1 X-ray microscopes: a short introduction

X-ray microscopes are systems in which an x-ray beam is used to illuminate a specimen, and some sort of x-ray image is obtained with a spatial resolution δ_r of micrometers to nanometers.[1] Some microscopes use an x-ray lens such as a Fresnel zone plate to produce a magnified image (Fig. 1.1), while others use an x-ray lens to produce a small beam spot through which the sample is raster-scanned while image data are collected (Fig. 1.2).

When using microscopes, one of the first questions asked is this: "What is the magnification?" This is an eminently sensible question to ask when one is looking at an image through the eyepieces of a visible light microscope, and indeed the objective lenses and eyepiece lenses in visible light microscopes are usually labeled in terms of their respective magnification, such as 40× and 10× to yield a net magnification of 400×. However, we do not recommend that you somehow contrive to make an x-ray eyepiece! Your eye does not directly register x-ray images, and in any case you do not wish to expose any part of yourself to such high doses of X rays (this will be discussed in Chapter 11). Because we are likely to view the same image at vastly different magnifications (ranging from printed images in journal papers, to images on computer screens, to very large images projected in conference rooms), it is far more convenient to instead talk about the spatial resolution δ_r of images (see Section 4.4.3), and a field of view which is the viewable width and height at the specimen's location. (A common practice that we strongly recommend is to place a scale bar on the image, which shows how large some defined distance would appear; see for example Fig. 4.60.) That is, an image might have a resolution of $\delta_r = 20$ nanometers (or nm), and a field of view of 10 micrometers (or μm) on a side. The continuous intensity variations $I(x, y)$ in Cartesian coordinates are almost always sampled onto a regular discrete array $I[i_x, i_y]$ with spacing Δ_x and array indices $i_x = 0, 1, \ldots, (N_x - 1)$, and corresponding values in y. Thus one might encounter an image with a picture element or pixel size of $\Delta_{x,y} = 10$ nm, and $N_x = 1024$ and $N_y = 768$ pixels, giving a field of view of 10.24×7.68 μm. The extension to 3D imaging involves volume elements or voxels, and the z direction.

Of course the image is just a particular representation of the object under study; for incoherent brightfield imaging, the image intensity $I(x, y)$ represents the magnitude squared of the wavefield at a particular plane, which hopefully is the downstream side of the specimen so that one obtains a pixel-by-pixel mapping of x-ray absorption in

[1] We follow the convention of the American Institute of Physics style guide, so that the noun is "X ray" and the adjective is "x-ray."

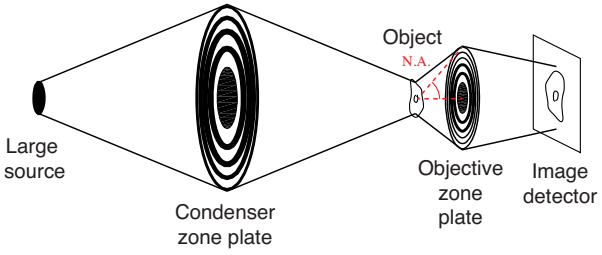

Figure 1.1 Schematic of a transmission x-ray microscope, delivering a full-field image. An x-ray source illuminates a specimen (often by using a condenser lens to image the source onto the specimen), and the transmitted wavefield is imaged by an objective lens onto a pixelated detector. The numerical aperture (N.A.) of the objective lens is indicated (lens radius divided by focal length; see Eq. 4.172).

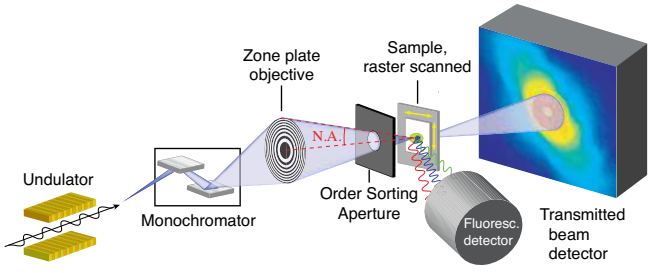

Figure 1.2 Schematic of a scanning x-ray microscope, delivering a scanned image. An x-ray source such as an undulator at a synchrotron light source is (optionally) monochromatized, and an objective lens with numerical aperture N.A. images this source (or an illuminated aperture) to produce a small focal spot through which a specimen is scanned. One detector might record the transmitted signal (either measuring the total signal, or measuring its redistribution such as with a pixelated detector), and other detectors such as an energy-resolving detector for x-ray fluorescence signals can be used. Figure modified from [de Jonge 2010a].

the specimen. In fact the image usually consists of this signal S due to the presence of contrast in the specimen, and noise N due to stray light, statistical fluctuations, or other causes; the signal-to-noise ratio (SNR) weighs their relative contributions (this is discussed in Section 4.8). As we shall see, some x-ray microscopes deliver multiple image signals, such as simultaneous absorption and phase contrast, or energy-dependent signals as will be discussed in Chapter 9.

1.1 How to read this book

Of course you should really read every word of this book, or even memorize it! But not all readers will need to be concerned with every detail, so here are a few suggestions:

- If you just want to get a feel for what x-ray microscopes can do, look at Chapter 12,

which summarizes a number of recent scientific applications of x-ray microscopy while providing representative images. You can then put this book on your shelf and pull it down when you need to read up on certain details.
- If you are wondering what type of x-ray microscope to use for a specific application, Chapter 6 provides an overview.
- If your main interest is in using x-ray absorption spectroscopy combined with imaging, see Section 9.1. If you are mostly interested in fluorescence imaging of the distribution of chemical elements in a specimen, see Section 9.2.
- Be aware of limitations due to ionizing radiation damage, as discussed in Chapter 11.

Many of the later chapters refer back to discussions of the fundamentals of x-ray physics in Chapter 3 and imaging physics in Chapter 4. In most cases there will be a cross-reference to the exact section or equation number.

1.2 Online appendices

Two short appendices available online at www.cambridge.org/Jacobsen[2] supplement this book:

- Online Appendix B contains further detail on how to calculate the visible and x-ray refractive index, and properties derived from it.
- Online Appendix C provides examples of the many different ways that the key formulae for maximum likelihood and estimation maximum approaches are written in the literature.

These are short enough to print out, if so desired.

1.3 Key mathematical symbols and formulae

One of the beauties of physics is that there is widespread agreement on the basic notation: we all know what $F = ma$ means, for example.

This is mostly but not completely true in x-ray optics and microscopy. Therefore we list our notation for some of the most important mathematical terms in x-ray microscopy in Table 1.1. There are certain instances where key terms and formulae are written in different ways within the community. Some write the x-ray refractive index as $n = 1 - \delta + i\beta$ whereas we use $n = 1 - \delta - i\beta$, as discussed in Box 3.4. Our usage of the terms "magnitude" and "amplitude" is discussed in Box 4.1. The definition of momentum transfer q varies in the literature, as discussed in Box 4.2. We discuss depth resolution δ_z and depth of field (DOF) in Box 4.7.

[2] See also www.cambridge.org/9781107076570

Table 1.1 Key mathematical symbols and their meaning in this book, along with the section where they first are described. See also Box 4.1 for our usage of the words "magnitude" and "amplitude." Additional photometric quantities are shown in Section 7.1.1.

Symbol	Meaning	Location
$\lambda = hc/E$	X-ray wavelength λ, photon energy E, and Planck's constant h (Eq. 3.2) multiplied by the speed of light c (Eq. 3.55).	Eq. 3.7
n_a and n_e	Atom (n_a) and electron (n_e) number density	Eqs. 3.21 and 3.22
Λ and σ	Mean free path (Λ) and cross section (σ)	Eq. 3.25
$(f_1 + if_2)$	Complex number of oscillator modes per atom, which varies with x-ray energy E.	Eq. 3.42
α	As used in $n = 1 - \alpha\lambda^2(f_1 + if_2)$	Eq. 3.66
μ	Linear absorption coefficient (μ) and inverse attenuation length (μ^{-1})	Eqs. 3.45 and 3.75
μ'	Mass absorption coefficient	Eqs. 3.78 and 9.3
$n = 1 - \delta - i\beta$	X-ray refractive index n with its phase-shifting part δ and absorptive part β	Eq. 3.67
θ_c'	Critical angle for grazing incidence reflectivity	Eq. 3.115
δ_r	Spatial resolution	Eq. 4.173
N.A.	Numerical aperture of an optic	Figs. 1.1 and 1.2, and Eq. 4.172
dr_N	Outermost zone width in a Fresnel zone plate	Eq. 5.27
δ_z	Depth resolution (depth of field is DOF = $2\delta_z$; see Eqs. 4.214 and 4.215)	Eq. 4.213
Δ_r	Pixel size (picture element size) at the object. The subscript r can be thought of as referring to real space rather than Fourier space, or a vector coordinate $\vec{r}$ with components in $\hat{x}$ and $\hat{y}$.	Eq. 4.87
Δ_u	Pixel size in Fourier space	Eq. 4.92
Δ_{det}	Size of a pixel on an area detector.	Eq. 4.93
N	Number of image pixels (as in N_x and N_y)	Eq. 4.87
u_x, u_y	Spatial frequencies, or wavelength-normalized diffraction angles $u_x = \theta_x/\lambda$, $u_y = \theta_y/\lambda$	Eqs. 4.32 and 4.88
$\mathcal{F}$	Fourier transform, as in $G(u_x) = \mathcal{F}\{g(x)\}$	Eq. 4.80
SNR	Signal-to-noise ratio, or S/N	Section 4.8.1
DQE	Detective quantum efficiency	Eq. 7.34
Θ	Contrast parameter	Eq. 4.238
Φ	Flux, in photons/second	Section 7.1.1
$\mathfrak{F}$	Fluence, in photons/area or photons/m^2	Section 7.1.1
I	Intensity	Eq. 4.3