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37

DIFFRACTION OF ELECTRONS AND LIGHT ON CRYSTAL LATTICE

1. Fundamentals

The explanation of the photoelectric effect given by A. Einstein in 1905 and the phenomenon of scattering of X-rays on free electrons observed in 1923 radically changed our views on the nature of electromagnetic waves.

Electromagnetic waves, although they exhibit properties characteristic of wave motion (diffraction, interference, etc.), in their interaction with an electron, behave as a stream of particles (photons) whose energy is equal to $h\nu$ (h – Planck's constant, ν- the frequency of the light wave) and momentum p is:

$$p = \frac{h\nu}{c} = \frac{h}{\lambda}\ , \qquad (1)$$

where c – speed of light, λ - wavelength.

It cannot be said that the nature of photons is a wave or a particle, only that they exhibit both wave and particle characteristics. This way of their behavior is called **wave-particle duality**.

In 1924, Louis de Broglie formulated de Broglie hypothesis claiming that all matter exhibits a wave-like nature. de Broglie wavelength λ associated with the matter particle is related to its momentum p through the Planck constant h:

$$\lambda = \frac{h}{p}\ . \qquad (2)$$

This means that a moving particle can exhibit wave-like behavior under certain conditions. Such a wave is called a particle wave or de Broglie wave.

It is worth noting that equation (2) can be obtained by transforming equation (1). This convergence is not accidental. At the base of de Broglie's hypothesis lies an assumption that wave-particle duality is a fundamental property of the whole matter, thus of both photons (of rest mass equal to zero!) and corpuscular particles (of rest mass different from zero). To ~~In order to~~ check the validity of de Broglie's hypothesis, it should be experimentally proved that particles exhibit wave phenomena, e.g., the phenomenon of interference or diffraction, fulfilling the relation (2).

To observe the phenomenon of interference, it is necessary to use a diffraction grating whose constant (i.e., the distance between slits) does not differ significantly from the length of the incident radiation (no more than two orders of magnitude). At the same time, particles should have significant energy to be able to penetrate very thin layers of matter. Then their momentum will be large, and according to formula (2) the de Broglie wavelength will become very small. This, in turn, imposes a condition for a very small value of diffraction lattice constant, much smaller than possible.

For example, electrons to penetrate an aluminum foil about 50 nm thick must have an energy of about 10 keV, but then their de Broglie wavelength is about 0.01 nm. This is a value smaller than the diameter of an atom. So how to make a diffraction grating with such small distances between slits? We do not have to make such a grating, as crystals fulfill their role. Atoms in a crystal are arranged periodically, and interatomic distances are a few Å (*Angstrom*) (1Å = 0,1 nm = 10^{-10}m), which makes them useful for observing the phenomenon of de Broglie wave interference. A description of the different types of crystalline bodies and definitions of the basic concepts related to crystal structure are given in Appendix A.

1.1. Diffraction of a wave on a crystal lattice

Suppose that a crystal is hit by a wave of length λ. **Each atom of the crystal interacting with it becomes itself a source of a new (secondary) spherical wave of the same length (Huyghens' principle)**. The secondary waves emitted by individual atoms will interfere with each other. To find the result of the interference in the general case, let us first consider the case when a plane wave interacts with only one atomic plane.

Since a crystal can be represented as a set of parallel atomic planes, creating a new wave can be described as a superposition (interference) of spherical waves created in particular atomic planes. These waves, after superposition, will be, depending on the difference of their optical paths, amplified or weakened, see Fig.1. The condition of amplification of the waves is that the difference of the optical paths is equal to a multiple of the wavelength.

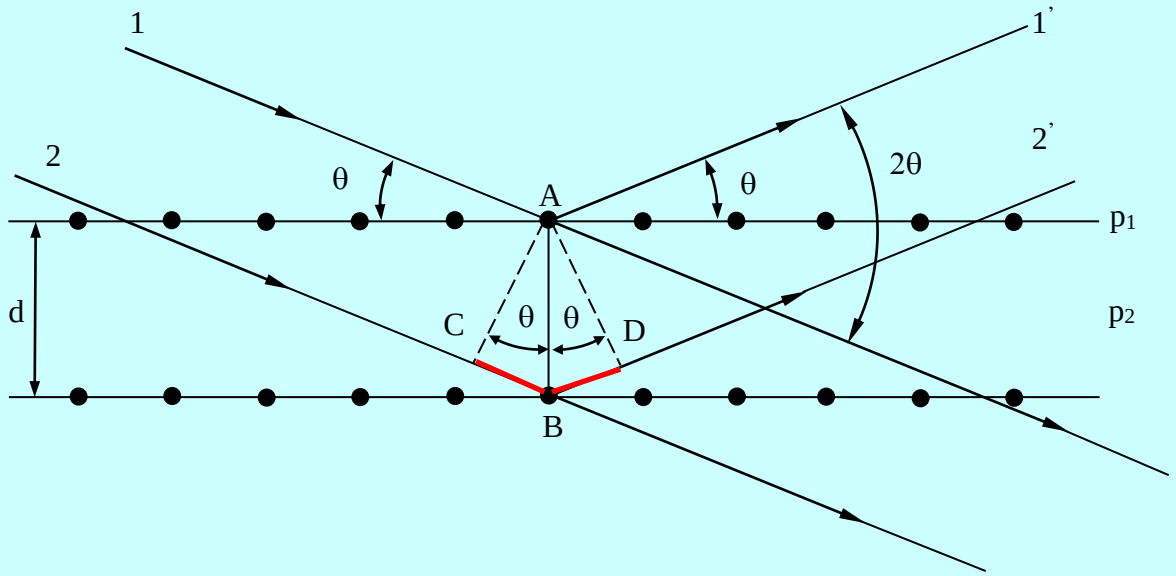

Fig.1 Diffraction of light on a crystal (1' is the direction in which the wave is amplified by interference)

From Figure 1, it follows that the difference of optical paths for points of space located in directions 1'and 2' for two consecutive atomic planes (p_1 and p_2) is: $CB + BD = 2d\sin\theta$ (the difference in paths is marked red in the figure). Interference gain will occur when it is equal to an integer multiple of the wavelength, i.e.:

$$2d\sin\theta = n\lambda \qquad (3)$$

where d - is the distance between the atomic planes and θ - is the angle between the direction of the incident beam and the atomic plane (so-called angle of slip - not to be confused with the angle of incidence!!!), while = 1,2,3,...(order of deflection). Equation (3) is called the **Bragg formula**.

Although obtaining Bragg's formula, we considered only the waves arising in only two consecutive atomic planes, and it turns out that it is also valid when a large number of these planes are involved. From Fig.1, it can also be seen that the angle between the direction in which interference maxima lie and the extension of the direction of the incident wave is 2θ.

The above-described mechanism of wave diffraction on a crystal is called Bragg diffraction (in literature, one can often meet the term "Bragg reflection"). However, it should be remembered that this is a special "reflection", i.e., it occurs only when the condition: $2d\sin\theta = n\lambda$. Thus, the Bragg phenomenon can only be observed for wavelengths comparable to the distance between interatomic planes (d of the order of 0.1 nm) and shorter. It is, therefore, possible to fulfill equation (3) for X-rays but impossible for visible light (λ = 400-700 nm).

Many families of atomic planes can be distinguished in crystals. For example, in the cross-section of the crystal shown in fig.2, apart from the planes p_1, p_2, p_3, ... planes can be distinguished t_1, t_2, t_3,..., s_1, s_2, s_3,..., u_1, u_2, u_3,... . Each family of planes listed here, characterized by its own

distance between planes d_i, can give the phenomenon described above as long as the Bragg condition is satisfied. For this reason, we obtain multiple directions of enhancement for different slip angles θ_i.

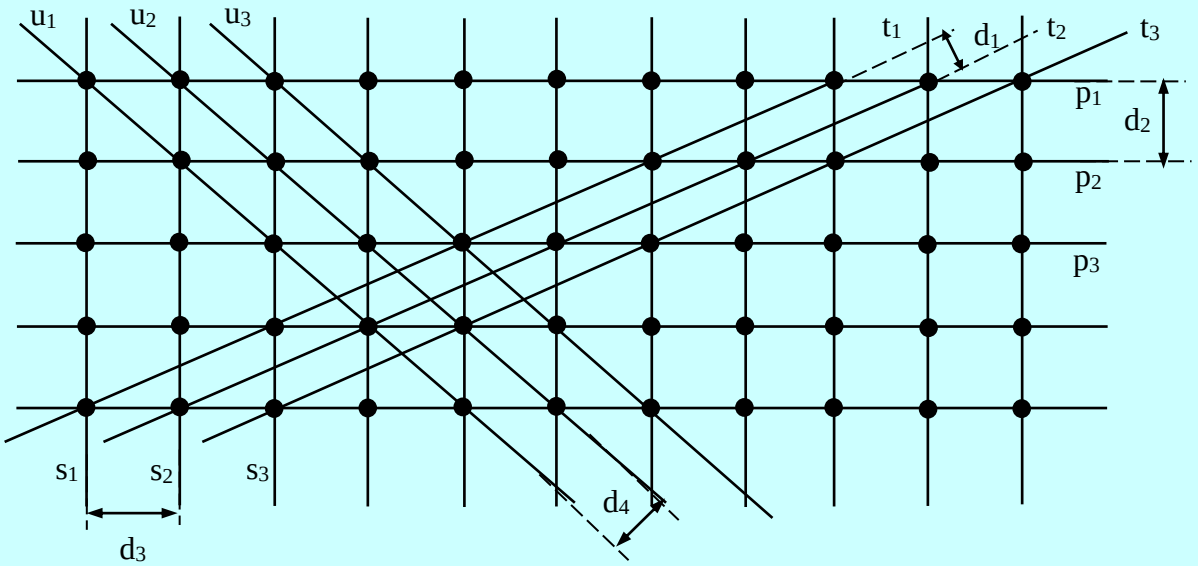

Fig.2 Examples of families of atomic planes in a crystal (in the figure, we see their projections on the plane of the figure)

If the crystal is rotated with respect to the axis coinciding with the direction of the incident beam, the amplified beams will start to stagger conical surfaces with an angle of dilation 4Θ. When a parallel and monochromatic wave falls on a polycrystal, i.e., a material containing a large number of small (micron-size) monocrystals (crystallites), oriented in a random way, we observe an effect like that of a crystal rotation. This is because there will always be a certain number of crystallites for which Bragg's condition will be fulfilled for a given angle Θ and then the reinforced beams will form the surfaces of cones with opening angles 4Θ. If we place a screen in the path of the amplified beams, we will observe circles on it (fig.3).

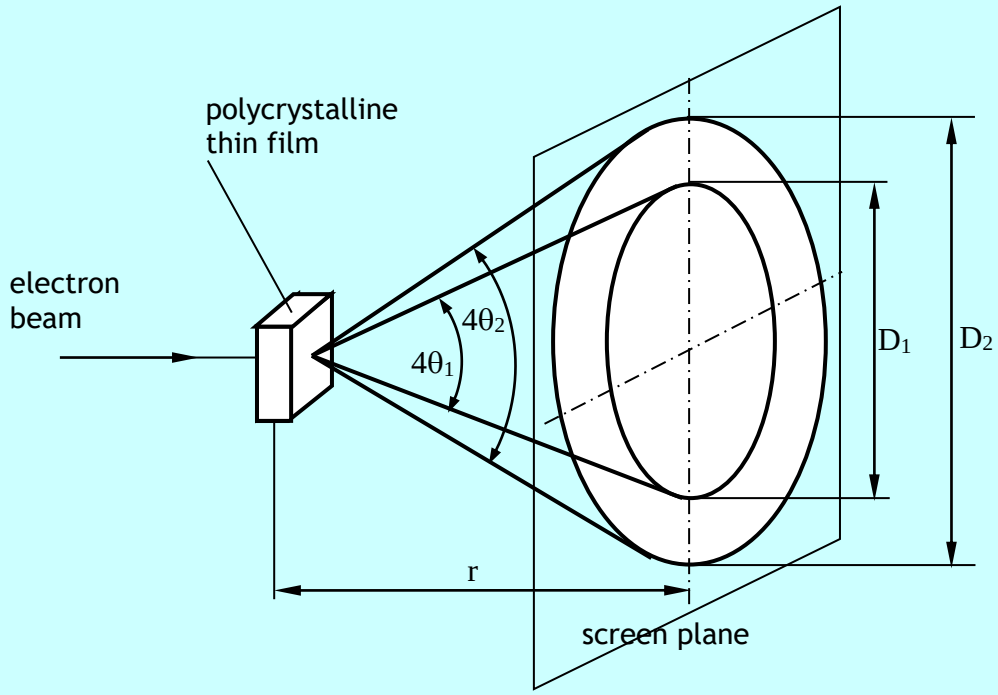

Fig.3 Bragg phenomenon for a polycrystalline sample.

1.2. The Thomson experiment

The considerations carried out earlier are the basis for understanding the experiment carried out by G. P. Thomson in 1927, confirming de Broglie's hypothesis. Thomson placed a thin gold foil (polycrystalline foil) in an oscilloscope tube behind a system of focusing anodes. Electrons falling on it were subjected to the phenomena discussed above (i.e., the phenomenon of interference), resulting in circles of different diameters on the screen D_i .

The ring system formed on the screen can be explained if we assume that the electron is associated with a wave whose length is determined by the formula: $\lambda=h/p$. It interacts with the polycrystalline film in the manner presented earlier. An additional argument for this assumption's validity is that the same arrangement of circles was obtained by irradiating the mentioned film with X-rays of a similar wavelength as the wavelength of electrons predicted by de Broglie. Thomson's experiment thus confirms the wave nature of the electron flux. The wave associated with the electron is a particle wave, the nature of which is described in detail in Appendix B.

To investigate the properties of matter waves (and to test de Broglie's hypothesis), a suitably prepared oscilloscope tube was used. A thin foil (aluminum or graphite) was placed in the path of the electron beam. Its thickness is about 50 nm. This thin film is transparent to electrons with energies above 8 keV. It is obtained by vacuum vapor deposition. The electrons emitted by the cathode of the oscilloscope tube are accelerated to the kinetic energy of $E_k=eU$ by the applied voltage U, which can be adjusted.

Since the distance between the foil and the screen is much larger than the diameter of the interference circles D obtained on the screen, according to Fig.3: $\sin 4\theta \approx 4\theta \approx D/r$ (r - film-screen distance), and hence: $\sin\theta \approx \theta \approx D/4r$.
By substituting the value calculated in this way $\sin\theta$ to Bragg's formula (3), we obtain:

$$\frac{dD}{2r} = n\lambda \qquad \textbf{(4)}$$

The value λ is found from equation (1), i.e., $\lambda = h/p$. The momentum of the electron p is calculated by knowing the voltage U from the classical relation between momentum and its energy eU, i.e., $eU=p^2/2m$ (e - charge of the electron, m – its mass). Relativistic change of mass of the electron at energies of the electric field used in the experiment introduces negligible uncertainty.
By substituting into Formula (4) the value λ calculated for the accelerating voltage U: $\lambda = \frac{h}{\sqrt{2meU}}$
and n = 1 (since only circles of the first order are visible), we obtain:

$$D = \frac{2rh}{d\sqrt{2meU}} \qquad \textbf{(5)}$$

The diameter of the interference circle D, coming from the same set of atomic planes, should be inversely proportional to the square root of the electron accelerating voltage U. If we obtain such a result, it will confirm the formula describing de Broglie's hypothesis.

1.3. Diffraction of light on a two-dimensional lattice

The second part of the exercise is to get acquainted with the diffraction of light on a regular two-dimensional lattice when the light beam falls on the lattice at right angles to the lattice plane. According to what was written in the previous part of the manual, each atom becomes a source of a new spherical wave. These waves interfere with each other, and the effect can be seen on a screen placed perpendicularly to the direction of the incident wave, at some distance from the lattice.

Let us consider a regular rectangular network. The amplification condition in such a case is that two Laue's equations are satisfied, which can be written as follows:

$$a\cos\Theta' = m\lambda$$

$$b\cos\Theta'' = n\lambda \qquad (6)$$

Where a, b - lattice constants, Θ` and Θ`` - angles between the direction of incidence of the light beam and the direction of amplification (amplified beams form cones with opening angles of 2Θ` and 2Θ``), *m* and *n* - arbitrary integers.

The solutions to each of Laue's equations are conical surfaces that form families on a screen-oriented direction parallel to the surface of the grid (and perpendicular to the direction of incidence of the light beam) hyperbolas. The common solution of both equations observed on the screen in the form of luminous points are points of intersection of hyperbolas. In the experiment conducted, the length of the light wave (0.6 m) is almost three orders of magnitude smaller than the distance between atoms in the crystal lattice under investigation (0.1 mm). For this reason, on the screen, the points are arranged on hyperbolas of very small curvature, visible actually as straight lines (curvature of hyperbolas cannot be noticed).

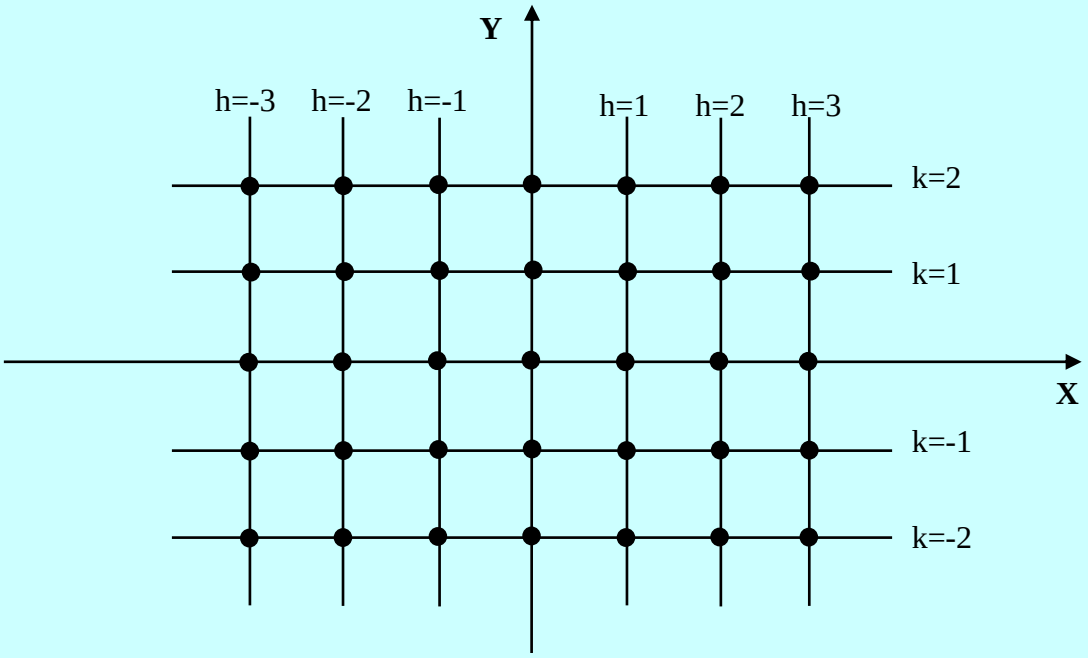

Fig.4 Screen appearance of diffraction case on the regular lattice - black points in the illustration are luminous points on the screen, the effect of the intersection of hyperbolas (definition of indices h and k)

We assign two indices to the luminous points on the screen (see figure 4) called Miller indices. The coordinates of the points are written as pairs of numbers (h, k), for example, (1, 1) (3, 1) (-2, 5), etc. The segment that connects the point (h, k) with the center of the diffraction image (i.e., with the point (0, 0)) is denoted H_{hk}. Knowledge of the length of light λ used in the experiment, the distance L of the screen from the crystal lattice, and the value of H_{kl} allow for the determination of the lattice constants of the tested lattice.

From the geometrical properties, we obtain the following formula:

$$tg\Theta_{hk} = \frac{H_{hk}}{L} \qquad (7)$$

Taking into account the well known relationship

$$d_{hk}\sin\Theta_{hk} = n\lambda \qquad (8)$$

we can calculate the constants d_{hk}, and from them, the lattice constants of the tested lattice. The method of determining the lattice constants depends on the type of network. Relationships between the lattice constants and the determined constants d_{hk} are the following:

$$d_{hk} = \frac{a}{\sqrt{h^2 + k^2}}$$ (regular lattice, lattice constant a)

$$d_{hk} = \frac{a}{\sqrt{\frac{4}{3}\left(h^2 + kh + k^2\right)}}$$ (hexagonal lattice, lattice constant a) **(9)**

$$d_{hk} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2}}}$$ (rectangular lattice, lattice constants a and b)

When the beam falls on a polycrystalline lattice, you should get concentric circles on the screen (as in electron diffraction). If the circles (rings) are not clearly visible, it means that the light beam covers only a few differently oriented monocrystalline areas.

2. Experiment

2.1. Electron diffraction - Thompson experiment

Implementation of the exercise

1. Familiarise yourself with the operation of the power supply unit for the oscilloscope tube (if in doubt, ask your instructor).
2. Make sure the electron accelerating voltage adjustment knob is in the zero position (turned to the "left") - if not, move it to this position.
3. Turn on the power supply and wait about 2 minutes for the cathode of the oscilloscope tube to warm up.
4. Turn the electron accelerating voltage regulation knob and observe the appearance of a spot on the screen (adjust its brightness as necessary).
5. Increase the electron accelerating voltage until rings appear (control brightness and sharpness of the image).
6. Measure the diameters D_i of all the rings visible on the screen as a function of the accelerating voltage U for at least 6 different voltages.
7. Turn the accelerating voltage control knob to zero (extreme left) and switch off the power supply.
8. Note the distance r (foil - screen).

Compilation of results

1. Verify that the results obtained are by formula (5), drawing a diagram of the dependence of the ring diameter D_i on $\frac{2rh}{\sqrt{2meU}}$ (i.e., the function depending on the inverse of the square root of the accelerating voltage), and find the value of the slope coefficient of the resulting straight line b and its uncertainty using the method of least squares (calculations with the aid of a computer program!!).
2. Calculate the distance between the atomic planes d and the uncertainty calculated by the Type A method from the results of the linear approximation. Calculate the uncertainty of Type B based on a single measurement point (take the necessary physical constants from tables). For the evaluation of the combined uncertainty, use the law of propagation of uncertainty.
3. Using the graph obtained and the χ^2 test, answer the question concerning the truth of the de Broglie hypothesis. Compare the obtained result with the values of interatomic distances in graphite crystals.

The figure below shows a diagram of the crystalline structure of graphite.

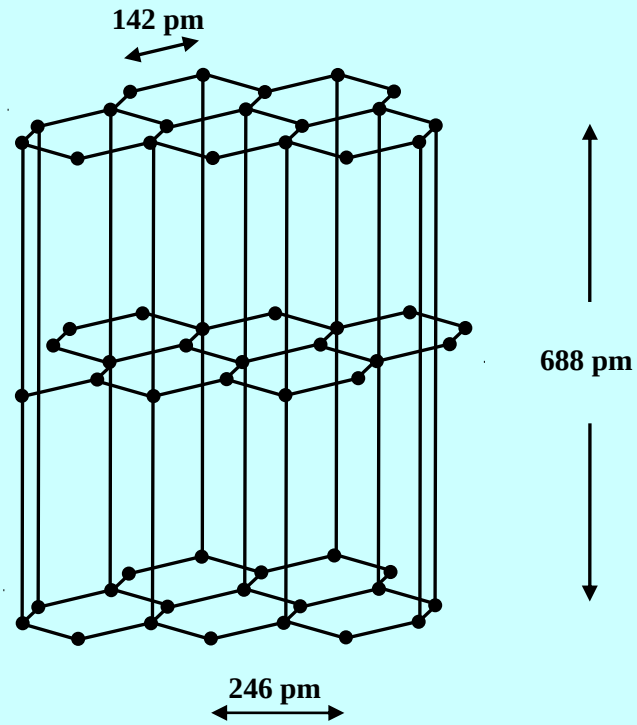

Fig.5 Graphite crystal lattice

The graphite layer through which the electron beam passes is polycrystalline. The long bonds between the individual layers are broken (fig.5), so the orientation of the cells is random. (Graphite is very "slippery" and spreads easily over the surface - this is the effect of the individual layers of carbon atoms moving against each other. On the other hand, graphite is very resistant to compression. For these reasons, it is used to produce various types of lubricants, particularly dry lubricants).

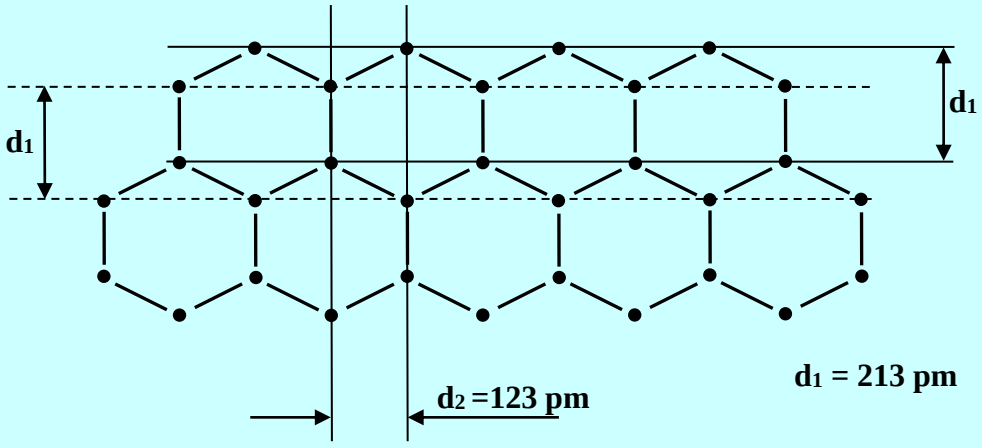

Fig.6 Interplane distances for the first two interference rings

4. **The report should answer the following questions:** Why are the intensities of the two rings comparable? Why are rings of higher interference orders or from other atomic planes not visible?

2.2. Diffraction of light on a crystal lattice

Implementation of the exercise

Two-dimensional models of different types of crystalline and polycrystalline lattices in the form of transparencies on photosensitive film are used to observe the diffraction of light on crystals. A semiconductor laser is used as the light source, generating light of the length specified on the laser holder. The laser is fixed on a base to which the slides are magnetically attached (the frames have magnetic strips at the bottom). Each slide has a marking (e.g., A1, C2, etc.). The tripod with laser should be placed in the marked position on the laboratory table at exactly the specified distance from the screen located on the vertical housing of the laboratory station (the distance between the slide and the screen must remain constant). The screen is equipped with a clip where the protocol is attached, and the resulting diffraction images are redrawn.

There is also an optical microscope on the bench, which is used to observe the network models and directly measure the network constants (using the micrometer slide of the microscope table or the spider web in the eyepiece).

In the instructions given below, the command "trace the image" means to place the protocol on the screen and to mark with a pen the most important elements of the resulting interference image.

1. Turn on the laser and place it in the position marked on the laboratory table so that the beam falls near the center of the screen.
2. Insert slides A1, B1, and C1 into the laser beam. Trace the resulting images onto the protocol.
3. Insert the slide marked D1 into the laser beam. Trace the resulting image onto the record.
4. Insert the slide marked B5 into the laser beam. Trace the resulting image onto the protocol.
5. Place all slides used in the exercise on the optical microscope table and measure the lattice constants directly.
6. Insert slides marked B2 and B3 into the laser beam.

Compilation of results

1. Compare the interference images for slides A1, B1, and C1. What was observed under the microscope? Which physical principle is confirmed by this part of the experiment?
2. Based on formulas (7), (8), and (9), calculate lattice constants for these crystalline networks. Compare the obtained result with measurements under a microscope.
3. Calculate the lattice constants for the D1 slide. Compare the result with the result obtained from measurements under the microscope.
4. Which crystal we are dealing with for slide B5. Determine the lattice constant by measuring the diameter of the interference ring. The result obtained should be compared with the result of measurements taken under the microscope. Can the interference image obtained for slide B5 be compared with the image obtained for electron diffraction in Thompson's experiment in the previous part of the exercise? The answer should be justified.
5. What are the crystal lattices shown in slides B2 and B3? Calculate the lattice constans.
6. For all lattice types, estimate the uncertainties of the determined lattice constants.

3. Questions

1. What assumption underlies the de Broglie hypothesis?
2. What conditions must be met for the interfering waves to be amplified?
3. Derive Bragg's formula.
4. What physical phenomenon is described by Laue's equations?
5. Draw and explain the interference image when light diffracts on a polycrystal.
6. Explain the essence of Thomson's experiment. What is the relationship between the diameter of the ring and the accelerating voltage?
7. Assume that a neutron and an electron have the same energy. Which particle corresponds to the larger de Broglie wavelength?

4. References

1. D. Halliday, R. Resnick, J. Walker, Podstawy fizyki, tom IV, PWN 2003
2. R. Eisberg i R. Resnick, Fizyka kwantowa – str. 78 PWN 1983
3. Cz. Bobrowski, Fizyka – krótki kurs, WNT 1993

APPENDIX A
The crystalline structure of solids

Based on how the atoms (or particles) are arranged, solids can be divided into monocrystalline, polycrystalline, and amorphous (amorphous) bodies. Monocrystals are those bodies in which the atoms are arranged regularly throughout the volume of the body - this is called long-range ordering. The distance between neighboring atoms is usually a few Angstroms (Å). The smallest cell whose repetition in all three directions gives a single crystal is called an **elementary cell**. An elementary cell is defined by the lengths of its sides (the so-called lattice constants) in three selected directions and the three angles that these sides form with each other. This experiment considers the simplest two-dimensional crystal lattice, as shown in Fig. 7.

The second type of crystalline body investigated in the experiment is polycrystals. These are bodies in which one can observe areas of monocrystalline structure arranged randomly in relation to each other. These areas (monocrystalline grains - crystallites) may be of the size of fractions of a micrometer, as well as of macroscopic dimensions. The natural state for most solids is the crystalline state, often monocrystalline, as the ordering energy of the atoms is lowest. In nature, beautiful and large-sized monocrystals can often be observed: salt crystals in Wieliczka, diamonds (carbon crystals!), etc. However, if the crystallization process is disturbed during crystal formation, a polycrystalline or even amorphous body is obtained.

Monocrystals are widely used in modern technology. They are the basis of all microelectronics; there would be no microprocessors, memories, electronic circuits, and computers without them. Most integrated circuits are manufactured on thin sheets of monocrystalline silicon. Every self-respecting student of the Warsaw University of Technology should know that the method of obtaining monocrystals by crystallization from a molten substance was developed by Jan Czochralski, an outstanding chemist and meteorologist, professor at the Warsaw University of Technology from 1930 until the end of the World War II. This method (known throughout the world as the Czochralski method) is still today the basic method for obtaining monocrystals with an incredible diameter of several tens of centimeters and length of several meters. The monocrystals are cut into slices a fraction of a millimeter thick, and on these slices, the ubiquitous integrated circuits are made.

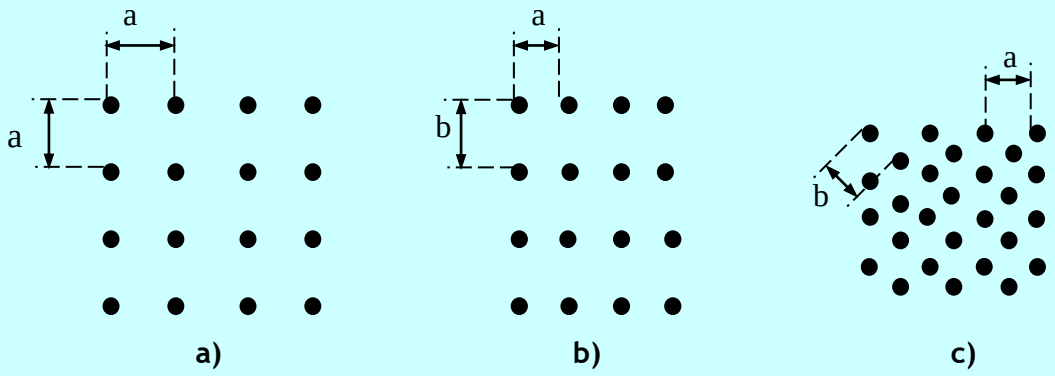

Fig.7 Two-dimensional crystal lattice types: a) regular lattice, b) rectangular lattice, c) hexagonal lattice

APPENDIX B
The nature of de Broglie's waves

In trying to answer this question, we will refer to an experiment. If, in Thomson's experiment, an electron beam of extremely small intensity is used, it can be assumed that single electrons fall on the film, single flashes of equal intensity will be observed on the screen. Most flashes will occur at the point where electrons pass straight through, but a number of flashes will be observed on the interference circles.

The appearance of single flashes clearly contradicts the possibility that the de Broglie wave is simply a ripple of electron matter. If this were the case, we would observe the whole interference pattern (i.e., a system of circles), although with very low intensity, already at the passage of a single electron.

However, the result of the experiment should not shake our conviction about the wave properties of the electron (properties, not nature), since flashes appeared (except for the place corresponding to the passage of electrons straight ahead) only on the interference circles. As shown above, the interaction of the wave (electron) with many atomic planes is needed, so the electron behaves like a wave. However, we cannot explain why a single electron interacts with atomic planes as a wave but with screen atoms as a corpuscle.

Analyzing the results of other experiments, one may formulate a conclusion: if a particle interacts with an object in such a way that it is impossible to determine with which part of the object the interaction takes place, then wave properties of the particle are revealed (interaction with atomic planes of thin-film crystals). However, when we can localize the interacting particle (e.g., interaction with specific atoms of the screen), then it interacts as a particle. In the region of accelerating electron, we can also exactly (in the range of field energy about 10 keV) trace the position and momentum of the particle. Interaction of the electron with the electric field in the oscilloscope lamp also allows for treating the electron as a particle.

To complete the picture, let us add that if in the experiment in question a photographic plate is placed behind the screen (instead of observing single flashes), then after long exposure, the image obtained on it will not differ in any way from the image observed on the screen at a high intensity of the electron beam. The latter result proves the statistical character of laws governing the behavior of particles. This view is represented by quantum mechanics, a theory to which the de Broglie hypothesis contributed. Quantum mechanics does not enter into the nature of de Broglie's waves but only deals with the description of the behavior of particles taking into account their wave properties.

The state of a particle in quantum mechanics is described by the wave function $\psi(x,y,z)$ with a mathematical form identical to the wave equation known from optics. The mathematical form of the wave function is found by solving the Schrödinger equation (the basic equation of quantum mechanics). Its interpretation is probabilistic (statistical). The square of the modulus of the function $\psi(x,y,z)$ is the probability density of finding a particle in a given point of space with x,y,z coordinates. Whereas the probability P of finding a particle in an element of the volume dV in the vicinity of a given point of space is:

$$P = |\psi(x, y, z)|^2 \, dV$$

The particle wave (de Broglie) is described by the function $\psi(x, y, z)$ having the form of the wave equation.