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STUDYING THE EFFECTS OF RADIATION DAMAGE USING X-RAY DIFFRACTION TECHNIQUES

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ANNOTATION

X-ray crystallography is an empirical scientific method used to elucidate the arrangement of atoms and molecules within a crystal. When an incident beam of X-rays encounters a crystal, its crystalline structure causes the X-rays to diffract into specific directions. By measuring the angles and intensities of these diffracted beams, a crystallographer can generate a three-dimensional representation of the electron density within the crystal. From this electron density map, valuable information can be derived, including the average positions of atoms within the crystal, their chemical bonds, the degree of disorder in the crystal lattice, and various other structural characteristics. X-ray crystallography serves as a powerful tool for understanding the internal structure and properties of crystalline materials.

Key words: *crystal, biological molecule, atomic-scale, mineral, X-ray crystallography;*

Since many materials can form crystals—such as salts, metal, mineral, semiconductors, as well as various inorganic, organic, and biological molecules—X-ray crystallography has been fundamental in the development of many scientific fields. In its first decades of use, this method determined the size of atoms, the lengths and types of chemical bonds, and the atomic-scale differences among various materials, especially minerals and alloys. The method also revealed the structure and function of many biological molecules, including vitamins, drugs, proteins and nucleic acids such as DNA. X-ray crystallography is still the primary method for characterizing the atomic structure of new materials and in discerning materials that appear similar by other experiments. X-ray crystal structures can also account for unusual electronic or elastic properties of a material, shed light on chemical interactions and processes, or serve as the basis for designing pharmaceuticals against diseases.

X-ray crystallography is related to several other methods for determining atomic structures. Similar diffraction patterns can be produced by scattering electrons or neutrons, and neutron scattering can be similarly interpreted by Fourier transformation. If single crystals of sufficient size cannot be obtained, various other X-ray methods can be applied to obtain less detailed information; such methods include fiber diffraction, powder diffraction and (if the sample is not crystallized) small-angle X-ray scattering (SAXS). If the material under investigation is only available in the form of nanocrystalline powders or suffers from poor crystallinity, the methods of electron diffraction, transmission electron microscopy and electron crystallography can be applied for determining the atomic structure.

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Wilhelm Röntgen discovered X-rays in 1895. Physicists were uncertain of the nature of X-rays, but soon suspected that they were waves of electromagnetic radiation. The Maxwell theory of electromagnetic radiation was well accepted, and experiments by Charles Glover Barkla showed that X-rays exhibited phenomena associated with electromagnetic waves, including transverse polarization and spectral lines akin to those observed in the visible wavelengths. Barkla created the x-ray notation, as well, noting in 1909 two separate types of diffraction beams, at first, naming them "A" and "B" and then supposing that there may be lines prior to "A", he started an alphabet numbering beginning with "K." Single-slit experiments in the laboratory of Arnold Sommerfeld suggested that X-rays had a wavelength of about 1 angstrom.

X-rays are not only waves but are also photons, and have particle properties causing Sommerfeld to coin the name, Bremsstrahlung, for this wavelike type of diffraction. Albert Einstein introduced the photon concept in 1905, but it was not broadly accepted until 1922, when Arthur Compton confirmed it by the scattering of X-rays from electrons. The particle-like properties of X-rays, such as their ionization of gases, had prompted William Henry Bragg to argue in 1907 that X-rays were not electromagnetic radiation. Bragg's view proved unpopular and the observation of X-ray diffraction by Max von Laue in 1912. confirmed for most scientists that X-rays are a form of electromagnetic radiation.

Crystals are regular arrays of atoms, and X-rays can be considered waves of electromagnetic radiation. Atoms scatter X-ray waves, primarily through the atoms' electrons. Just as an ocean wave striking a lighthouse produces secondary circular waves emanating from the lighthouse, so an X-ray striking an electron produces secondary spherical waves emanating from the electron. This phenomenon is known as elastic scattering, and the electron (or lighthouse) is known as the scatterer.

X-rays are used to produce the diffraction pattern because their wavelength λ is typically the same order of magnitude (1–100 angstroms) as the spacing d between planes in the crystal. In principle, any wave impinging on a regular array of scatterers produces diffraction, as predicted first by Francesco Maria Grimaldi in 1665. To produce significant diffraction, the spacing between the scatterers and the wavelength of the impinging wave should be similar in size. For illustration, the diffraction of sunlight through a bird's feather was first reported by James Gregory in the later 17th century. The first artificial diffraction gratings for visible light were constructed by David Rittenhouse in 1787, and Joseph von Fraunhofer in 1821. However, visible light has too long a wavelength (typically, 5500 angstroms) to observe diffraction from crystals. Prior to the first X-ray diffraction experiments, the spacings between lattice planes in a crystal were not known with certainty.

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