Scattering and Diffraction

2

CHAPTER PREVIEW

The electron is a low mass, negatively charged particle. As such, it can easily be deflected by passing close to other electrons or the positive nucleus of an atom. These Coulomb (electrostatic) interactions cause the electron scattering which is the process that makes TEM feasible. We will also discuss how the wave nature of the electron gives rise to diffraction effects. What we can already say is that if the electrons didn't scatter, then there would be no mechanism to create TEM images or diffraction patterns and no source of spectroscopic data. So it is essential to understand both the particle approach and the wave approach to electron scattering in order to be able to interpret all the information that comes from a TEM. Electron scattering from materials is a reasonably complex area of physics, but it isn't necessary to develop a detailed comprehension of scattering theory to be a competent microscopist.

We start by defining some terminology that recurs throughout the book and then we introduce a few fundamental ideas that have to be grasped. These fundamental ideas can be summarized in the answers to three questions.

- What is the probability that an electron will be scattered when it passes near an atom?
- If the electron is scattered, what is the angle through which it is deviated?
- Does the scattering event cause the electron to lose energy or not?

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

The answer to the first question concerning the probability of scattering is embodied in the ideas of cross sections and mean free paths, so we define these concepts in this chapter. The angle of scattering, usually determined through the differential cross section, is also important because it allows you as TEM operator to control which electrons form the image, and therefore what information is contained in the image. We will develop this point much further when we talk about image contrast in Part III of the book. To answer the third question we must distinguish elastic and inelastic scattering. The former constitutes most of the useful information in diffraction patterns obtained in the TEM, discussed in Part II, while the latter is the source of X-rays and other spectroscopic signals discussed in Part IV. The distinction between electrons that lose energy and those that don't is important enough that we devote the subsequent two chapters to each kind of electron and expand on the basic ideas introduced here.

The electron beam is treated in two different ways: in electron scattering it is a succession of particles, while in electron diffraction it is treated by wave theory. The analogy to X-rays or visible light would be to compare a beam of photons and an electromagnetic wave. However, we must always remember that electrons are charged particles and that Coulomb forces are very strong.

Scattering and Diffraction

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2.1. WHY ARE WE INTERESTED IN ELECTRON SCATTERING?

We need to know about electron scattering because it is fundamental to all electron microscopy (not just TEM). You know well that your eye cannot see anything unless it interacts with visible light in some way, for example through reflection or refraction, which are two forms of scattering. Similarly, we cannot see anything in electron microscope images unless the specimen interacts with, and scatters, the electrons in some way. Thus any nonscattering object is invisible, and we will come across situations where "invisibility" is an important criterion. In the TEM we are usually most interested in those electrons that do not deviate far from the incident electron direction. This is because the TEM is constructed to gather these electrons primarily and they also give us the information we seek about the internal structure and chemistry of the specimen. Other forms of scattering, such as electrons which are scattered through large angles, including backscattered and secondary electrons, are also of interest and we will not neglect them, although they are of the greatest interest to SEM users and give surface-sensitive information, such as topography.

In this chapter we introduce the fundamental ideas of electron scattering, then in the next two chapters we discuss the two principal forms of scattering, namely elastic and inelastic. Both forms are useful to us, but you'll see that the latter has the unfortunate side effect of being responsible for specimen damage and ultimately limits what we can do with a TEM.

To give you some feel for the importance of electron scattering, it is worth illustrating at this stage the basic principles of the TEM. You will see in due course that in a TEM we illuminate a thin specimen with electrons in which the electron intensity is uniform over the illuminated area.

> We will often refer to incident and scattered electrons as "beams" of electrons, because we are dealing with many electrons, not an individual electron; these electrons are usually confined to well-defined paths in the microscope. For example, the electron beam that comes through the specimen, parallel to the direction of the incident beam, is an important beam, which we will term the *direct beam.*

As the electrons travel through the specimen, they are either scattered by a variety of processes or they may remain unaffected by the specimen. The end result is that a nonuniform distribution of electrons emerges from the exit surface of the specimen, as shown schematically in Figure 2.1. It is this nonuniform distribution that contains all the structural and chemical information about our specimen. So everything we learn about our specimen using TEM can be attributed to some form of electron scattering.

We'll see in Chapter 9 that the electron microscope is constructed to display this nonuniform distribution of electrons in two different ways. First, the *angular distribution* of scattering can be viewed in the form of scattering patterns, usually called diffraction patterns, and the *spatial distribution* of scattering can be observed as contrast in images of the specimen. A simple (and fundamental) operational step in the TEM is to use a restricting aperture, or an electron detector, of a size such that it only selects electrons that have suffered more or less than a certain angular deviation. Thus, you as operator have the ability to choose which electrons you want to use and thus you control what information will be present in the image. Therefore, to comprehend these images, you have to understand what causes electrons to scatter in the first place.

We devote the whole of Part II to diffraction phenomena and the whole of Part III to images. Then, Part IV deals with ways in which we use inelastic scattering to

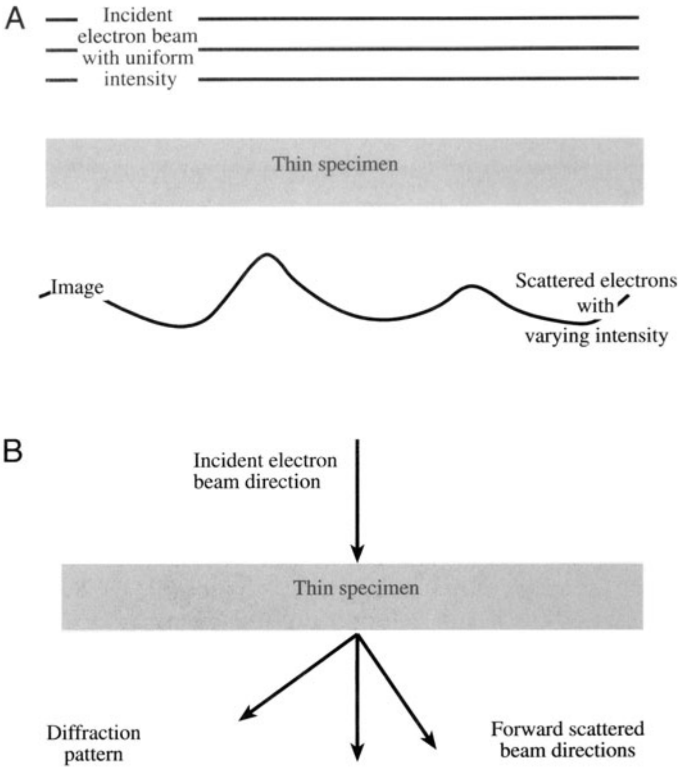

Figure 2.1. (A) A uniform intensity of electrons, represented by the flat line, falls on a thin specimen. Scattering within the specimen changes both the spatial and angular distribution of the emerging electrons. The spatial distribution (intensity) is indicated by the wavy line. (B) The change in angular distribution is shown by an incident beam of electrons being transformed into several forward-scattered beams.

study the chemistry of the specimen. So electron scattering is the theme that permeates this text and connects all aspects of TEM.

2.2. TERMINOLOGY OF SCATTERING

Electron scattering can be grouped in different ways. We've already used the most important terms *elastic* and *inelastic* scattering. These terms are simply descriptions of scattering that results in no loss of energy and some measurable loss of energy, respectively. In this case we tend to consider the electrons as particles, and scattering to involve some interaction like billiard balls colliding. However, we can also separate scattered electrons into *coherent* and *incoherent*, which refers of course to their wave nature. These distinctions are related, since elastic electrons are usually coherent and inelastic electrons are usually incoherent. Let's assume that the incident electron waves are coherent, that is they are essentially in step (in phase) with one another and of a fixed wavelength, governed by the accelerating voltage. (We'll see that this isn't a bad assumption in most circumstances.) Then coherently scattered electrons are those that remain in step and incoherently scattered electrons have no phase relationship after interacting with the specimen.

The nature of the scattering can result in different angular distributions. Scattering can be either *forward scattering* or *back scattering* (usually written as one word) wherein the terms refer to the angle of scattering with respect to the incident beam and a specimen normal to the beam. (Note: you will sometimes see the term forward scattering used in another sense.) If an electron is scattered through < 90° then it is forward scattered, and if > 90° it is backscattered. These various terms are related by the following general principles, summarized in Figure 2.2.

- Elastic scattering is usually coherent, if the specimen is thin and crystalline.

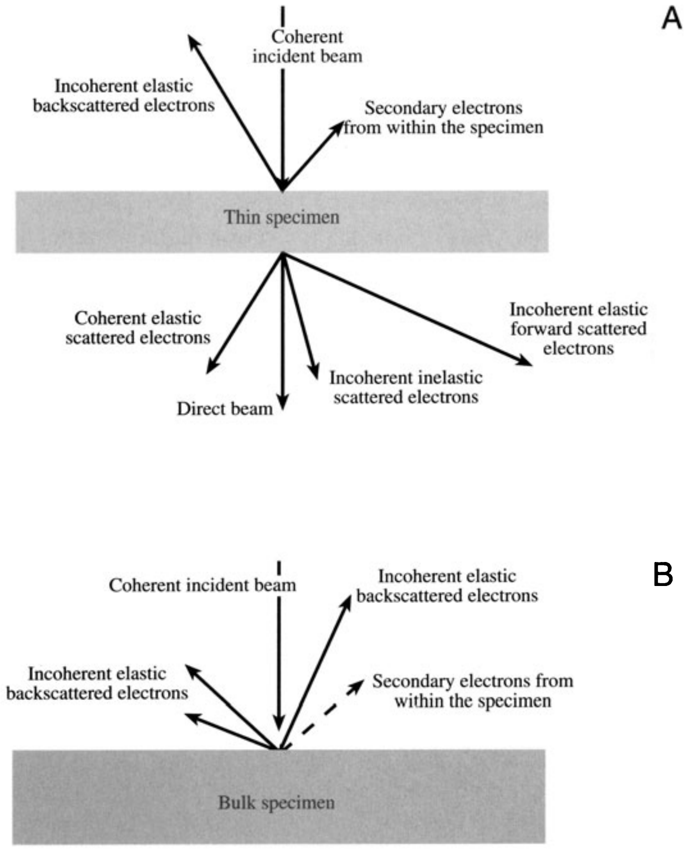

Figure 2.2. Different kinds of electron scattering from (A) a thin specimen and (B) a bulk specimen: a thin specimen permits electrons to be scattered in both the forward and back directions while a bulk specimen only backscatters the incident beam electrons.

- Elastic scattering usually occurs at relatively low angles (1–10°), i.e., in the forward direction.
- At higher angles (> ~10°) elastic scattering becomes more incoherent.
- Inelastic scattering is almost always incoherent and relatively low angle (<1°) forward scattering.
- As the specimen gets thicker, less electrons are forward scattered and more are backscattered until primarily incoherent backscattering is detectable in bulk, nontransparent specimens.

The notion that electrons can be scattered through different angles is related to the fact that electrons can also be scattered more than once. Generally, the more scattering events, the greater the angle of scatter, although sometimes a second scattering event can redirect the electron back into the direct beam so it appears to have undergone no scattering. The simplest scattering process is *single scattering* and we often approximate all scattering within the specimen to a single scattering event (i.e., an electron either undergoes a single scattering event or it suffers no scattering). We'll see that this is often a very reasonable assumption if the specimen is very thin (something you can control). If the electron is scattered more than once we use the term *plural scattering,* and if it is scattered >20 times we say *multiple scattering*. It is generally safe to assume that, unless you have a particularly grim specimen, multiple scattering will not occur. The greater the number of scattering events, the more difficult it is to predict what will happen to the electron and the more difficult it is to interpret the images, diffraction patterns, and spectra that we gather. So once again we emphasize the importance of creating thin specimens so that the single scattering assumption is plausible.

In the transmission electron microscope we utilize the electrons that go through a specimen; it is important to note that such electrons are not simply "transmitted" in the sense of visible light through window glass. Electrons are scattered mainly in the forward direction, i.e., parallel to the incident beam direction. We might ask what percentage of the electrons are forward scattered and how does this vary with the thickness and atomic number of the "target" atom? This scattering is a direct consequence of the fact that there is such a strong interaction between electrons and matter.

> Forward scattering causes most of the signals used in the TEM.

Forward scattering includes elastic scattering, Bragg scattering, the events called diffraction, refraction, and inelastic scattering. Because of forward scattering through our thin specimen, we see a diffraction pattern or an image on the viewing screen, and detect an X-ray spectrum or an electron energy-loss spectrum outside the optical column. But don't neglect backscattering; it is an important imaging mode in the SEM.

2.3. THE CHARACTERISTICS OF ELECTRON SCATTERING

When physicists consider the theory of electron interactions within a solid, they usually consider scattering of electrons by a single, isolated atom, then progress to agglomerations of atoms, first in amorphous solids and then in crystalline solids. When an electron encounters a single, isolated atom it can be scattered in several ways, which we will cover in the next two chapters. For the time being let's imagine simply that, as shown in Figure 2.3, the electron is scattered through an angle θ (radians) into some solid angle Ω measured in steradians (sr). Often we assume that θ is small enough such that sin θ ≈ tan θ ≈ θ. When θ is this small, it is often convenient to use milliradians or mrads; 1 mrad is 0.0573°, 10 mrads is ~0.5°.

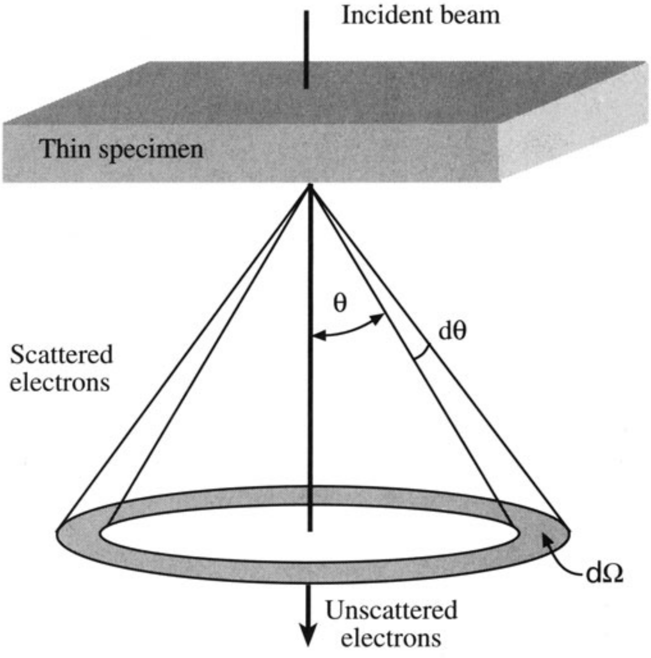

Figure 2.3. Electron scattering by a single isolated atom. The electrons are scattered through a semiangle θ and the total solid angle of scattering is Ω. An incremental increase in scattering angle *d*θ gives an incremental increase in a solid angle *d*Ω.

A convenient definition of a small angle is 10 mrads.

The characteristics of the scattering event are controlled by factors such as the electron energy and the atomic number/weight of the scattering atom. When we consider a specimen rather than a single atom, factors such as the thickness, density, and crystallinity of the specimen also become important. To understand these variables, we need to examine the physics of scattering in more detail.

2.4. THE INTERACTION CROSS SECTION

The chance of a particular electron undergoing any kind of interaction with an atom is determined by an interaction *cross section*. The concept of a cross section is well described by the following analogy given by Rudolf Peierls (Rhodes 1986).

> If I throw a ball at a glass window one square foot in area, there may be one chance in ten that the window will break and nine chances in ten that the ball will just bounce. In the physicist's language this particular window, for a ball thrown in this particular way, has a disintegration (inelastic!) cross section of 0.1 square feet and an elastic cross section of 0.9 square feet.

So each possible interaction has a different cross section which depends on the energy of the particle, in our case the beam energy. The cross section (for which we'll use the letter Q or the Greek σ) has units of area, not square feet as used in Peierls's analogy, but a tiny fraction of a square centimeter termed a "barn." One barn is 10^{-24} cm^2 [that's $(10^{-4}\text{Å})^2$] and the name arises because of the perverse sense of humor of some of the early atomic physicists who considered that this area is "as big as a barn door." Note again the use of non-SI units (cm^2) which persists in the literature, although we can easily define the barn as 10^{-28} m^2. The cross section does *not* represent a physical area, but when divided by the actual area of the atom it represents a *probability* that a scattering event will occur. So the larger the cross section, the better the chances of scattering.

We can look at scattering in two different, but equivalent, ways. First, following Hall (1953), since we are ignoring different kinds of scattering, we can talk about the *total* scattering cross section for the isolated atom, σ_T, which is simply the sum of all elastic and inelastic scattering cross sections such that the total σ_T is

$$\sigma_T = \sigma_{\text{elastic}} + \sigma_{\text{inelastic}} \qquad [2.1]$$

We can define the cross section (an area) in terms of the *effective radius* of the scattering center, r

$$\sigma = \pi r^2 \qquad [2.2]$$

where r has a different value for each of the scattering processes. For example, in the case of elastic scattering, which we'll see is most important in TEM image and diffraction pattern formation, the radius is given as

$$r_{\text{elastic}} = \frac{Ze}{V\theta} \qquad [2.3]$$

where V is the potential of the incoming electron, charge e, which is scattered through an angle greater than θ by atoms of atomic number Z. At first sight this equation seems dimensionally incorrect, since Z and θ are numbers. But V is in volts, so e has to be defined in esu such that the whole term has units of distance. This expression is useful because it indicates the general behavior of electrons in the TEM; i.e., usually electrons scatter less at high kV and high angles, and are scattered more by heavier atoms than light atoms.

Second, following Heidenreich (1964), if we instead consider that the specimen contains N atoms/unit volume, we can define the total cross section for scattering from the specimen (in units of cm^{-1} or m^{-1}) as

$$Q_T = N\,\sigma_T = \frac{N_0 \sigma_T \rho}{A} \qquad [2.4]$$

where N_0 is Avogadro's number (atoms/mole), and A is the atomic weight (g/mole) of the atoms in the specimen which has density ρ (so $NA = N_0\rho$). Thus Q can be regarded as the number of scattering events per unit distance that the electron travels through the specimen. If the specimen has thickness t, then the probability of scattering from the specimen is given by

$$Q_T\, t = \frac{N_0 \sigma_T (\rho\, t)}{A} \qquad [2.5]$$

The product of ρ and t is called the "mass-thickness" of the specimen (e.g., doubling ρ produces the same effect as doubling t) and we'll come across this term again when we discuss image contrast and also X-ray absorption. Equation 2.5 is an important expression, since it contains all the variables that affect the scattering probability from a real specimen. We'll use it again when we consider how certain kinds of image contrast arise in the TEM.

Expressions for the cross section become more complicated as they are modified to give better approximations for the scattering in a real specimen. For example, the expression for r_{elastic} which we would substitute in the cross-section equation for elastic scattering (equation 2.2) neglects any screening effects of the electron cloud around the nucleus, which obviously acts to reduce the Z effect. However, the more complex equations don't alter the basic scattering behavior predicted by the simple equations we've just given. If you want to see a fuller description of scattering, then read Chapter 1 by Newbury in Joy *et al.* (1986). If you're a glutton for punishment, the classical text on scattering is by Mott and Massey (1965).

Because of all the variables that affect σ and Q, it is only possible to give a ball-park value for the cross section. For TEM electron energies, the elastic cross section is almost always the dominant component of the total scattering. If you look ahead to Figure 3.3, typical small-angle elastic cross sections for transition metals bombarded by 100-keV electrons are ~10^{-22} m^2 (~10^{-18} cm^2). This is a good number to remember especially when you are considering the probability that a 100-keV electron will be elastically scattered. Inelastic cross sections range from ~10^{-22} m^2 down to 10^{-26} m^2 (100 barns), depending on the specific type of scattering and the material.

2.5. THE MEAN FREE PATH

Instead of using an area to describe the interaction, we can use a length since the distance an electron travels between interactions with atoms is clearly going to be an important concept. The total cross section for scattering can be expressed as the inverse of the mean free path, λ. This new parameter is then the average distance that the electron travels between scattering events. This distance is important because, if we know what it is, we can work out how thin we have to make our specimen so plural scattering is not significant, thus making it easier to interpret our images and spectroscopic data. Because the dimensions of Q are $(\text{length})^{-1}$ there is a simple expression for the mean free path λ which has units of length

$$\lambda = \frac{1}{Q} = \frac{A}{N_0\,\sigma_T\,\rho} \qquad [2.6]$$

Typical values of λ for scattering at TEM voltages are of the order of tens of nm, so single scattering approximations imply specimen thicknesses of this order. It is, unfortunately, conventional to use λ to denote the mean free path; it is *not* the wavelength of the electron. From this equation we can define a probability of scattering p as the electron travels through a specimen thickness t

$$p = \frac{t}{\lambda} = \frac{N_0\,\sigma_T\,(\rho\, t)}{A} \qquad [2.7]$$

which is just $Q_T t$ of equation 2.5.

2.6. THE DIFFERENTIAL CROSS SECTION

Because of the importance of the angle of scattering we need to introduce the concept of the *differential cross section* $d\sigma/d\Omega$. This term describes the angular distribution of scattering from an atom. As shown in Figure 2.3, electrons are scattered through an angle θ into a solid angle Ω and there is a simple geometrical relationship between the θ and Ω

$$\Omega = 2\pi(1-\cos\theta) \qquad [2.8]$$

and therefore

$$d\Omega = 2\pi \sin\theta\, d\theta \qquad [2.9]$$

So the differential scattering cross section can be written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{2\pi\sin\theta}\frac{d\sigma}{d\theta} \qquad [2.10]$$

Now, we can calculate σ for scattering into all angles which are greater than θ by integrating equation 2.10. This yields

$$\sigma_\theta = \int_\theta^\pi d\sigma = 2\pi\int_\theta^\pi \frac{d\sigma}{d\Omega}\sin\theta\, d\theta \qquad [2.11]$$

The limits of the integration are governed by the fact that the values of θ can vary from 0 to π, depending on the specific type of scattering. If we work out the integral we find that σ decreases as θ increases (which makes physical sense). Since $d\sigma/d\Omega$ is often what we measure experimentally, equation 2.11 gives us an easy way to determine σ for an atom in the specimen: σ for all values of θ is simply the integral from 0 to π. From this we can use equation 2.4 to give us the total scattering cross section from the whole specimen, which we will see later allows us to calculate the TEM image contrast. So we can now appreciate, through a few simple equations, the relationship between the physics of electron scattering and the information we collect in the TEM.

Our knowledge of the values of σ and λ is very sketchy, particularly at the 100–400 keV beam energies used in TEMs. Cross sections and mean free paths for particular scattering events may only be known within a factor of two, but we can often measure θ very precisely in the TEM. We can combine all our knowledge of scattering to predict the electron paths as a beam is scattered through a thin foil.

This process is called Monte Carlo simulation because of the use of random numbers in the computer programs; the outcome is always predicted by statistics!

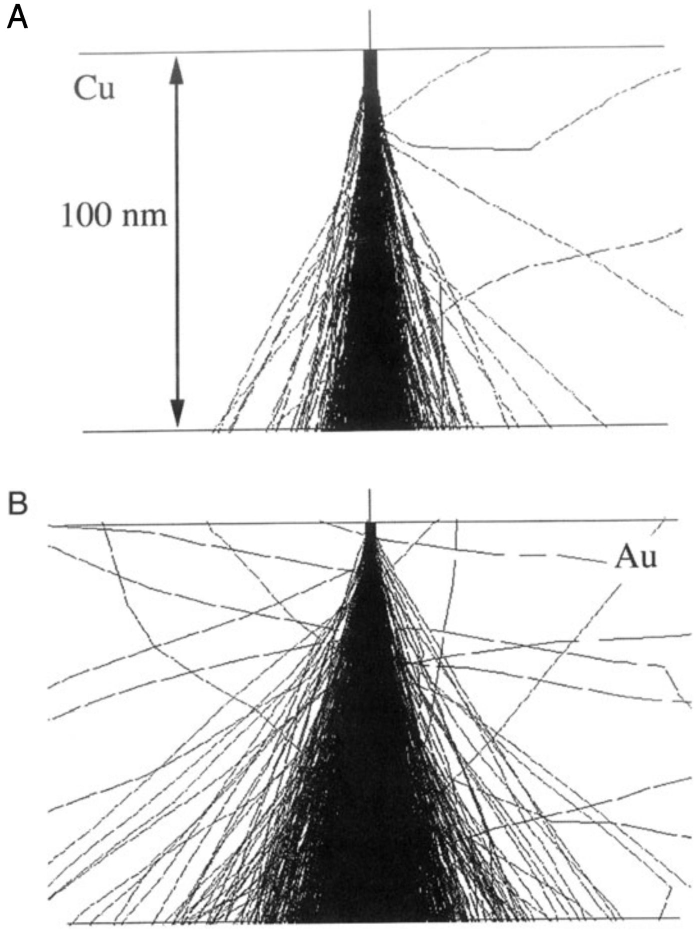

Figure 2.4. Monte Carlo simulation of the paths followed by 10^3 100-keV electrons as they pass through thin foils of (A) copper and (B) gold. Notice the increase in scattering with atomic number.

The Monte Carlo calculation was first developed by two of the United States' foremost mathematicians, J. von Neumann and S. Ulam at Los Alamos in the late 1940s. Ulam actually rolled dice and made hand (!) calculations to determine the paths of neutrons through deuterium and tritium which proved that Teller's design for the "Super" (H-bomb) was not feasible (Rhodes 1995). Monte Carlo methods are more often used in SEM image calculations (see, e.g., Newbury *et al.* 1986, Joy 1995), but they have a role in TEM in determining the expected spatial resolution of microanalysis. Figure 2.4 shows two Monte Carlo simulations of electron paths through thin foils.

2.7. OTHER FACTORS AFFECTING SCATTERING

By selecting electrons of a certain scattering angle (choosing a θ), you are changing the effective scattering cross section (σ_θ), because the scattering strength generally decreases as the angle of scattering increases. Therefore, there will generally be less scattering at higher angles, which explains why we said at the start of the chapter that we are mainly interested in forward scattering in the TEM. Most of the scattered electrons are within ±5° of the unscattered beam.

You also have control of the scattering cross section in other ways. First, the accelerating voltage, which determines the electron energy E_0 (eV), will affect the cross section as implied in equation 2.3 (specifically for elastic scattering). In fact, for all forms of scattering, the total cross section decreases as E_0 increases. Therefore, intermediate and higher voltage TEMs will result in *less* electron scattering than typical 100-kV instruments and, as we'll see in Chapter 4, this has important implications for electron beam damage in delicate specimens, such as polymers.

Q decreases as E_0 increases. Electron scattering at 300 kV will be smaller than at 100 kV.

We shall see later that the effect of the atomic number of the specimen is more important in elastic than inelastic scattering and, as Z increases, elastic scattering dominates. This behavior helps when we consider ways to enhance scattering (and therefore contrast) in low Z materials such as polymers.

2.8. COMPARISON TO X-RAY DIFFRACTION

There is a very good reason why electrons are used in microscopy: they have a "suitable interaction" with matter. Most descriptions of the interaction of electrons with matter are based on scattering. You will come across such topics as kinematical scattering, dynamical scattering, elastic scattering, inelastic scattering, etc., and we will use the formalism of a scattering factor to describe the process mathematically. It is this scattering process that varies with the structure or composition of the specimen, permitting us ultimately to image a microstructure, record a diffraction pattern, or collect a spectrum. Historically, it was diffraction that provided most of the crystallographic information we have about materials, and the majority of those studies used X-rays. This is why X-ray diffraction is so well documented in the scientific literature. A good understanding of X-ray diffraction helps considerably in understanding electron diffraction; however, the primary processes by which electrons are scattered are very different from the processes by which X-rays are scattered.

X-rays are scattered by the *electrons* in a material through an interaction between the negatively charged electrons and the electromagnetic field of the incoming X-rays. The electrons in the specimen respond to the applied field of the X-ray flux, oscillating with the period of the X-ray beam. These accelerated charged particles then emit their own electromagnetic field, identical in wavelength and phase to the incident X-rays. The resultant field which propagates radially from every scattering source is called the scattered wave.

Electrons are scattered by *both* the electrons and the nuclei in a material; the incoming negatively charged electrons interact with the local electromagnetic fields of the specimen. The incoming electrons are therefore directly scattered by the specimen; it is not a field-to-field exchange as occurs in the case of X-rays. Consequently, electrons are scattered much more strongly than X-rays.

2.9. FRAUNHOFER AND FRESNEL DIFFRACTION

Diffraction of visible light is well understood, so we should carry over as much of the analysis as possible. If you have any experience with diffraction of visible light you will have encountered Fraunhofer and Fresnel diffraction.

- Fraunhofer diffraction occurs when a flat wavefront interacts with an object. Since a wave emitted by a point becomes planar at large distances, this is known as far-field diffraction.
- Fresnel diffraction occurs when it's not Fraunhofer. This case is also known as near-field diffraction.

So why discuss these topics now? We will see later that electron diffraction patterns correspond closely to the Fraunhofer case while we "see" the effects of Fresnel diffraction in our images.

In TEM we will find both forms of diffraction. We will briefly go through the Huygens explanation of how a wave propagates, then consider Fraunhofer diffraction from two slits (Young's slits), and then extend this to many slits. There are two reasons for reviewing this analysis:

- It reminds us that coherent interference is purely a matter of physical optics.
- We can review the concept of phasor diagrams, which we'll use in later chapters.

Huygens explained the propagation of any wavefront by imagining that each point on the wavefront itself acts as a new source for a spherical wavelet. The wavelets interfere with one another to give the new wavefront and the process is repeated.

2.10. DIFFRACTION OF LIGHT FROM SLITS

When we place a pair of very narrow slits in front of a wavefront, we select just two of the Huygens wavelets; these wavelets then must have the same phase at the slits. As they propagate past the slits, their phases differ, depending on the position of the detector. The important term is the path difference $L = d \sin \theta$ as shown in Figure 2.5. The two wavelets propagating in direction $\mathbf{r}$ are out of phase by $2\pi L/\lambda$. If d and λ are such that this phase difference is actually a multiple of 2π, then the rays are again in phase. Therefore, there is an inverse relationship between d and θ for a given d; as d decreases, $\sin \theta$ increases.

> The inverse relationship between d and θ occurs solely due to the positions of the slits. We'll come across an identical relationship when we talk about electron diffraction in Section 3.11.

When we extend this analysis to more than two slits we see the same result, but with added subsidiary peaks. The origin of the subsidiary peaks can best be illustrated by considering a series of phasor diagrams. (We'll find similar diagrams useful when we discuss TEM images in Chapter 26.) These diagrams plot the amplitude and phase of the scattered wave as illustrated, for the case of five slits, by the polyhedra in Figure 2.6; in other words, when we add the amplitudes of beams we must take account of their phase. When θ is zero, the rays experience no phase shift and we simply add all of the ampli-

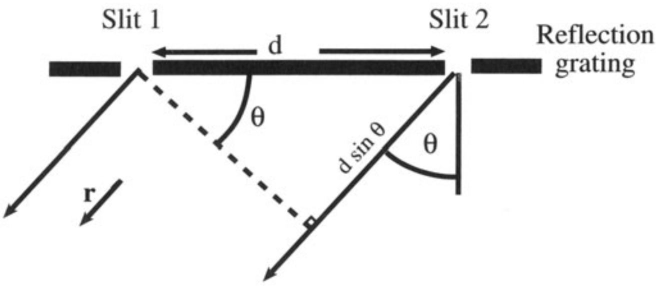

Figure 2.5. An incident plane wave is scattered by two slits, distance d apart. The scattered waves are in phase when the path difference $d \sin \theta$ is $n\lambda$.

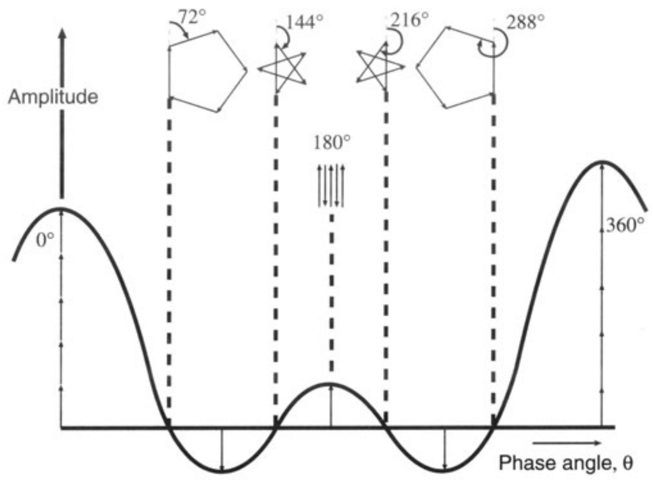

Figure 2.6. A phasor diagram showing how the total amplitude produced by summing five waves produced by five slits varies with the phase angle (how much each wave is out of phase) between the different waves. The arrows show the individual phasors from each slit.

tudes; as θ increases the rays become out of phase, but the phasors can still add to give a large resultant vector. When θ is exactly 72° (360°/5 for five slits), the phasor diagram is a closed pentagon and the resultant amplitude is zero. This process repeats at 144° (2 × 360°/5) and 216° (3 × 360°/5). In between these values at 108° (1.5 × 360°/5) we produce a local maximum in amplitude which is repeated at 180° (2.5 × 360°/5). If we plot the amplitude as a function of θ, we produce the curve with a series of subsidiary maxima shown in Figure 2.6.

Now what happens if we allow the slit to have some width as shown in Figure 2.7A? Each slit produces a phasor diagram as shown in Figures 2.7B and C; i.e., the rays from within a single slit will interfere with each other to modify the polyhedra in Figure 2.6. The amplitude from a single slit varies as $A = A_0\, \phi^{-1} \sin \phi$, where ϕ is the phase $\lambda^{-1}\pi w \sin \theta$ for a single slit of width w. If we imagine just one slit, we would see a zero in the phasor diagram when $\phi = \pm n\pi$ as shown in Figure 2.7D.

Without going into the detailed math, we can replace the slit of width w by a circular hole or aperture of diameter D. The resulting peak width in the plot of amplitude versus θ then has a maximum of $1.22\lambda D^{-1}$ which is shown in Figure 2.8.

Because of the circular symmetry of the aperture, the calculation needed to obtain the number 1.22 involves the use of Bessel functions, which you can find in texts on physical optics.

The disk of diameter $1.22\lambda D^{-1}$ is named after Airy and will be one of the fundamental limits on the achievable resolution in TEM, as we discuss in Chapter 6. If we introduce *any* aperture into *any* microscope, we will limit the ultimate resolution of the instrument. As the diameter of the aperture, D, decreases, the minimum resolvable spacing, r, increases. This equation also suggests that decreasing λ (increasing the accelerating voltage) will improve resolution: as λ decreases, r decreases.

The final step is to consider the amplitude scattered from many slits which each have a width, w. The result is shown in Figure 2.9, where we've increased λ/w relative to Figure 2.7.

The important point about this analysis for TEM is that we'll see the same relationship in later chapters, where the slits will be replaced by an aperture, by many atoms, or by a thin specimen.

2.11. COHERENT INTERFERENCE

To expand on this point, consider an infinite plane wave described by the usual characteristics of amplitude and phase. We can describe the wave function for this wave by the expression

$$\psi = \psi_0 e^{i\phi} \qquad [2.12]$$

where ψ_0 is the amplitude and ϕ the phase of the wave. The phase depends on position x, such that if x changes by one wavelength λ, the phase difference is 2π. Stated another way, the phase difference $\Delta\phi$ between any two monochromatic (same wavelength) waves is related to the path difference Δx they must travel in going from source to detector. The relationship is

$$\Delta\phi = \frac{2\pi}{\lambda}\Delta x \qquad [2.13]$$

Figure 2.10 will help you visualize the relationships between the path difference and phase difference for monochromatic waves. Coherent interference between waves relies on the fact that the waves add amplitudes with attention to phase. If all waves scattered by all of the atoms in the specimen are to interfere coherently, they must all differ in phase by integral multiples of 2π. Clearly, this condition requires that the path differences traveled by all of the waves be integer multiples of the wavelength of the incident wave. We can ensure this by requiring that the scattering centers

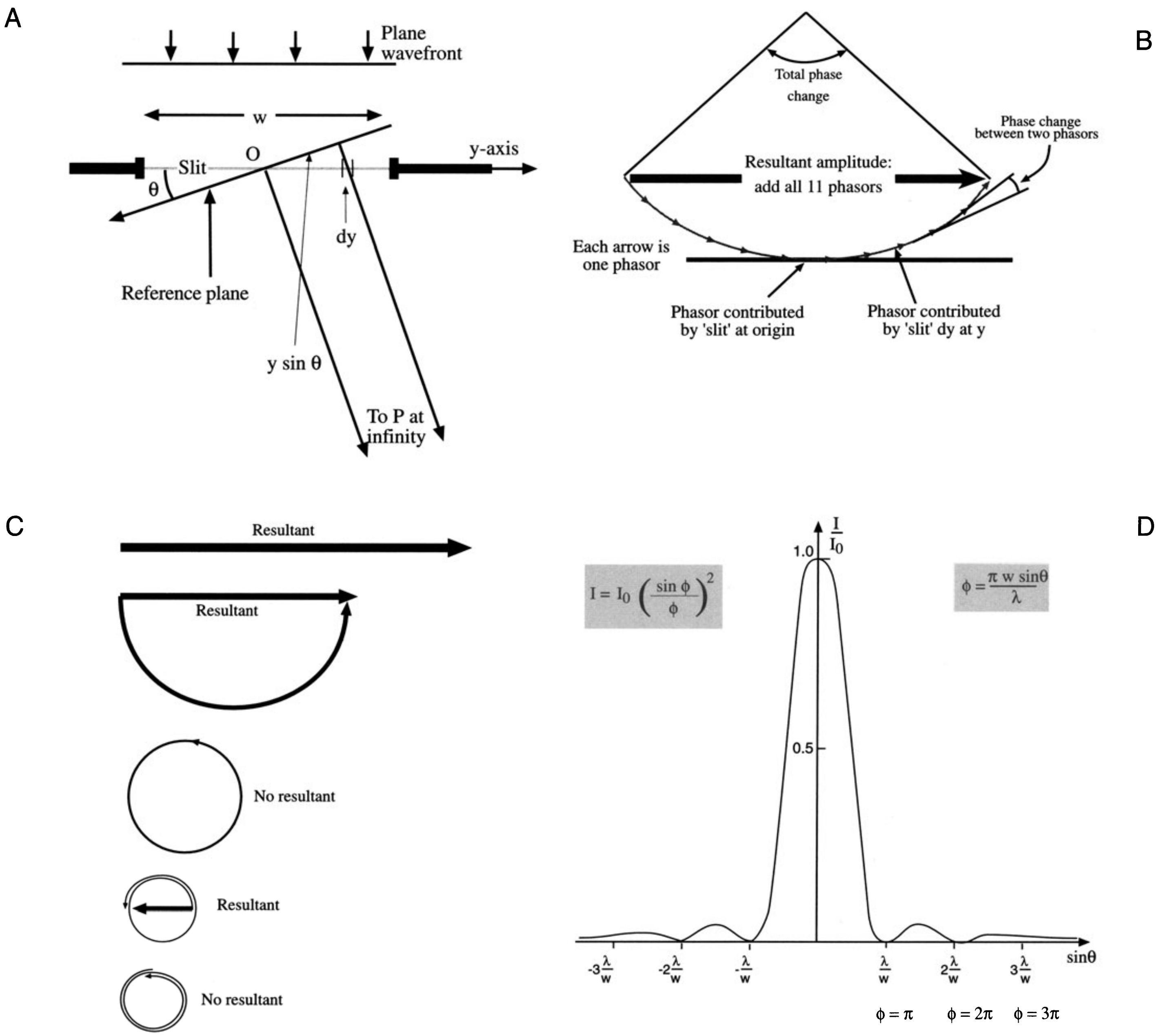

Figure 2.7. (A) Geometry for the scattering from an individual slit. (B) How the phasors from within an individual slit can be added to give the total phasor for the slit shown in (A). (C) How a single slit can produce a beam which has zero amplitude for certain values of θ in (A). The circles are directly comparable to the polyhedra in Figure 2.6. The total length of the phasor increments (from each *dy*) is the same in each figure. (D) A plot of the resulting intensity for scattering from the slit shown in Figure 2.5; this is known as the Fraunhofer diffraction pattern from a single slit; *w* is the slit width defined in (A).

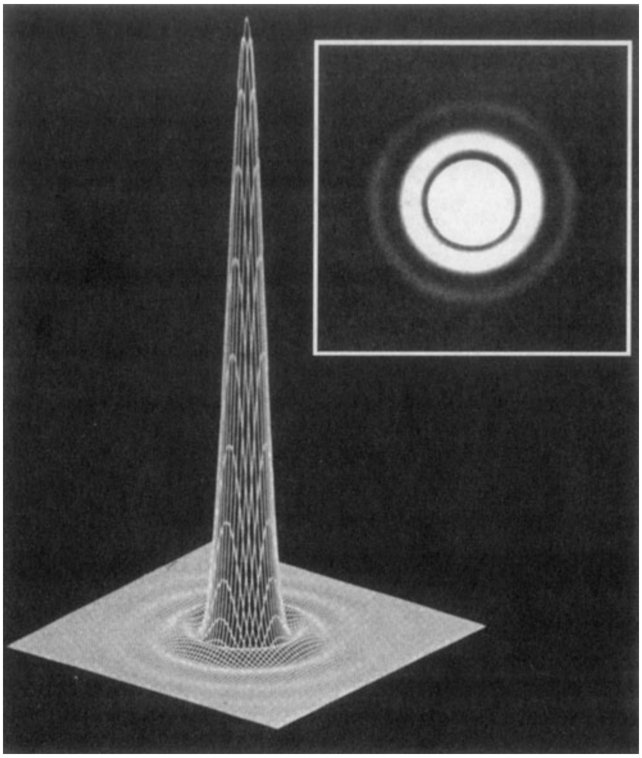

Figure 2.8. The visible-light intensity produced by a 0.5-mm-diameter circular aperture and the observed Airy rings (inset).

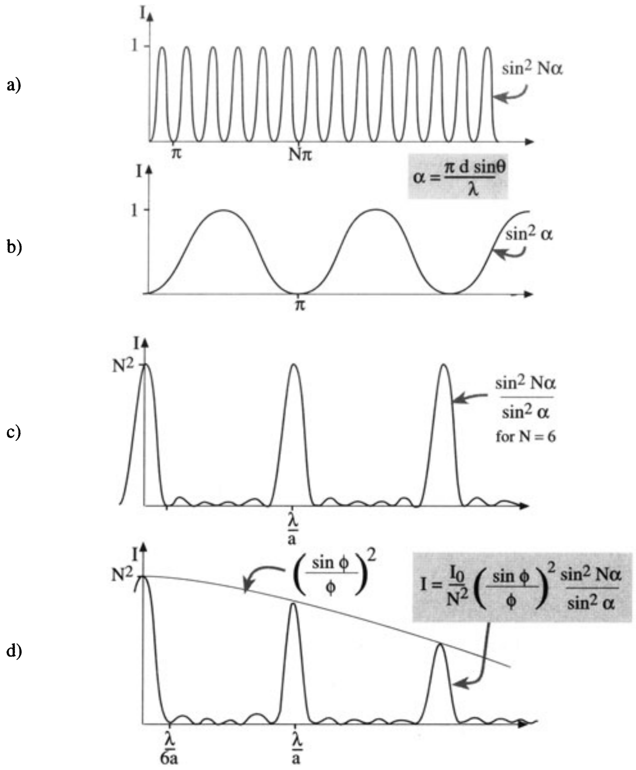

Figure 2.9. The scattered intensity from N slits (shown here for $N = 6$) where each slit would give the intensity shown in (B). (C) is the curve in (A) divided by curve in (B) and (D) is the curve in (C) multiplied by the curve in (Figure 2.7D). The distance d, the separation of the slits, and ϕ are defined in Figures 2.5 and 2.7. (λ/w has been increased compared to Figures 2.7 and 2.8 for simplicity.)

be periodically spaced. Fortunately this is true for all crystals, and the mathematical description of coherent interference is simplified (Part II).

2.12. A WORD ABOUT ANGLES

Since angles are so important in the TEM (you can control some of them and the specimen controls others) we want to try to be consistent in our terminology.

- We can control the angle of incidence of electrons on the specimen and we will define the semiangle of incidence as α, as summarized in Figure 2.10.
- In the TEM we use apertures or detectors to collect a certain fraction of the scattered electrons and we will define any semiangle of collection as β.
- We will define all scattering semiangles controlled by the specimen as θ. This may be a specific angle, such as twice the Bragg angle, where $\theta = 2\theta_B$ (see Section 11.4), or a general scattering semiangle θ.

2.13. ELECTRON DIFFRACTION PATTERNS

We've mentioned a couple of times that the TEM is uniquely suited to take advantage of electron scatter because it can form a picture (diffraction pattern) of the distribution of scattered electrons, which we'll discuss in Part II in much more detail. To understand fully how a diffraction pattern is formed in the TEM, you need to go to Chapter 6 to see how electron lenses work, and then to Chapter 9 to find how we combine lenses to form the TEM imaging system. But before we take you through these concepts it is worth just showing a few of the many kinds of diffraction patterns that can be formed in the TEM. At this stage, all you have to do is imagine that a photographic film is

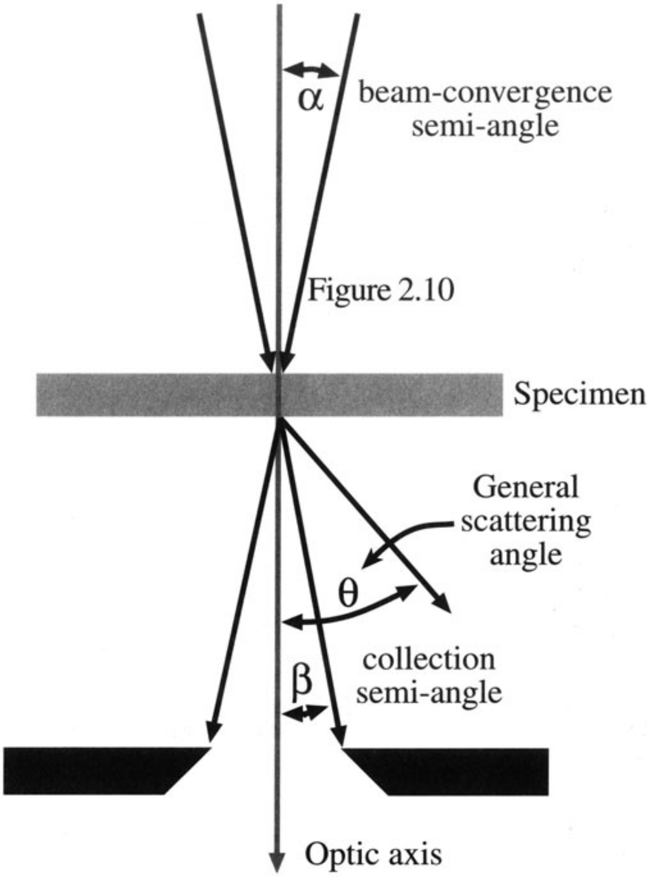

Figure 2.10. Definition of the major semiangles in TEM. Any incidence/convergence semiangle of the beam is termed α; any collection semiangle is β and general scattering semiangles are θ.

placed directly after the thin specimen and that electrons scattered by the specimen as in Figure 2.1B impinge directly on the film. Under these circumstances, the greater the angle of scatter, the further off center the electron hits the film. Thus distances on the film correspond to angles of scatter at the specimen. This relationship is different than the usual interpretation of images in which distances correspond to distances in the specimen, but it is critical to our understanding of diffraction patterns.

Even using this simple description, however, you can comprehend some of the basic features of diffraction patterns. Figure 2.11 is a montage of several kinds of diffraction patterns, all of which are routinely obtainable in a TEM. You can see that several points we've already made about scattering are intuitively obvious in the patterns. First, most of the intensity is in the direct beam, in the center of the pattern, which means that most electrons are *not* scattered but travel straight through the specimen. Second, the scattered intensity falls with increasing θ (increasing distance from the direct beam), which reflects the decrease in the scattering cross section with θ. Third, the scattering intensity varies strongly with the structure of the specimen. You'll see much more of this in Part II.

So far, in fact, we've only considered the amplitude of the electron wave and we've neglected the phase. When a wave is scattered, it will change its phase with respect to the incident wave. This is because a wave cannot change direction and remain in step with a wave that is unscattered. The phase of the scattered wave is most important in the specific topic of phase-contrast images, which are the principal form of high-resolution atomic-level images such as shown back in Figure 1.2. We'll also come across the importance of the phase of the scattered wave when we consider the intensity of diffracted electron beams and the intensity in diffraction contrast images. But at this stage all you need to know is that the electrons in the beam are in phase when they hit the specimen and the process of scattering, in any form, results in a loss of phase between the scattered and direct beams.

CHAPTER SUMMARY

Remember that electrons are strongly scattered because they are charged particles. This is the big difference compared to X-rays. Thus electrons are scattered by the electron cloud and by the nucleus of an atom. Remember X-rays are only scattered by the electron cloud. (In case you are physics oriented, a quantum mechanical calculation does give the same distribution as the classical calculation for the Coulomb force.)

We have defined three important parameters in this chapter:

σ	the scattering cross section of one atom
λ	the mean free path (average distance between scattering events)
$d\sigma/d\Omega$	the differential scattering cross section of one atom

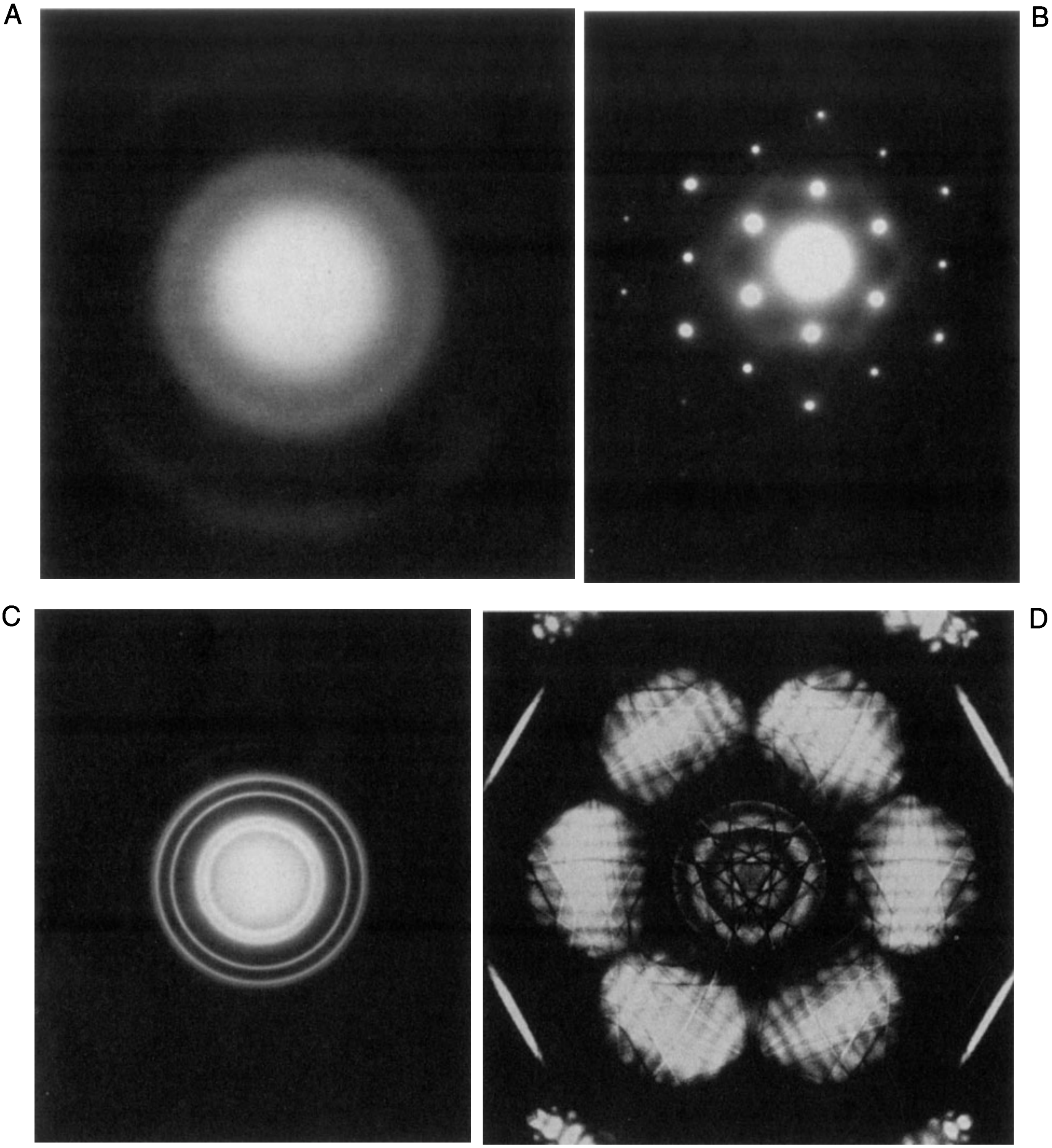

Figure 2.11. Several kinds of diffraction patterns obtained from a range of materials in a conventional 100 kV TEM: (A) amorphous carbon, (B) an Al single crystal, (C) polycrystalline Au, (D) Si illuminated with a convergent beam of electrons. In all cases the direct beam of electrons is responsible for the bright intensity at the center of the pattern and the scattered beams account for the spots or rings that appear around the direct beam.

Finally, a note on grammar! Should we discuss electron scatter or electron scattering? Electrons are scattered and we observe the results of this scattering (a gerund), but in fact we see the scatter (noun) of the electrons which can be measured. However, we'll use electron "scattering" to denote the effect and to be consistent with the popular usage which goes back to the early work of Bragg and others.

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