However, as the kV increases, the radius of the Ewald sphere increases and the diffraction spots appear to move closer together.

It is very important for TEM that because λ is small, the radius of the Ewald sphere, λ^{-1}, is large and hence the Ewald sphere is quite flat. Note that this is very different from what we find in LEED or a typical back-reflection Laue X-ray pattern. The result is that we

Table 12.2. Particular Values of λ and λ^{-1} as a Function of Accelerating Voltage

E	λ (Å)	Radius, λ^{-1} (Å^{-1})	$(v/c)^2$
100 keV	0.03701	27.02	0.3005
120 keV	0.03349	29.86	0.3441
200 keV	0.02508	39.87	0.4834
300 keV	0.01969	50.80	0.6030
400 keV	0.01644	60.83	0.6853
1 MeV	0.008719	114.7	0.8856

see many spots in the DP. Some values of the radius of the Ewald sphere are given in Table 12.2.

You'll find it a useful exercise to generate this table yourself using a spread-sheet. Use the values from Chapter 1: $m_0 = 9.109 \times 10^{-31}$ kg, $c = 2.998 \times 10^{8}$ ms^{-1}, $h = 6.626 \times 10^{-34}$ Nms, and 1eV = 1.602×10^{-19} Nm.

CHAPTER SUMMARY

When combined with the Ewald sphere construction, the reciprocal lattice gives us a very simple way of thinking about diffraction. When the sphere exactly cuts through a point, Bragg's Law or the Laue equations are exactly satisfied. When the sphere just misses a point, we define a distance **s** to quantify this excitation error. In other words, **s** is a measure of where we cut the relrod. Ideally, you will become as familiar with tilting reciprocal lattices in space as you are with tilting real lattices in your specimen holder. Remember that the lattices are rigidly connected to one another: when one turns the other does by exactly the same amount. Although Lilliput does not exist, reciprocal space does—at least for the electron microscopist!

Keep in mind the geometry and the dimensions.

- The Ewald sphere has a radius of $1/\lambda$ and always passes through the point O in the reciprocal lattice.
- Reciprocal lattice dimensions are Å^{-1} or nm^{-1}. Since 10 Å = 1 nm, 1 Å^{-1} = 10 nm^{-1}.

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