# Exp. B 10: Experiment with X-Rays

1. Literature

Keywords: Generation of x-rays, continous x-ray spectrum, Bohr's model of the atom, Term scheme of atoms, characteristic spectrum, Moseley's law, absorption spectrum, crystal lattice, Bragg's law of reflection, detection of x-rays, x-ray counting tube

2. Basics

2.1 Continous X-Ray Spectrum

X-rays can be generated using an (evacuated) x-ray tube (see schematic view in Fig. 1). Free electrons are generated by thermionic emission from a hot cathode C, focussed with the aid of a *Wehnelt cylinder* W and accelerated towards an anode A by a high anode voltage U_A.

When the electrons reach the anode, most of them gradually lose their kinetic
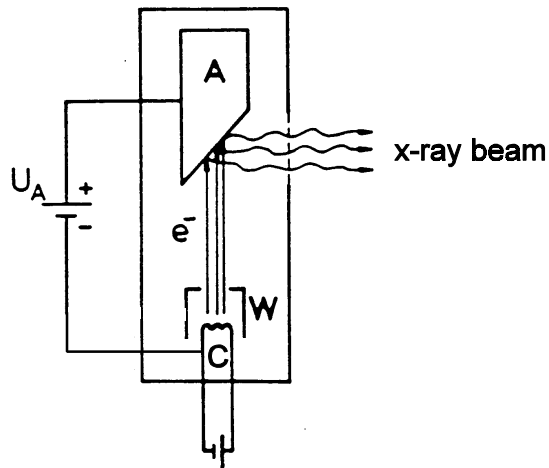
Fig. 1:

X-ray tube (schematic)

energy ($\frac{1}{2} mv^2 = eU_A$) during many collisions with the atoms of the anode material (eg. Tungsten or Copper) due to the Coulomb interaction (what is this?). The main part of their kinetic energy is converted simply into heat (i.e. atomic vibrational energy of the anode material), the remaining (smaller) part is converted into electromagnetic radiation. Among the latter, x-rays are generated within a continous spectrum, the so called *Bremsstrahlung* ("white x-ray light"), first

discovered by W. Röntgen (1895).
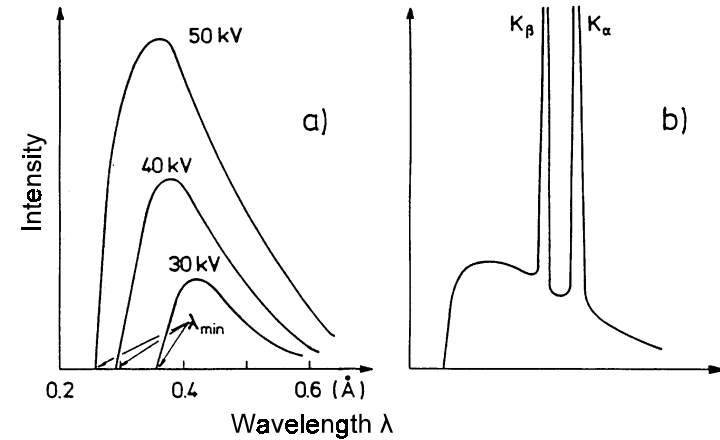
Fig. 2: a) continuous, b) continuous and characteristic x-ray spectrum (schematic)

Fig. 2 a shows the intensity of continueous x-ray spectrum vs. wavelength for various accelerating voltages. The spectral intensity is independent of the anode material and exhibits a short wave length cutoff λ_{min}, where the intensity drops to zero. At the cutoff wavelength λ_{min}, depending only on the accelerating voltage U_A, the kinetic energy of an electron is converted into radiation energy within a single process according to the following relation

$$\frac{1}{2}mv^2 = eU_A = h\nu_{max} = \frac{hc}{\lambda_{min}} .$$

(1)

This means that the maximum frequency ν_{max} or the minimum wave length $\lambda_{min} = c/\nu_{max}$ of the continous x-ray spectrum for a certain voltage U_A are solely determined by the charge of the electron e and Planck's constant h.

For many technical purposes, as in the present experiment, the acceleration voltages U_A are in the range 20 to 50 kV; thus the wave lengths are (according eq. 1) in the range of less than 1 Å (= 10^{-10} m = 0.1 nm = 100 pm).

2.2 Characteristic Spectrum

The x-ray spectrum observed often exhibits in addition to the continous spectrum shown in fig. 2a very high intensities at certain discrete wave lengths, which are characteristic for the atoms of the anode material (see eg. fig. 2b). These *spectral lines* are caused by energetic transitions of electrons across the different energetic states within the atoms of the anode material.

The physical origin of the characteristic x-ray spectrum is easily explained with the aid of Bohr's model of the atom (compare with Fig. 3). At the impact of the
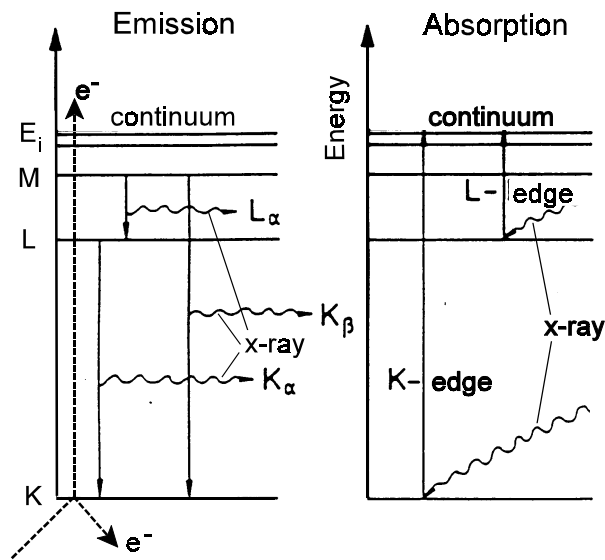

Fig. 3: term scheme with electronic transistions of the atom,
left: at emission, right: at absorption of x-rays

accelerated electron with an atom of the anode material, another electron, e.g., from the (energetically lowest, inner) K-shell, is removed and struck into the high energy continuum of the metal. The remaining hole in the K-shell is filled up by an electron from, e.g., the (energetically next higher) L-shell. At this transition, a certain amount of energy ΔE corresponding to the energy diffrence between the L- and the K-shell is released and emitted as electromagnetic radiation with the energy quantum $\Delta E = h\nu = hc/\lambda$ (*x-ray photon*). At the transition from, e.g., L to

K, the so called K_α x-ray line appears in the spectrum.

Transitions from the M-shell to the K-shell generate the K_β line, similarly the transitions from M to L generate the L_α line, etc. The characteristic spectrum is thus generated according to the energy levels of the atoms of the anode material. Both frequency or wavelength of these x-ray lines depend on the square of the atomic number Z of the considered element. For the K_α line the eq.

$$\nu_{K_\alpha} = \frac{3}{4}(Z - \sigma)^2 Ry , \quad \sigma = 1 \qquad (Moseley's \ Law) , \tag{2}$$

holds with the *Rydberg frequency* $Ry = 3.29 \cdot 10^{15} \ s^{-1}$. The *screening constant* σ accounts for the screening of the charge $+Ze$ of the nucleus by the remaining K-shell electron.

2.3 Absorption Spectrum

The weakening of x-rays in material is caused, first, by *classical* (elastic) *scattering* (changing the photon's momentum without changing its energy), second, by *Compton scattering* (partial transfer of photon energy to free or weakly bound electrons), and, third, by absorption. The capability of matter to absorb x-rays is described by the coefficient of absorption τ_A. It strongly depends on the atomic number Z (number of atomic electrons) and on the wavelength λ of the radiation ($\tau_A \sim Z^4\lambda^3$). At the absorption of x-rays, the whole photon energy is transfered to inner shell electrons being excited into higher energy states. From Fig. 3, it is evident that at the absorption of x-rays, no characteristic absorption lines - like the emission lines - can be observed. Otherwise, this would mean that, e.g., for the K_α line the excitation of one K-electron to the L-shell would be necessary. This shell and the other shells, M, N etc., are usually occupied. Therefore, only the excitation into states with $E \geq E_i$ (ionization energy), into the so called *continuum* is possible, and an absorption spectrum, as shown schematically in Fig. 4, is observed. Besides the increase of $\tau_A \sim \lambda^3$, the spectrum exhibits K, L, M, .. absorption edges (corresponding the excitation energies of K, L, M, ..electrons) at certain wavelengths λ - characteristic for the absorbing material. The corresponding frequencies, e.g., ν_K for K-electron excitation, depend on the atomic number of the absorbing element similar to that given by eq. (2)

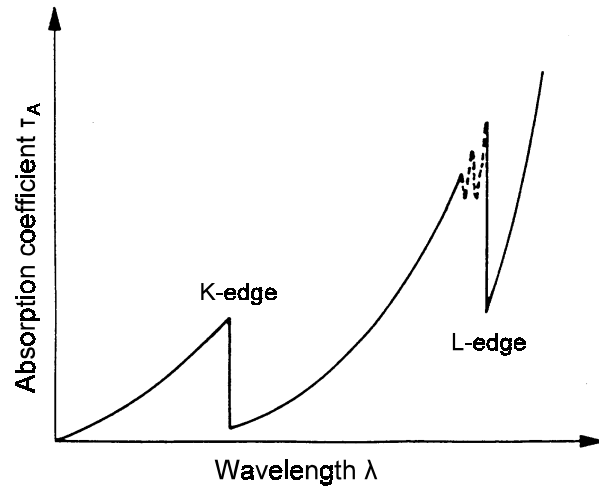$$\nu_K = (Z - \sigma)^2 Ry , \quad \sigma \approx 1 . \tag{3}$$

Fig. 4: X-ray absorption spectrum (schematic)

A suitable combination of anode material (in the present experiment copper, Z=29) and absorbing filter material (here nickel, Z=28) placed into the emitted x-ray beam, allows to obtain an x-ray emission spectrum (continuous and characteristic Cu spectrum), which is weakened very much at short wavelengths so that essentially only the Cu K_α line remains, i.e., monochromatic x-rays with $\lambda_{K\alpha} = 1.54$ Å = 154 pm.

2.4 Detection of X-Rays

X-rays can be detected through the use of their ionizing effect. The intensity of the radiation can be measured, e.g., by measurement of the current pulses through ionization chambers or counting tubes, or by the determination of the blackening of photo plates. The functioning of a simple counting tube, the *Geiger-Müller-tube* (used in the present experiment), is illustrated schematically in Fig. 5:
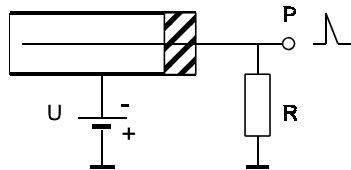

Fig. 5: Geiger-Müller tube

The tube consisting of a metal housing with a thin foil at one end is filled with inert gas (e.g. Argon) and some additional alcohol vapor. A thin steel wire (insulated from the housing) is streched along the center of the tube and connected through a resistor R (>1MΩ) to ground. The housing is negatively charged against the center wire by a high voltage, U≈500V. If the x-rays traverse the tube, they ionize single gas atoms, and the electrons are accelerated toward the center wire causing more ionization on their way resulting finally into a complete discharge of the tube (limited in time by the alcohol vapor). The discharge current across the resistor generates a voltage pulse at P which is counted.

2.5 Bragg Reflection of X-Rays

The wave nature of x-rays was first established in 1906 by Barkla, who was able to exhibit their polarization. In 1912 a method was devised to actually measure the wavelengths. Max v. Laue recognized that the wavelengths hypothesized for x-rays were about on the same order of magnitude as the spacing between adjacent atoms in crystals. He, therefore, used crystals to diffract x-rays with their regular lattices acting as a kind of a three dimensional grating. The diffraction of x-rays in crystals and their subsequent interference, characteristic for their wave nature, results in a diffraction pattern dependent on the x-ray wavelength and the spacing between the atoms. The regular arrays of atoms in crystals (in the present experiment NaCl, Sodium chloride with simple cubic symmetry) "reflect" x-rays with a single wavelength λ only at certain angles. Since the radiation penetrates the crystals, the "reflection" occurs at many atomic planes (selected families of atomic arrays) and actually depends on the distance d between the planes.
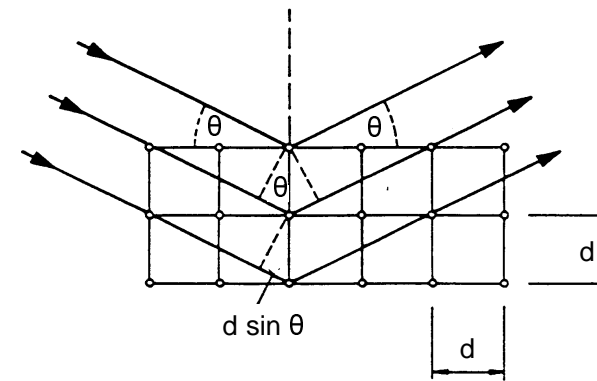

Fig. 6: Bragg reflection at a single crystal

This is illustrated schematically in Fig. 6. A monochromatic beam falls onto the parallel p lanes of atoms (separated b y distance d) with the a ngle θ and is "reflected" at the same angle. Constructive interference of the reflected beam, i.e., the so called *Bragg reflection,* only takes place if the path difference between x-rays reflected at adjacent planes is $\lambda, 2\lambda, 3\lambda..$, i.e., $n\lambda$, where n is an integer. According to the geometric situation scetched in Fig. 6, the condition for Bragg reflection is simply

$$n\lambda = 2d\sin\theta_n \qquad (Bragg^{/}s\ Law)\ . \qquad\qquad (4)$$

The "reflection" of radiation at atoms is actually a scattering and an interference process. The electronic shells (-Ze) of every atom of the crystal subjected to the field of the electromagnetic radiation are forced to vibrate around the nuclei (+Ze) and thereby emit radiation with the same frequency as the incoming radiation in almost all directions. This radiation is intensified by constructive interference at angles given according eq. (4) and annihilated at other angles. Since the interference maxima, if plotted vs. reflection angle, are very sharp, one gets the impression that the radiation is reflected at certain angles θ_1, θ_2, etc.

Using Bragg's law one can determine the spacing d of an unknown lattice if the wavelength λ of the monochromatic x-ray beam is known, or vice versa λ, if the

lattice spacing d of the crystal is known. The first condition is important for the determination of unknown crystal structures. Generally, the application of x-rays is of high technological importance in studying materials.

1. Assignment of tasks

1.Task: With the X-ray machine, the intensity (pulse rate R of the Geiger Müller counter tube) of x-rays reflected on a LiF single crystal has to be determined depending on the refraction angle θ for five different anode voltages U_{AS}. The refraction angle has to be transformed into the wavelength λ by bragg´s law taking into account the lattice distance of the Li F crystal (d_{LiF} = 201.4 pm).

From the curves R(λ), the short-wave limit λ_{min} of the X-ray spectrum has to be determined graphically. With these values and the linear equation:
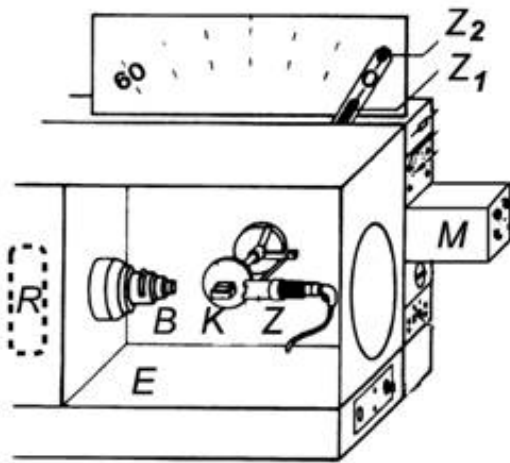
$$e\ U_{AS} = h*f_{max}$$

the Planck constant h should be derived from the slope of the plotted equation.

2.Task: With the X-ray machine (Mo-Anode and included Zr-filter: λ_{Ka}= 71.1 pm) the Bragg angles have to be determined for a NaCl single crystal.

Calculate the lattice distance d of NaCl and compare it with the literature value d_{NaCl} = 282.5 pm.

2. Experimental set-up

Fig. 2.1:

X-ray machine with X-ray tube (R), experimental chamber (E), aperture (B), crystal (K), counting tube (Z), pointer 1 (Z_1), pointer 2 (Z_2), motor drive (M)

Fig. 2.1 shows the X-ray machine used in the experiment, Fig. 2.2 shows the entire experimental setup schematically. The X-ray radiation generated by the Molybdenum X-ray tube enters the experimental chamber through an aperture (collimator) into which a filter (e.g. Zr-film) can be inserted. The filtered X-ray hit the crystal (LiF or NaCl), which is attached to a vertical axis that rotates to the beam direction. The angular position θ of the crystal surface (=crystal planes) to the incident X-ray beam is indicated with a pointer Z_1 on an angular scale. Around the same axis of rotation, the counting tube for the intensity measurement of the reflected X-ray radiation can be rotated, whose angular position 2θ to the incident X-ray beam is indicated with a second longer pointer Z_2.

Both angle positions are adjustable. Via a mechanical coupling it is ensured: when adjusting one the other is tracked accordingly. At the position $2\theta = \theta = 0$, both pointer Z_1 and Z_2 are on top of each other. Note that in this position there is no reflection of the crystal and the direct Xray beam hits partially directly onto the Geiger-Müller counter which should be avoided during experiment. Therefore all experiments will start with a minimum angle of $\theta = 3°$. *Note!* The motor drive is powered by a 12 V voltage source.

According to the angular position of the motor, a voltage in the range $\pm$3V is picked up at a potentiometer, which is connected to the motor axis by means of a slip clutch, which is located at the input C of the interface.

The pulse rate R of the Geiger-Müller-counter (proportional of the radiation intensity) is registered via the input F of this interface, so that an automatic recording of the counting rate $R(\theta)$ or $R(\lambda)$ (at known network plane distance using the Bragg equation) is possible.
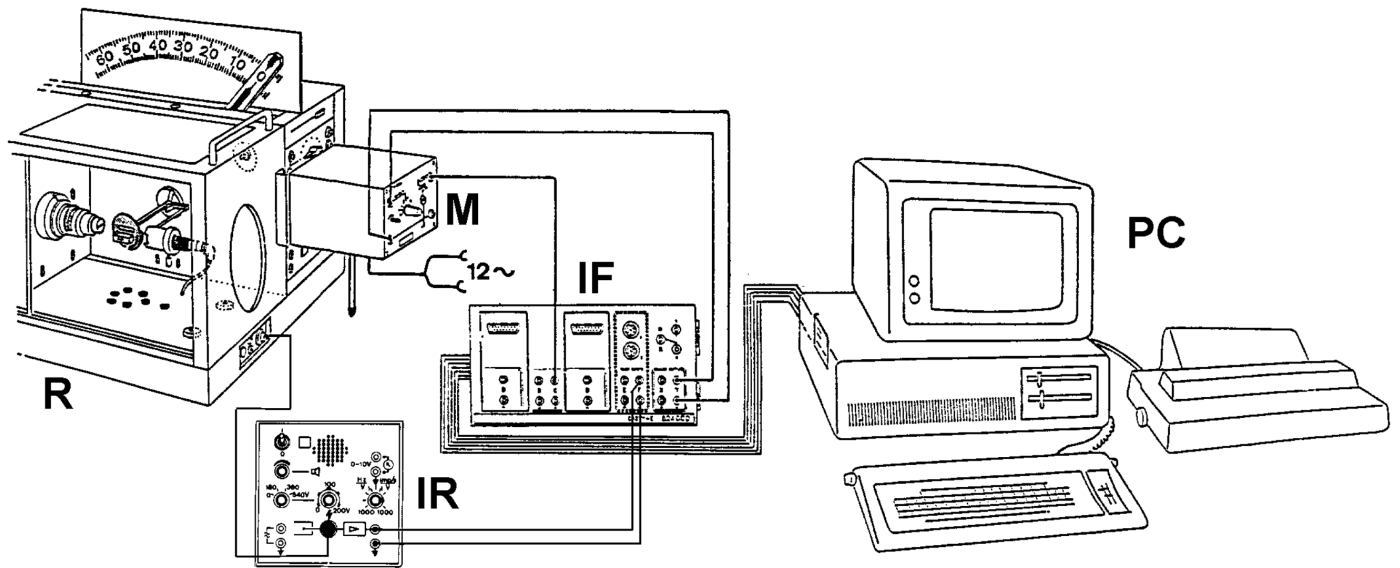
The use of a computer also makes it possible to immediately graphically display and assess the rate R(θ) during the measurement on the monitor.

In addition, it should be noted that the emission current of the X-ray tube remains constant during the measurement (approx. 1 mA). This is controlled with a DC meter. An AC volt meter is used to determine the gradually adjustable (1,…,8) anode voltage U_A. This is determined by the measured effective value of the AC voltage U over the relationship

$$U_A = \sqrt{2} \times 10^3 U$$

To shield the environment from the X-ray radiation of the tube, the X-ray tube itself and the experimental chamber are enclosed by steel plates and lead glass windows. The lateral window can only be opened when the anode voltage is switched off, e.g. for mounting the crystal. The operation of the X-ray tube (switched on anode voltage) is indicated by a red warning lamp on the top of the device.

3. Experimentation and evaluation

3.1 Start of experiment, angle calibration and angle correction

First, the X-ray machine (initially without high voltage), the rate meter, and finally the power supply of the actuator must be adjusted.

In general, a calibration of the angle adjustment of the motor is necessary before the start of the experiment. For this purpose, the menu item *Calibration/Ranges (Kallibrieren/Bereiche)* is selected, then *angle calibration (Winkelkalibrierung),* then *start/stop*, after which the voltage U of the motor potentiometer shown on the screen is driven to the value of approx. -2.95 V, which should correspond to the angular position $2\theta = \theta = 0$. A slight adjustment of the hands is necessary by the keys +/-/S (larger / smaller angle / stop). The zero position is confirmed by *F2,* i.e. the set voltage value is assumed to be $2\theta = \theta = 0$.

The angle $2\,\theta = 60^0$ is then approached with the *+/-/S* keys. The voltage now displayed in the screen corresponds to $\theta = 30^0$, which is confirmed again by *F2.* After that, the calibration is finished and can be exited with *ESC.*

In the evaluation of the measured angles, it must be taken into account that the spectra have an offset of an angle Δ. This angular error Δ depends strongly on the used crystal surface and its position in the crystal holder and is provided for the 1st task, since no filter (monochromator) can be used here. The angular error Δ for the 2nd task can be determined using the Bragg equation. If $\theta_1{}^m$ and $\theta_2{}^m$ are the measured angles for the maximum intensity in 1st and 2nd order, the angle correction is $\Delta = \theta_1 - \theta_1^m = \theta_2 - \theta_2^m$. With the boundary condition, that the corrected angles θ_1 and θ_2 result in the same mesh plane spacing for NaCl ($d_{NaCl} = 282.5\ pm$), one ends up with the relation to calculate Δ:

$$\tan \Delta \;=\; \frac{\sin \theta_2^m \;-\; 2 \sin \theta_1^m}{2 \cos \theta_1^m \;-\; \cos \theta_2^m}$$

3.1.1. 1st Task:

The measurement is carried out with the LiF crystal **without** filter for 5 different anode voltages (levels 4 – 8 on the scale). The respective voltages U_{eff} have to be noted and the high voltage U_A has to be calculated (see equation above)

Before the 1st measurement:

parameters: Angle range: θ: 3-10⁰, step: 0.1⁰

Torzeit: t: 1s

d_{LiF} = 201.4 pm

Measurement: start: F1

After each measurement series:

Print screen: Determine minimum angle θ_{min}

Substract $\Delta = 0.7°$

After all series of measurements of the 1st task:

Derive λ_{min} with Bragg´s law ($\lambda_{min} = 2d_{LiF}\sin{(\theta_{min})}$) .

Calculate $f_{max} = c \: / \: \lambda_{min}$

Plot the linear equation of U*e versus h*f$_{max}$ following from the energy conservation

$$U * e = h * f_{max}$$

Determine the Planck constant h from the slope of the graph using linear regression and compare to literature. Please note that your fit curve must go through (0;0) point (function y=kx).

3.1.2. 2nd Task:

The measurement is to be carried out with NaCl crystal and **with** Zr filter, voltage level 8 to determine the lattice distance of NaCl

Before measuring:

parameters: Angle range θ: 3-25⁰,

Torzeit: t: 1s

Measurement: start: F1

After the measurement:

Print screen:

Determine the peak angles for n=1,2,3

Calculate Δ

from the first two maxima with the equation given above

Derive d_{NaCl} for all 3 Maxima

Get an average and compare it with the literature value

4. Questions for Self-checking

1) How does an *X-ray tube work?*

2) Which different *X-ray spectra* are distinguished (drawing)?

3) Why is there a short-wave limit of the *Bremsstrahlung*?

4) What is the origin of the X-ray *characteristic spectrum*?

5) How do we prove that X-ray are electromagnetic waves?

6) What is *Bragg's Law*?

7) How does a *counter tube work?*

Appendix: Analysis of Errors

1. Systematic and Statistical Errors

Every result of a measured ph ysical quantity inevitably contains an error. To evaluate the e xperimental result obtained, it i s, therefore, n ecessary to give a n estimate of the numerical error(s) inherent to the experimental quantity.

There are different kinds of errors: systematic and random, i.e., statistical. Systematic errors are caused by the measurement system and can be recognized from the fact that the measured numerical value is strictly too large or too small as compared to those obtained when using other methods of measurement or theory. To minimize systematical errors, one has to change the experimental setup, i.e., the apparatus or the measuring procedure. Alternatively, the numerical result has to be corrected p roperly to account for the systematic e rrors involved in the measurement.

A statistical error arises due to random postive a nd n egative deviations of the actually measured value from the mean or precise experimental value. If, e.g., the measured length o f a distance is not exactly that of a ce rtain nu mber of scale divisions, on e has to estimate a more a ccurate value by interpolation, thus a statistical error may result. On the other hand, the displayed (analog or digital) value of, e.g., a measured voltage can vary with time, i.e., fluctuating around an unknown (average) value. Thus, by evaluation of a time averaged value, or by the choice of the measurement moment, a statistical error may arise as well. Statistical errors are c haracterized b y a probability distribution, which d etermines the probability of a measured deviation from the precise (true), i.e., most probable value (expectation value). The more a measurement is repeated, the more precisely are the probability distribution and the most probable value determined and the less becomes the statistical (measuring) uncertainty (see below).

2. Average Value, Standard Deviation, Statistical Uncertainty

The best evaluation for the most probable value of a measured quantity x out of n different single measurements x_i is obtained b y taking the *arithmetic average value* $\overline{x}$

$$\overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \ . \tag{1}$$

Very o ften a shortened no tation is used in the literature c ontaining statistical equations with expressions of sums, where the lower and upper summation limit and the summation index is suppressed:

$$\overline{x} = \frac{1}{n} \sum x \ . \tag{2}$$

This shortened notation will be used in the following text.

Once the average value is known, the moduli of differences $|x_i - \overline{x}|$, denoting the deviations of single measuring results from the average value, give some estimate for the precision of the measurements. Because of numerical reasons, the moduli of the differences are replaced by the squares $(x_i - \overline{x})^2$ and the *standard deviation* s is defined by

$$s = \sqrt{\frac{\sum (\overline{x} - x)^2}{n - 1}} \ , \quad n > 1 \ . \tag{3}$$

The standard deviation gives the statistical average error of a *single* measurement. By introducing the (positive) square root, the quantity s has the same units as the measured qu antity and is therefore c omparable with it. The division b y n - 1 instead by n takes into account, that for only a single measurement (n = 1) no statistical statement can be given, i.e., s is not defined.

The equation defining the standard deviation is usually not that given by eq. (3). All pocket calculators use instead the fully equivalent equation

$$s = \sqrt{\frac{\sum x^2 - \frac{1}{n}(\sum x)^2}{n - 1}} \ , \quad n > 1 \ , \tag{4}$$

because, when using eq. (4), not the single measured values x, but only the sum $\sum x$ and the sum of the square $\sum x^2$ has to be stored.

Besides the calculation of the average value and the standard deviation, it is often interesting to consider the value of the statistical uncertainty of the average value as well. This is because $\overline{x}$ is just a guess of the result x according eq. (2), which for a small number n o f single measurements, can b e very unprecise. The

statistical measuring uncertainty u is a measure of the (statistical average) error of the average value $\bar{x}$:

$$u = \frac{s}{\sqrt{n}} = \sqrt{\frac{\sum x^2 - \frac{1}{n}(\sum x)^2}{n(n-1)}} \quad , \quad n > 1 \ . \tag{5}$$

While the standard deviation s as a measure of the statistical spread of single measured values x_i approaches a finite value > 0 with increasing n, the statistical measuring uncertainty u of the average value $\bar{x}$ decreases with increasing n and approaches zero at large n.

Very often the measured values x_i are so called "normally" distributed, i.e., their relative probabilities are given by the *Gaussian distribution function* $\varphi(x)$:

$$\varphi(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) \ . \tag{6}$$

The integral

$$P(x_1, x_2) = \int_{x_1}^{x_2} \varphi(x)\,dx \ , \tag{7}$$

gives the probability that the values x_i (for a large number of measurements $n \to \infty$) lie within the interval (x_1, x_2). As shown by Fig. 1, the function $\varphi(x)$ is symmetric around the most probable value x_0 (the expectation value) and has the shape of a bell with a full width at half maximum of somewhat more than 2σ.

For very large n, the average value $\bar{x}$ determined from the measuring series approaches the value x_0 of the function $\varphi(x)$, and the standard deviation s approaches the value σ. The probability that the result x_i of a single measurement lies within the interval $\bar{x} \pm s$, i.e., $x_0 \pm \sigma$, amounts according to eq. (7) to about 68 %, for the interval $x_0 \pm 2\sigma$ to about 95 % and for $x_0 \pm 3\sigma$ already 99.7 %. Similar relations are valid for the statistical measuring uncertainty u of the average value: the probability of the true value x_0 lying within the so called (unit) *range of*
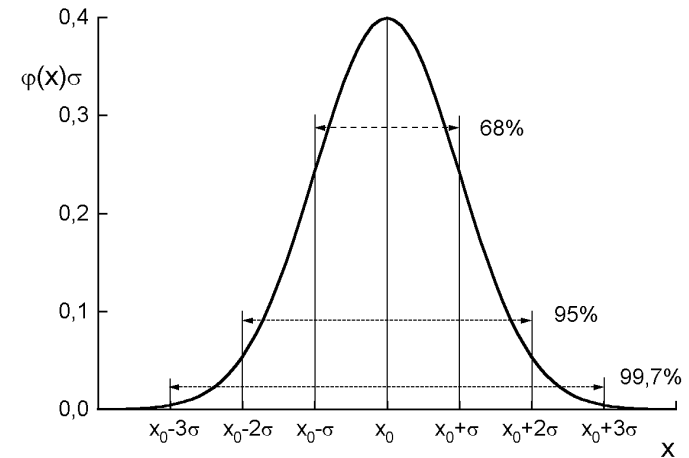
Fig. 1: Gaussian distribution function $\varphi(x)$ with most probable value x_0 and intervals $x_0 \pm \sigma$, $x_0 \pm 2\sigma$, and $x_0 \pm 3\sigma$ for relative frequencies 68%, 95%, and 99,7% of measuring value x_i

confidence $\bar{x} \pm u$ is about 68 %, for the twofold and threefold range of confidence $\bar{x} \pm 2u$ and $\bar{x} \pm 3u$ about 95 % and 99.7 %, respectively.

One has to take into consideration, however, that the evaluation of the statistical measuring uncertainty or the range of statistical confidence for the value $\bar{x}$ is physically reasonable only in combination with the evaluation of possible systematic errors. The total error of a result obtained from a measurement is always the sum of moduli for systematic and statistical errors. It is, therefore, not useful to repeat a measurement very often just for minimizing the statistical error if the evaluated systematic error exceeds the former by orders of magnitude.

Example 1: In the experiment B10 (experiment with x-rays) the lattice constant d of NaCl is to be determined from the Bragg reflection using Bragg's law

$$n\lambda = 2d\sin\theta_n \quad ,$$

with the wavelength $\lambda = 154$ pm and the measured Bragg angles θ_n (n = 1, 2, 3).

Typical values are given in the table below.

n	θ_n (°)	d_n (pm)
1	16.0	279.4
2	33.2	281.3
3	55.15	281.5

Using these values the following are found:

the average value: d = 280.73 pm,

the standard deviation: s = 1.16 pm,

the statistical uncertainty u of the average value d , u= 0.67 pm,

Finally,

d = (280.73 ± 0.67) pm = 280.73 pm ± 0.2 % ,

if no error (statistical or systematic) in the measured angles θ_n is considered. (Otherwise see example 2 below!)

Notice: Any estimated error should no t contain more than 2 o r 3 d ecimal positions. The final result is to be rounded correspondingly. Very often it does not make any sense and only simulates precision to present the many decimal places displayed by a pocket calculator.

Additional notice: Comparison of the result for d given above with the value d_{NaCl} = 282.0 p m, known from the literature, and with those obtained u sing other experimental setups in the laboratory, reveals a systematic deviation o f θ_n (of roughly 0.5% - depending on the system used - because of inaccurate adjustments). In this case, the value of the statistical uncertainty presented is not significant at all to estimate the (actual true) error of d. If u is replaced by the standard deviation s, the result

d = (280.73 ± 1.16) pm = 280.73 pm ± 0.4 %

can account to a better extent the actual error but this presentation does not solve the p roblem principally, i.e., ho w the systematic e rror present in this case is properly taken into account. One possibility to solve the problem is to take into consideration that an inherent (constant) systematic e rror $\Delta\theta^s$ (because of

misalignment of both the crystal and the detector) has to be taken into account when using Bragg's law for the evaluation of θ from the experimental data, i.e., $\theta = \theta^m + \Delta\theta^s$, where θ^m is the measured value. Since in the experiment considered the task is not to validate Bragg's law but to determine the lattice constant d, we state that Bragg's law is valid in any order n, i.e., that the value of d is independent of n. Combining Bragg's law, e.g., for n = 1 and 2, $\Delta\theta^s$ can be calculated with the values in the table of example 1 from

$$\tan\Delta\theta^s = \frac{\sin\theta_2^m - 2\sin\theta_1^m}{2\cos\theta_1^m - \cos\theta_2^m} , \quad \Delta\theta^s = -0.2° .$$

Using this systematic correction $\Delta\theta^s$ of the angle θ^m, the values d_1 = 282.8 pm; d_2 = 282.8 pm (i.e., $d_1 = d_2$) and d_3 = 282.2 pm are obtained. Thus, the average of the corrected result for d is

d = 282.6 pm ,

which is closer to the value d_{NaCl} = 282.0 pm known from the literature than the value d = 280.73 p m presented above, without t aking into consideration the correction of the systematic error.

3. Propagation of Errors

Generally, the determination of a physical quantity y requires the measurement of several single (different) parameters x_1, x_2, ... In this context, the question arises how far the single errors Δx_i resulting from the measurement of the individual parameters determine the uncertainty Δy of the quantity y. If the errors Δx_i are small as comparted to x_i, the function y expanded into a power series of the errors Δx_i around the values x_i is approximately given by the terms linear in Δx_i . The error Δy resulting, e.g., from a single error Δx_i is given by

$$\Delta y \bigg|_{x_{j\neq i}=const} = \frac{\partial y}{\partial x_i} \Delta x_i .$$

(8)

To estimate the *largest possible absolute error* $(\Delta y)_{max}$ by taking into account all possible single errors Δx_i, the following relation is defined:

$$(\Delta y)_{max} = \left| \frac{\partial y}{\partial x_1} \Delta x_1 \right| + \left| \frac{\partial y}{\partial x_2} \Delta x_2 \right| + \dots \qquad (9)$$

Example 2: In the experiment B10 (experiment with x-rays, see also example 1) the lattice constant d of NaCl is to be determined from the Bragg reflection using the relationship

$$n\lambda = 2 d_n \sin\theta_n , \quad d = \frac{1}{3}\sum d_n = \frac{\lambda}{6}\left(\frac{1}{\sin\theta_1} + \frac{2}{\sin\theta_2} + \frac{3}{\sin\theta_3} \right) ,$$

with the wavelength $\lambda = 154$ pm and the measured Bragg angles θ_n ($n = 1, 2, 3$). Assuming a statistical error $\Delta\theta = \pm 0.25° = 0.0044$ of every measured angle θ_n, the maximum statistical error Δd_{max} is according to eq. (9)

$$(\Delta d)_{max} = \left| \frac{\partial d}{\partial\theta_1} \Delta\theta_1 \right| + \left| \frac{\partial d}{\partial\theta_2} \Delta\theta_2 \right| + \left| \frac{\partial d}{\partial\theta_3} \Delta\theta_3 \right|$$

$$= \frac{\lambda\Delta\theta}{6}\left(\frac{\cos\theta_1}{\sin^2\theta_1} + \frac{2\cos\theta_2}{\sin^2\theta_2} + \frac{3\cos\theta_3}{\sin^2\theta_3} \right) .$$

Taking the numerical θ-values presented in example 1 we obtain

$(\Delta d)_{max} = 0.112$ ($12.65 + 5.58 + 2.55$) pm $= 2.33$ pm; $\quad (\Delta d)_{max} / d = 0.83$ %

It is noted that the error contribution from the first Bragg angle θ_1 is the largest one, because the error $\Delta\theta_1/\theta_1$ is the largest one, consistent with the observation in the table of example 1, where the deviation of ($d_1 - d_{NaCl}$) is the largest one too.

Example 3: In the experiment B8 (determination of the specific charge e/m of the electron) the ratio e/m is determined from measurements of the acceleration voltage U and of the current I through the coils with radius R for an electron beam with circular radius r.

$$\frac{e}{m} = 2\left(\frac{R}{0.715\,\mu_0\,n} \right)^2 \frac{U}{(rI)^2}$$

Since e/m is a product of powers of the variables R, U, r, and I, the expression of the *largest possible relative error* of e/m is rather simple. Taking into account the errors ΔR, ΔU, Δr, and ΔI, the largest possible relative error of e/m is given by

$$\left[\frac{\Delta(e/m)}{(e/m)} \right]_{max} = \frac{1}{e/m}\left(\left| \frac{\partial(e/m)}{\partial R}\Delta R \right| + \left| \frac{\partial(e/m)}{\partial U}\Delta U \right| + \left| \frac{\partial(e/m)}{\partial r}\Delta r \right| + \left| \frac{\partial(e/m)}{\partial I}\Delta I \right| \right)$$

$$= \left| \frac{2\Delta R}{R} \right| + \left| \frac{\Delta U}{U} \right| + \left| \frac{2\Delta r}{r} \right| + \left| \frac{2\Delta I}{I} \right| . \qquad (10)$$

Typical estimates of errors and values of measured quantities are

$\Delta R = \pm 2$ mm	$R = 20$ cm	$\Delta R/R = 0.01$
$\Delta U = \pm 6$ V	$U = 200$ V	$\Delta U/U = 0.03$
$\Delta r = \pm 0.5$ mm	$r = 3$ cm	$\Delta r/r = 0.017$
$\Delta I = \pm 90$ mA	$I = 2$ A	$\Delta I/I = 0.045$

resulting in

$$\left[\frac{\Delta(e/m)}{(e/m)} \right]_{max} = 0.02 + 0.03 + 0.034 + 0.09 = 0.174 .$$

4. Graphs and Linear Regression

In experimental physics, the aim is often to validate a theoretically predicted functional dependence of two quantities x and y by a measurement. In simple cases, the quantities x and y are linearily connected, i.e.,

$$y = a + bx . \qquad (11)$$

Since every measurement is inherent with an error, the data (x_i, y_i) in a graph y_i vs. x_i will scatter more or less around a straight line drawn through the data points. It is the task to find an optimum straight line balancing the deviations due to errors (i.e. that line which would represent the data if the errors were absent). This is the *regression line*. It can be simply done by a *visual estimate*, i.e., by drawing a suitable straight line with a ruler. A more objective way to construct the regression

line is the *least mean square fit*; the calculation of the parameters a and b of eq. (11) (a: intercept on y-axis, b: slope of line) with the condition

$$\sum (a + bx - y)^2 ,$$

being an absolute minimum. If this is the case, a and b fulfil the condition

$$\frac{\partial}{\partial a} \sum (a + bx - y)^2 = 0, \quad \frac{\partial}{\partial b} \sum (a + bx - y)^2 = 0 . \qquad (12)$$

Differentation yields the equation system

$$an + b\sum x = \sum y \quad , \qquad a\sum x + b\sum x^2 = \sum xy , \qquad (13)$$

with the solution

$$a = \frac{\sum y \sum x^2 - \sum x \sum xy}{n\sum x^2 - (\sum x)^2} , \qquad b = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - (\sum x)^2} . \qquad (14)$$

Note: For a regression line through the origin of the coordinate system, i.e. for the line $y = bx$ (a = 0) the corresponding solution is

$$b = \frac{\sum xy}{\sum x^2} \qquad (15)$$

The linear regression algorithm using the method of the least mean squares is almost always applied to find an optimum fit to the data. It is (besides the (arithmetic average) the most frequently used algorithm and, therefore, is included in many pocket calculators.

When using the (critical) regression coefficient R^2, one has to be cautious. With R^2 the quality of fit functions with several independent measuring series can be compared. The coefficient of a single measuring series, however, has no physical meaning.

In cases where the quantity Y(X) does not linearly depend on X, it may be possible to find a proper transformation $Y(X) \rightarrow y(x)$ so that a linear relationship

$y = a + bx$ holds.

Some examples are given in the following table:

function Y(X)	transformation		y = a + b x	
	y(X,Y)	x(X,Y)	a	b
A X^B	ln (Y)	ln (X)	ln (A)	B
A exp (BX)	ln (Y)	X	ln (A)	B
A X + B X^3	Y / X	X^2	A	B