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INTRODUCTION

1.1 The discovery

Near the end of the nineteenth century, Röntgen was experimenting with cathode ray tubes—vacuum tubes similar to old-fashioned computer monitors. After placing a metal target in the electron beam, he noticed that phosphor behind a wood screen glowed and nearby photographic plates became exposed even though protected from light. Röntgen realized that these effects must be due to some unknown, “x” radiation, and he quickly began to investigate, placing various objects in the beam (including his wife’s hand—the famous image is shown in Figure 1-1).

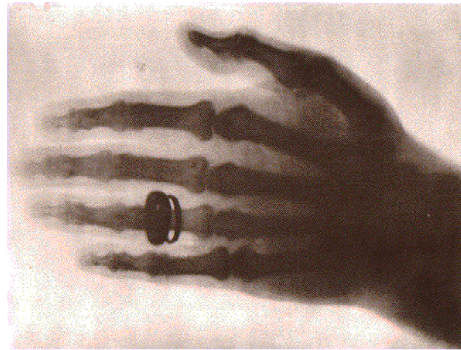


FIGURE 1-1. An x-ray image of Frau Röntgen’s hand, from *On a new kind of rays*, *Nature* 53 (January 23, 1896): 274–76.

This commonly told story of the discovery of x rays is a classic tale of serendipity. Imagine it—a laboratory in Würzburg, Germany, cluttered with all the latest scientific apparatus of 1895: vacuum tubes, photographic plates, jars and sheets of phosphors and metals, and an excited scientist randomly applying high voltages. Suddenly he notices the phosphor on the other side of the room is glowing, and William Conrad Röntgen is on his way to receiving the first Nobel Prize in Physics. Shortly into his investigations, he happens to see the outline of the bones in his wife’s hand exposed on a photographic plate, and the field of diagnostic imaging is born.

As with most great advances, the real story is a bit more deliberate. Röntgen, along with several of his contemporaries, including Tesla and Hertz, was actively engaged in research on the emissions from cathode ray tubes. The inventor of his tube, Crookes, had previously seen shadows on photographic plates, and may have suggested that Röntgen investigate them. However, Röntgen did quite quickly realize the significance of his observations and rapidly began identifying many of the characteristics of

x rays—for example, the dependence of penetration on density and the lack of significant refraction—as well as pioneering some of their applications.

Today, x rays are important not only for medical imaging and baggage inspection but also for astronomical observations, for materials analysis, for structure determination of viruses and pharmaceuticals, for fluorescence analysis in manufacturing quality control, and for fraud detection in art. An increasing interest in x-ray astronomy was one of the major forces behind the development of x-ray optics in the latter half of the last century. Mirror systems similar to those developed for astronomy also proved useful for synchrotron beamlines. Just as x-ray tubes were an accidental offshoot of cathode ray research, synchrotron x-ray sources were originally parasitic to particle physics: the synchrotron radiation was an unwanted consequence of accelerating the particles, because it removes energy from the particle beam. The subsequent development of specialized synchrotron sources with increasing brightness and numbers of beamlines led to creation of a whole new array of x-ray tools and a consequent demand for an increasing array of optics.

The rapid development of x-ray optics also has been symbiotic with the development of detectors and compact sources. Detectors developed for particle physics, medicine, and crystallography have found application across the different fields. Similarly, the increasing capabilities of x-ray systems have stimulated the development of new science, with ever-growing requirements for intensity, coherence, and spatial and energy resolution. X-ray diffraction and fluorescence were early tools during the rapid development of materials science after World War II. More recently advancements have been made to meet the demands of shrinking feature sizes and allowed defect concentrations in semiconductors. The use of x-ray diffraction, especially the development of dedicated synchrotron beamlines, has also been stimulated by the growing demands for rapid protein crystallography in biophysics and pharmaceutical development.

1.2 What is an x ray?

Despite Röntgen's early identification of his unknown, “x” rays as longitudinal vibrations of the ether (this was just nine years after the Michelson-Morley experiment), x rays proved to be simply light waves, electromagnetic radiation, with very short wavelengths. The definition of the wavelength range considered to be in the x-ray regime differs somewhat among fields and applications, but is typically between 0.1 and 10 Å (0.01 to 1 nm). Longer wavelengths are considered to be in the range of extreme ultraviolet (EUV), and shorter wavelengths are generally considered to be in the gamma ray regime (although some fields make a distinction that “gamma ray” refers only to the products of nuclear reactions).

The usual relation holds between wavelength λ and wavenumber κ (the magnitude of the wavevector),

$$\lambda = \frac{2\pi}{\kappa}. \quad (1-1)$$

Quantum mechanics gives us the relationships between wavevector and momentum,

$$\vec{p} = \hbar \vec{\kappa} \Rightarrow \lambda = \frac{h}{p}, \quad (1-2)$$

where h is Planck's constant and, as usual,

$$\hbar = \frac{h}{2\pi}. \quad (1-3)$$

Relativity gives us the relationship between momentum and energy U ,

$$U^2 = (Mc^2)^2 + p^2c^2 \Rightarrow p = \frac{\sqrt{U^2 - (Mc^2)^2}}{c} = \frac{U}{c}, \quad (1-4)$$

since, as photons are massless, $M=0$. Thus, wavelength and energy are related by

$$U = \frac{hc}{\lambda}, \quad (1-5)$$

where c is the speed of light. Expressing h in units of $\text{eV} \cdot \text{s}$, and c in units of $\text{\AA}/\text{s}$ gives the useful result that

$$hc \approx 12.4 \text{ keV} \cdot \text{\AA}. \quad (1-6)$$

Thus, the wavelength range from 10 to 0.1 \AA corresponds to 1.2 to 124 keV in photon energy. For comparison, a visible light photon with a wavelength of 0.5 μm corresponds to a photon energy of 2.5 eV, or 2.5×10^{-3} keV. Quantum mechanics also gives us the relationship between photon energy and frequency ν ,

$$U = h\nu, \quad (1-7)$$

which gives us the expected relationship between wavelength and frequency,

$$\lambda = \frac{hc}{U} = \frac{c}{\nu}. \quad (1-8)$$

EXAMPLE 1-1

- a) What are the wavelength and frequency of the 8 keV x rays frequently used for protein crystallography experiments?

From equation 1-5,

$$\lambda = \frac{hc}{U} \approx \frac{12.4 \text{ keV} \cdot \text{\AA}}{8 \text{ keV}} \approx 1.55 \text{ \AA}.$$

From equation 1-8,

$$\nu = \frac{c}{\lambda} \approx \frac{3 \times 10^{18} \text{ \AA}/\text{s}}{1.55 \text{ \AA}} \approx 1.9 \times 10^{18} \text{ Hz} \approx 1.9 \text{ exahertz} \approx 1.9 \text{ EHz}.$$

- b) For comparison, what is the wavelength of an electron with a kinetic energy of 8 keV?

The difference between the photon and electron wavelengths arises in applying equation 1-4, because the electron is not massless. The kinetic energy is the

difference between the total energy U and the rest mass energy, which for small (nonrelativistic) momentum is

$$\begin{aligned} K_e &= U - M_e c^2 = \sqrt{(M_e c^2)^2 + p^2 c^2} - M_e c^2 \\ &= M_e c^2 \sqrt{1 + \frac{p^2 c^2}{(M_e c^2)^2}} - M_e c^2 \approx M_e c^2 \left(1 + \frac{1}{2} \frac{p^2 c^2}{(M_e c^2)^2} \right) - M_e c^2 = \frac{p^2}{2M_e} \end{aligned}$$

which is the expected, classical result. Then,

$$\begin{aligned} \lambda &= \frac{h}{p} = \frac{h}{\sqrt{2M_e(K_e)}} \approx \frac{(6.6 \times 10^{-34} \text{ J} \cdot \text{s})}{\sqrt{2(9.1 \times 10^{-31} \text{ kg})(8 \times 10^3 \text{ eV}) \left(\frac{1.6 \times 10^{-19} \text{ J}}{1 \text{ eV}} \right)}} \\ &\approx 1.4 \times 10^{-11} \frac{\text{kg} \frac{\text{m}^2}{\text{s}^2} \text{s}}{\sqrt{\text{kg}^2 \frac{\text{m}^2}{\text{s}^2}}} \approx 1.4 \times 10^{-11} \text{ m} \approx 0.14 \text{ Å}. \end{aligned}$$

The electron wavelength is more than a factor of 10 smaller than that of the x ray with the same kinetic energy.

1.3 What makes x rays useful?

The wavelength of x rays is in the angstrom range, similar to the spacing of atoms in a crystal. Thus, the arrays of atoms in a crystal can act as a diffraction grating for x rays. The 1914 Nobel Prize in Physics was awarded to Laue for the first demonstration of diffraction of x rays by a crystal. The 1915 prize went to William Henry Bragg and William Lawrence Bragg for the development of the theory that allows for association of crystal structure with the diffraction pattern. X-ray crystallography is routinely used today for applications such as verifying the crystal quality of films grown on silicon wafers, detecting stress in airplane engines, and determining the structure of proteins to understand their function in cancer growth. Diffraction is also used as a way to control

the direction or wavelength of x rays used in a particular experiment, just as gratings are used for visible light. The 1936 Nobel Prize in Chemistry was awarded to Peter Debye for, among other things, development of the theory of diffraction from powders and liquids.

Short-wavelength, high-energy photons are not easily absorbed—their high energy and momentum makes them difficult to stop. This means that x rays easily pass through materials such as human tissue for radiography or luggage for baggage inspection, as shown in Figure 1-2, or the dark paper Röntgen had used to protect



FIGURE 1-2. Baggage x-ray imaging, Gemini Dual-Energy system. The color images are produced by comparing absorption at two different x-ray photon energies. Copyright 2016 American Science and Engineering, Inc.

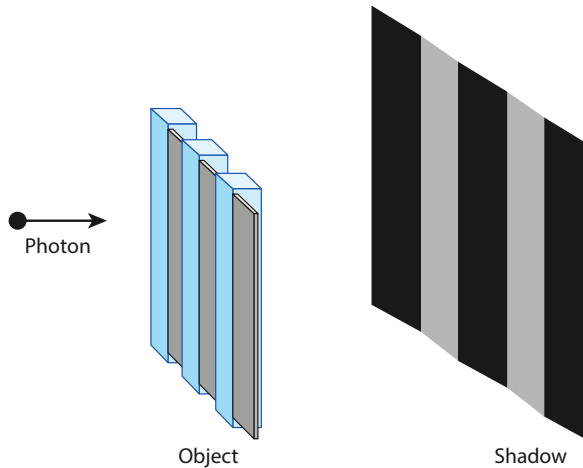


FIGURE 1-3. Making a shadow image.

his photographic plate. Absorption increases with the electron density of the material but is lower for higher-energy photons.

By way of analogy, consider an object with thick and thin regions like that of Figure 1-3. If the object was made with alternating painted plywood and tissue paper, you could map out the areas of tissue paper by throwing balls at the object and letting them mark the wall behind the object when they passed through. If the object was constructed of thick wood and bricks, you would need higher-momentum projectiles, perhaps bullets, to make a shadow. However, bullets would do a poor job of making a shadow image of the tissue paper area, because they would pass through the plywood as well. Thus, high-energy (“hard”) x rays are used for inspecting vehicles and steel cargo containers, as shown in Figure 1-4. Since almost all the hard x rays would pass through a thinner object or one with a lower atomic number, creating very little shadow, lower-energy (“softer”) x rays must be used to diagnose a broken hand.

Because x rays barely interact with materials, their index of refraction in any material is only slightly different from unity. This results in sharp shadows for radiography, because the rays are hardly refracted, but means it is very difficult to make refractive optics such as the lenses normally used for visible light. The penetrating nature of

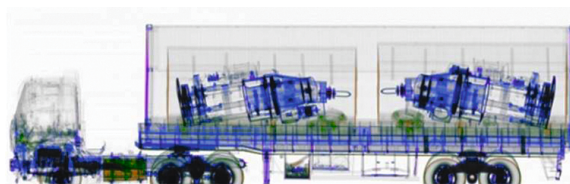


FIGURE 1-4. High-energy x-ray images of a cargo truck, OmniView Dual-Energy Transmission system. Copyright 2016 American Science and Engineering, Inc.

x rays also makes it difficult to construct optics such as Fresnel zone plates, or even pinholes for pinhole cameras, since the masking material must be thick compared with the dimensions of the apertures.

The energy of an x-ray photon, in the kiloelectronvolt range, is very much larger than the sub-electronvolt range typical for valence electron transitions in materials. Hence, x-ray properties are relatively insensitive to chemical state, unlike the changes in color or opacity that can easily be induced for visible light. However, x-ray energies are similar to ionization energies for *core* electrons and thus can be used to probe for characteristic atomic transitions. X-ray absorption spectroscopy and x-ray fluorescence are extremely important for elemental analysis. The 1924 Nobel Prize in Physics was awarded to Siegbahn for developing the field of x-ray spectroscopy.

1.4 The layout of the text

Any x-ray application or experiment requires an x-ray source and some material for the x-ray to interact with, including, in most cases, a detector. The next section of the book discusses methods of generating x rays. While some sources are naturally occurring—radioactive materials, black holes—the most common technique for generating x rays in the laboratory is by accelerating electrons, which generates a continuum (bremsstrahlung or synchrotron radiation) and characteristic emission lines (the same lines used for fluorescence analysis). X rays can also be emitted by blackbody radiation from very hot plasmas such as the sun, or those created by very intense lasers. The mechanisms for x-ray interactions with matter (including x-ray detection) are discussed in part III. These include absorption, scattering, refraction, reflection, and diffraction. Applications and optics enabled by these interactions are included in this section. The solutions to end-of-chapter problems are given in the appendix.

1.5 The elusive hyphen

Just as the definition of an x ray varies between applications, so does its hyphenation and capitalization, and you will encounter several styles. Grammatically, “x” is a modifier, like “optical,” so no hyphen is required. When the noun string is used as an adjective, as in x-ray beam, the hyphen is necessary. For example, when a child says “I am three years old,” you refer to him or to her as a “three-year-old child.” Some journals are very strict about removing extraneous hyphens. In other journals, it is the practice to always use the hyphen and/or to capitalize the *x*.

Problems

SECTION 1.2

1. Planck’s constant, h , is $6.6 \times 10^{-34} \text{ J} \cdot \text{s}$. 1 eV is the energy associated with an electron charge, $q_e \approx 1.6 \times 10^{-19} \text{ Coul}$, in a potential of 1 V. The speed of light is approximately $3 \times 10^8 \text{ m/s}$. Verify equation 1-6.
2. What is the wavelength of 30 keV x rays?

Further reading

General references for x-ray topics

- Jens Als-Nielsen and Des McMorrow, **Elements of Modern X-ray Physics**, John Wiley & Sons, 2001.
- Eric Lifshin, **X-ray Characterization of Materials**, John Wiley & Sons, 1999.
- A. G. Michette and C. J. Buckley, **X-ray Science and Technology**, Institute of Physics Publishing, 1993.
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- E. Spiller, **Soft X-ray Optics**, SPIE Press, 1994.
- David Attwood and A. Sakdinawat, **X-Rays and Extreme Ultraviolet Radiation: Principles and Applications**, Cambridge University Press, 2016.

Relativity

- D. Halliday, R. Resnick, and J. Walker, **Fundamentals of Physics**, 10th ed., John Wiley & Sons, 2013, chapter 37.

Historical references

- Arthur Stanton, Wilhelm Conrad Röntgen on a new kind of rays: Translation of a paper read before the Würzburg Physical and Medical Society, *Nature* 53 (1895): 274–76.
- New York Times*, February 16, 1896, Nature of the X Rays.