Analysis of the energy distribution of light which is diffracted by a hexagonal netting. The light diffraction pattern is an optical transform of a two dimensional pattern and helps to identify the netting’s axes of symmetry.

Measurements of electron diffraction can reveal the atomic structure of crystals and allow one to find the length of chemical bonds. An effective electronic charge of each atom in the crystal acts upon the incident electron beam as a netting of narrow pinholes, and Fourier transforms the de Broglie wavelength of the projectile electron accelerated at fixed voltage into a wave packet.

Phase 1 – Electrons are accelerated by a voltage, V

\[ V \rightarrow K = eV \rightarrow p = \sqrt{2mE} = \frac{h}{\lambda} \rightarrow \lambda = \frac{h}{p} \]

where \( E = mc^2 \) and \( k = \frac{2\pi}{\lambda} \)

Solving the Schrödinger equation:

\[ i\hbar \frac{\partial \psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(r,t)}{\partial r^2} + U(r)\psi(r,t) \]

with free boundary conditions for the projectile electron leads to a delocalized plane wave \( \psi(r,t) = \Delta \frac{e^{i(kr-\omega t)}}{\sqrt{A}} \) for a single de Broglie particle.

Phase 2 – The Fourier transform of free electrons into wave packets

1. The Heisenberg Uncertainty Principle sets up the mechanism to create wave packets.
2. Inside the atom of the crystal the projectile electron now has a spreading in \( \lambda = \Delta \lambda \frac{2\pi}{p} \)
3. Therefore, it becomes a wave packet

\[ \psi(r,t) = \sum_{m} \Delta \frac{e^{i(k_{m}r-\omega_{m}t)}}{\sqrt{A}} \]

Phase 3 – The fast passage of the projectile electrons through the crystal

1. Pauli Exclusion Principle forbids the projectile electrons to inhabit the atom. The characteristic time of transmission through an atom is \( \Delta \tau = \frac{\lambda}{\Delta K} \), where \( \Delta K = \frac{h}{\lambda} \) represents the uncertainty in the kinetic energy value of the projectile electron.
2. Inside the atomic region of size \( \Delta r \), the electronic wave packet of width \( \Delta k = \frac{1}{\Delta \lambda} \) in the momentum space travels with a group velocity \( v = \frac{\Delta K}{\Delta p} \).

The electron diffraction pattern is produced by electron transmission. The projectile electron experiences a strong Coulomb repulsion from the sp² hybrid bonding orbital of the L-shell and is pushed toward the atomic core. Therefore, the projectile interacts with an electronic charge density located around the atomic nuclei. The periodic structure of the graphite crystal creates long ‘channels’ formed by Carbon atoms which act as infinitely long ‘slits’. The ‘slits’ act as a 2D netting and produce a diffraction pattern. The interference and diffraction pattern is analyzed by measuring the separation of peaks (\( \Delta y \)) and the position of the first minimum of diffraction with respect to the central maximum.

**Energy Distribution Function (Infinite Slit Approximation)**

**Electron Diffraction by Crystal - Theory**

**Experimental Analysis**

**Experimental signal**

**Crystal's unit cell**

**3D diffraction pattern**

**Crystal Lattice**

(a) A hexagonal layer of graphite illustrated with atomic slits and (b) the valence charge density of the 2p² electronic subshell in a single plane. Contours are drawn as the electron density decreases from the center of the covalent bond.

**Analysis of the electron diffraction pattern for a graphite crystal:**

(1) Interference peaks are located at \( d \sin \beta = n \lambda \) with \( n \) a small integer with a separation distance \( \Delta \lambda \).

(2) We calculate the distance between the atomic 'slits': \( \Delta \lambda = \frac{\lambda}{d} \)

For \( V = 8250 \) volts \( \Rightarrow \lambda = 0.135 \) Å

\( L = 17.355 \) cm \( \Rightarrow d = 2.11 \) Å

(3) We calculate the lattice constant a:

\[ a = d \cos 30^\circ = 2.44 \text{ Å} \]

(4) The diffraction envelope vanishes where the 5th maximum of interference (n = 9) is missing:

\[ d \sin \beta = n \lambda \] and \( \sin \beta = \frac{n \lambda}{d} \)

(5) The C-bond length \( b \) defined as \( d / \sqrt{3} \) for a hexagonal crystal is 1.40 Å, which is 0.7% smaller than the accepted theoretical value (2.46 Å).

**Heisenberg Uncertainty Principle in electron diffraction by transmission:**

- The accelerating voltage of 8250 volts gives a linear momentum of 91.82 keV/c.
- From \( \Delta r \) we find \( \Delta p = h / \Delta r = 8.58 \) keV/c.
- The Fourier transform of the projectile has spreading: \( \Delta \lambda = \frac{h}{p} \Rightarrow \Delta \lambda = 0.02 \) Å.
- The projectile's kinetic energy of 8250 eV has a spreading \( \Delta \lambda = (m / p^2)E = 15411 \text{ eV} \).
- The group velocity of the projectile's wave packet is \( v = \Delta \lambda / \Delta \lambda = 0.179 \) Å/c.
- Characteristic time of the Pauli Exclusion Principle: \( \Delta t = h / \Delta \lambda = 4.27 \times 10^{-18} \) sec.