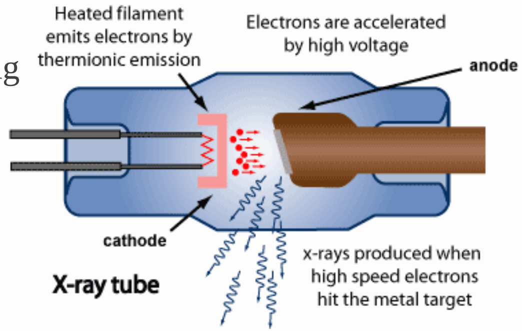
STRUCTURAL BIOLOGY

Live Session- Week 4
22 Feb, 2022

Summary

Week_4_Lecture_1: About Production of X-rays and its properties.

1. Electromagnetic radiation are X-rays, radio waves, microwaves, infrared, visible light, ultraviolet, and gamma rays and are distinguished by the amount of energy carried by the individual photons.
2. X-rays were produced by accelerating electrons through an electrical voltage and stopping them in a target.



Question 1: Electrons in X-ray tube were accelerated by

a. **High Voltage**
b. **Electromagnetic radiation**
c. **Magnetic field**

Solution: A small increase in the filament/cathode voltage emits electrons from a cathode, electrons are ***accelerated by high voltage***, and allow them to hit an anode, which emits X-ray photons.

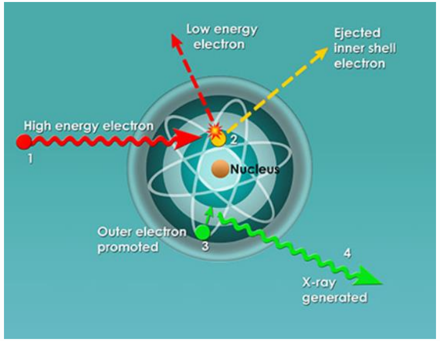
Question 2: In X-ray tube, when electron travel from cathode to anode, electron velocity is raised from

a. **Zero to speed of light**
b. **Zero to half of the speed of light**
c. **Zero to double the speed of light**

Solution: The velocity of electron is raised from zero to half the speed of light and called as projectile or moving electron. The interaction results in the conversion of electron kinetic energy into thermal energy and electro magnetic energy (such as infrared radiation and X-rays)

Week_4_Lecture_1: About Production of X-rays and its properties.

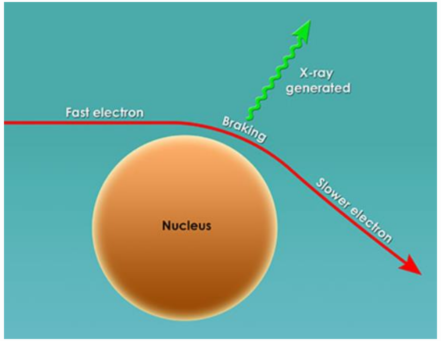
1. There are two types of X-ray generated: characteristic radiation and bremsstrahlung radiation.
2. When a high energy electron collides with an inner shell electron both are ejected from the atom leaving a hole in the inner layer. This is filled by an outer shell electron with a loss of energy emitted as an X-ray photon.
3. When an electron passes near the nucleus it gets slowed down and path is deflected. Energy lost is emitted as a bremsstrahlung X-ray photon.



Question 3: Percentage of bremsstrahlung X-ray within the X-ray beam

- **a. ~ 80 %**
- **b. ~ 50%**
- **c. ~ 20%**

Solution: Approximately 80% of the population of X-rays within the X-ray beam consists of X-rays generated in this way. As a result of characteristic and bremsstrahlung radiation generation, a spectrum of X-ray energy is produced.



Question 4: Factor effecting the wavelength of produced X-rays

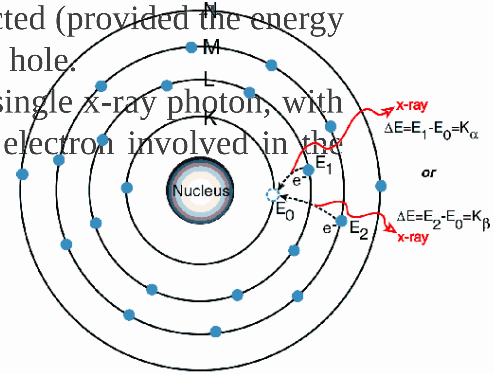
- **a. Tube current or voltage**
- **b. Anode**
- **c. Both**

Solution: This spectrum can be manipulated by changing the X-ray tube current or voltage settings, or by adding filters to select out low energy X-rays and anode material.

Many devices that use a high voltage and a source of electrons, produce X-rays as an unwanted byproduct of device operation. These are called incidental X-rays.

Week_4_Lecture_1: About Production of X-rays and its properties.

1. Fast-moving electrons interaction with K-shell electron causes the production of characteristic radiation.
2. **Characteristic radiation** is a type of energy emission relevant for X-ray production. This energy emission happens when a fast-moving electron collides with a K-shell electron, the electron in the K-shell is ejected (provided the energy of the incident electron is greater than the binding energy of K-shell electron) leaving behind a hole.
3. An outer shell electron fills this hole (from the L-shell, M-shell, etc.) with an emission of a single x-ray photon, with an energy level equivalent to the energy level difference between the outer and inner shell electron involved in the transition.



Question 5: When electron falls from L shell to K-shell, the x-ray emitted is

- **a. K alpha x-rays**
- **b. K-beta x-rays**
- **c. L alpha x-rays**

When an electron falls (cascades) from the L-shell to the K-shell, the x-ray emitted is called a K-alpha x-ray. Similarly, when an electron falls from the M-shell to the K-shell, the x-ray emitted is called a K-beta x-ray.

Question 6: The wavelength of K alpha radiation using Cu and Mo as Anode

- **a. 0.9 and 0.3 A^0**
- **b. 1.54 and 0.7 A^0**
- **c. 1 and 1 A^0**

Solution: Each element differs in nuclear binding energies, and characteristic radiation depends on the binding energy of particular element. The wavelength of X-rays produced by copper was 1.54 A and molybdenum was 0.7 A (useful as the high energy X-rays are absorbed less).

Question: Why Cu used in X-ray crystallography studies

Solution: Copper is the efficient conductor of heat and K alpha emission is relatively intense.

Summary

Week_4_Lecture_2: This lecture is about journey to 3D level.

1. A crystalline solid is distinguished by the fact that the atoms making up the crystal are arranged in a periodic fashion i.e., there is basic arrangement of atoms that is repeated throughout the entire solid.
2. The crystals appear exactly the same at one point as it does at other equivalent points. The periodicity in a crystal is defined in terms of a symmetric array of points in space called the lattice.

Question 7: Regular repetitive part of a lattice called as

- **a. Unit cell**
- **b. Edge**
- **c. Centre**

Solution: In every case, the lattice contains a volume or cell that represents the entire lattice and is regularly repeated throughout the crystal.

1. In crystallography, symmetry is used to characterize crystals, identify repeating parts of molecules, and simplify both data collection and nearly all calculations. Also, the symmetry of physical properties of a crystal such as thermal conductivity and optical activity must include the symmetry of the crystal.
2. An object is described as *symmetric* with respect to a *transformation* if the object appears to be in a state that is identical to its initial state, after the transformation.

Question 8: What are the symmetry operations in crystallography

- **a. Rotation**
- **b. Translation**
- **c. both**

Solution: In crystallography, most types of symmetry can be described in terms of an apparent *movement* of the object such as some type of rotation or translation (means shift from one point space to another). The apparent movement is called the symmetry *operation*. The locations where the symmetry operations occur such as a rotation axis, a mirror plane, an inversion center, or a translation vector are described as *symmetry elements*.

Summary

Week_4_Lecture_2: This lecture is about journey to 3D level.

1. The locations where the symmetry operations occur such as a rotation axis, a mirror plane, an inversion center, or a translation vector are described as *symmetry elements*.
2. Knowing the symmetry of the crystal reduces data collection by reducing the number of unique reflections to collect and may be useful for phase determination.
3. The crystal lattice is the ***symmetrical three-dimensional structural arrangements of atoms, ions or molecules (constituent particle) inside a crystalline solid as points.*** It can be defined as the geometrical arrangement of the atoms, ions or molecules of the crystalline solid as points in space.
4. Characteristics of Crystal Lattice
    a) In a crystal lattice, each atom, molecule or ions (constituent particle) is represented by a single point.
    b) These points are called lattice site or lattice point.
    c) Lattice sites or points are together joined by a straight line in a crystal lattice.

Question 9: The 3 dimensional view of the lattice is

a. Bravais Lattices
b. Miller index
c. Both

Solution: When we connect the straight lines, we can get a three-dimensional view of the structure. This 3D arrangement is called Crystal Lattice also known as Bravais Lattices. The Bravais lattice is the basic building block from which all crystals can be constructed.

Summary

Week_4_Lecture_2: This lecture is about journey to 3D level.

The unit cell is defined as the smallest repeating unit having the full symmetry of the crystal structure. Crystal structure is described in terms of the geometry of arrangement of particles in the unit cell.

Question 10: Number of parameters of 3 D unit cell

a. **3 edges**
b. **3 angles**
c. **both**

Solution: There are six parameters of a unit cell. These are the 3 edges which are a, b, c and the angles between the edges which are α, β, γ. The edges of a unit cell may be or may not be perpendicular to each other.

Types of Unit cells:

1**. Primitive Unit Cells**

When the constituent particles occupy only the corner positions, it is known as Primitive Unit Cells.

2. **Centered Unit Cells**

When the constituent particles occupy other positions in addition to those at corners, it is known as Centered Unit Cell.

Question 11: Types of centered unit cells

a. **Body centered**
b. **Face centered**
c. **End centered**
d. **All**

Solution: There are 3 types of Centered Unit Cells:

a) **Body Centered:** When the constituent particle at the centre of the body, it is known as Body Centered Unit cell.

b) **Face Centered:** When the constituent particle present at the centre of each face, it is known as Face Centered Unit cell.

c) **End Centered:** When the constituent particle present at the centre of two opposite faces, it is known as an End Centered Unit cell.

Summary

Week_4_Lecture_3: Crystal symmetry.

A Symmetry operation is an operation that can be performed either physically or imaginatively that results in no change in the appearance of an object. There are 3 types of symmetry operations: rotation, reflection, and inversion.

1. Rotational Symmetry

The axis along which the rotation is performed is an element of symmetry referred to as a rotation axis. The following types of rotational symmetry axes are possible in crystals

1-Fold Rotation Axis - An object that requires rotation of a full 360° in order to restore it to its original appearance has no rotational symmetry. Since it repeats itself 1 time every 360° it is said to have a 1-fold axis of rotational symmetry.

2-fold Rotation Axis - If an object appears identical after a rotation of 180°, that is twice in a 360° rotation, then it is said to have a 2-fold rotation axis (360/180 = 2).

Question 12: In 3 fold, 4 fold and 6 fold, objects repeat upon rotation of

a. 120^0, 120^0, 120^0
b. 120^0, 180^0, 240^0
c. 120^0, 90^0, 60^0

Solution:

3-Fold Rotation Axis- Objects that repeat themselves upon rotation of 120° are said to have a 3-fold axis of rotational symmetry (360/120 =3), and they will repeat 3 times in a 360° rotation.

4-Fold Rotation Axis - If an object repeats itself after 90° of rotation, it will repeat 4 times in a 360° rotation.

6-Fold Rotation Axis - If rotation of 60° about an axis causes the object to repeat itself, then it has 6-fold axis of rotational symmetry (360/60=6).

Summary

Week_4_Lecture_3: Crystal symmetry.

2. Mirror Symmetry

1. A mirror symmetry operation is an imaginary operation that can be performed to reproduce an object. The operation is done by imagining that you cut the object in half, then place a mirror next to one of the halves of the object along the cut.
2. If the reflection in the mirror reproduces the other half of the object, then the object is said to have mirror symmetry. The plane of the mirror is an element of symmetry referred to as a ***mirror plane.***

3. Center of Symmetry

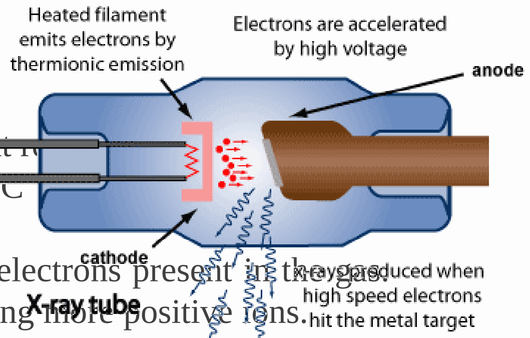
1. Another operation that can be performed is inversion through a point. In this operation lines are drawn from all points on the object through a point in the center of the object, called a symmetry center.
2. The lines each have lengths that are equidistant from the original points. When the ends of the lines are connected, the original object is reproduced inverted from its original appearance.

4. Inversion*:*

1. In the symmetry operation called inversion, lines are drawn from all points on the object through a point in the centre of the object.
2. This is called a symmetry centre. The lines each have lengths that are equidistant from the original points

Summary

Week_4_Lecture_4: Lecture 4 is about instrumentation in X-ray crystallography.



1. **Crookes tube**s are also called as cold cathode tubes, do not have a heated filament that r
2. Instead, electrons are generated by the ionization of the residual air by a high DC the cathode and anode electrodes in the tube.
3. The electric field accelerates the small number of electrically charged ions and free electrons present in the gas. The electrons collide with other gas molecules, knocking electrons off them and creating more positive ions.
4. All the positive ions are attracted to the cathode. When they strike it, they knock large numbers of electrons out of the surface of the metal, which in turn are repelled by the cathode and attracted to the anode or positive electrode.

1. **Sealed tubes** has the heated filament that emits electrons by thermo ionic emission. Electrons are accelerated by a high voltage, x-rays were produced when high speed electron hit the metal target.

Question 13: The speed of rotation in anode rotation

a. 6000 rpm
b. 1000 rpm
c. 3000 rpm

Solution: Rotating anodes allow the electron bean sweep a larger area of the anode, thus redeeming the advantage of a higher intensity of emitted radiation along with reduced damage to anode compared to its stationary state. The speed of anode rotation is around 6000 rpm

Week_4_Lecture_4: Lecture 4 is about instrumentation in X-ray crystallography.

Question 14: Which devices absorb all the x-rays except the narrow beam that passes between the gaps?

a. Monochromator
b. Sealed tubes
c. Collimator
d. X-ray detector

Solution: A **collimator** is a device which narrows a beam of particles or waves. To narrow can mean either to cause the directions of motion to become more aligned in a specific direction (i.e., make collimated light or parallel rays), or to cause the spatial cross section of the beam to become smaller (**beam limiting device**).

1. Collimators are used for X-ray, gamma-ray, and neutron imaging because it is difficult to focus these types of radiation into an image using lenses.
2. A **monochromator** is an optical device that transmits a selectable narrow band of wavelengths of light or other radiation chosen from a wider range of wavelengths available at the input.
3. Monochromators are of two types:
    a. Interface filters (Use a threshold for X-ray absorption edge).
    b. Crystal Monochromators, which are further classified as Flat and curved crystal monochromators
4. Advantages of mono chromatic rays:
    a. Improve resolution
    b. Improve signal to noise ratio
    c. Simplify data processing

Summary

Week_4_Lecture_4: Lecture 4 is about instrumentation in X-ray crystallography.

1. X-ray detectors are devices used to measure the flux, spatial distribution, spectrum, and/or other properties of X-rays.

1. Detectors can be divided into two major categories:
    a. Imaging detectors (such as photographic plates and X-ray film (photographic film), now mostly replaced by various digitizing devices like image plates or flat panel detectors) and
    b. Dose measurement devices (such as ionization chambers, Geiger counters, and dosimeters used to measure the local radiation exposure, dose, and/or dose rate).
2. In photographic method, to record the position and intensity of x-ray beam, a plane or cylindrical film is used. The blackening of the developed film is expressed in terms of density units. These are mainly used in diffraction studies.
3. Solid state detectors use semiconductors to detect x-rays. Direct digital detectors directly convert x-ray photons to electrical charge and thus a digital image.
4. Indirect systems may have intervening steps, first step is converting x-ray photons to visible light, and then an electronic signal. Both systems typically use thin film transistors to read out and convert the electronic signal to a digital image.

Summary

Week_5_Lecture_5: Lecture 5 is about Data collection and processing

1. When a crystal is mounted and exposed to an intense beam of X-rays, it scatters the X-rays into a pattern of spots that can be observed on a screen behind the crystal. The relative intensities of these spots provide the information to determine the arrangement of molecules within the crystal in atomic detail.
2. To collect all the necessary information, the crystal must be rotated step-by-step through 180°, with an image recorded at every step; actually, slightly more than 180° is required to cover reciprocal space (the **reciprocal lattice** represents the Fourier transform of another lattice (usually a Bravais lattice).
3. Each spot corresponds to a different type of variation in the electron density; the crystallographer must determine *which* variation corresponds to *which* spot (*indexing*), the relative strengths of the spots in different images (*merging and scaling*) and how the variations should be combined to yield the total electron density (*phasing*).
4. **Data processing begins with *indexing* the reflections.** This means identifying the dimensions of the unit cell and which image peak corresponds to which position in reciprocal space. A byproduct of indexing is to determine the symmetry of the crystal, i.e., its *space group*.
5. A **space group** is the symmetry group of an object in space, usually in three dimensions. The elements of a space group (its symmetry operations) are the rigid transformations of an object that leave it unchanged

Summary

Week_5_Lecture_5: Lecture 5 is about Data collection and processing

Miller indices

Vectors and planes in a crystal lattice are described by the three-value Miller index notation. This syntax uses the indices ℓ, *m*, and *n* as directional parameters.

By definition, the syntax (ℓmn) denotes a plane that intercepts the three points i.e., the Miller indices are proportional to the inverses of the intercepts of the plane with the unit cell (the basis of the lattice vectors).

Point groups

The crystallographic point group or *crystal class* is the mathematical group comprising the symmetry operations that leave at least one point unmoved and that leave the appearance of the crystal structure unchanged. These symmetry operations include

a. *Reflection*, which reflects the structure across a *reflection plane*
b. *Rotation*, which rotates the structure a specified portion of a circle about a *rotation axis*
c. *Inversion*, which changes the sign of the coordinate of each point with respect to a *center of symmetry* or *inversion point*

Space groups

In addition to the operations of the point group, the space group of the crystal structure contains translational symmetry operations. These include:

a. Pure *translations*, which move a point along a vector
b. *Screw axes*, which rotate a point around an axis while translating parallel to the axis.
c. *Glide planes*, which reflect a point through a plane while translating it parallel to the plane.