Atomic and nuclear physics

X-ray physics
Detection of x-rays

## Fluorescence of a luminous screen due to x-rays

Objects of the experiment

- Detecting x-rays by observing the fluorescence of a luminous screen.
- Transillumination of objects with different absorption characteristics.
- Investigating the dependence of brightness and contrast of the luminous screen on the emission current and tube high voltage.

Principles

Very soon after *W. C. Röntgen*'s discovery of x-rays in 1895, researchers were quick to apply the fact that x-rays can be "observed" on a luminous screen in medical examinations. At that time, the most common type of luminous screen was barium-platinum-cyanide, which fluoresces bright green; today, yellow-green zinc-cadmium-sulfide is used almost exclusively. The fluorescent substance is applied to lead glass, which protects the observer from the harmful effects of x-rays.

Fluorescence is a luminous phenomenon that occurs in certain materials when these are exposed to light, x-ray or particle radiation. The energy of the incident radiation is used to excite or ionize the atoms and molecules; when these return to the ground state, a portion of this energy is released in the form of visible light. The transitions are extremely rapid ($< 10^{-5}$ s), so that fluorescence can only be observed during irradiation (in contrast to phosphorescence).

The ability of x-rays to pass through opaque materials and bodies make them particularly useful in diagnostic applications. Depending on the composition of the irradiated object, the radiation is attenuated to a greater or lesser extent. That is why the images on the luminous screen reveal details of the internal structure of objects. In this experiment, this fact is demonstrated using a simple object, e.g. a pocket calculator, which has parts made of materials with different absorption properties. This experiment investigates the effect of the emission current I of the x-ray tube on the brightness and the effect of the tube high voltage U on the contrast of the luminous screen.
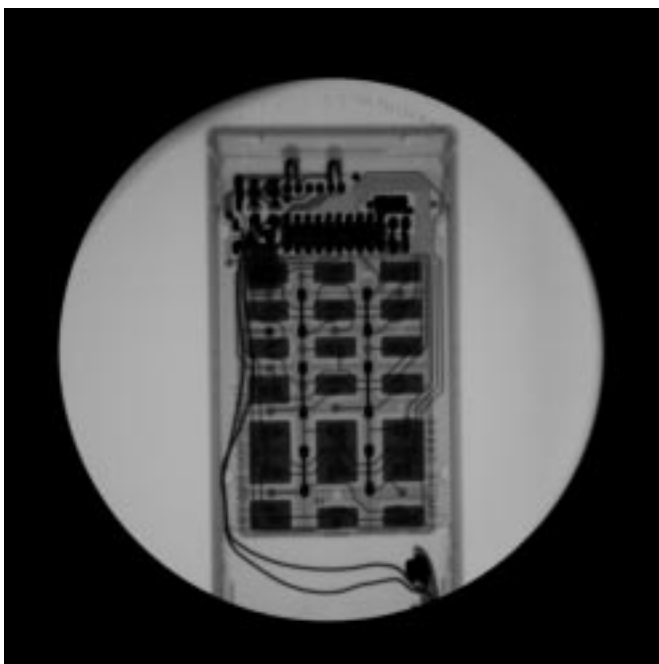
Luminous-screen image of a pocket calculator

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Apparatus

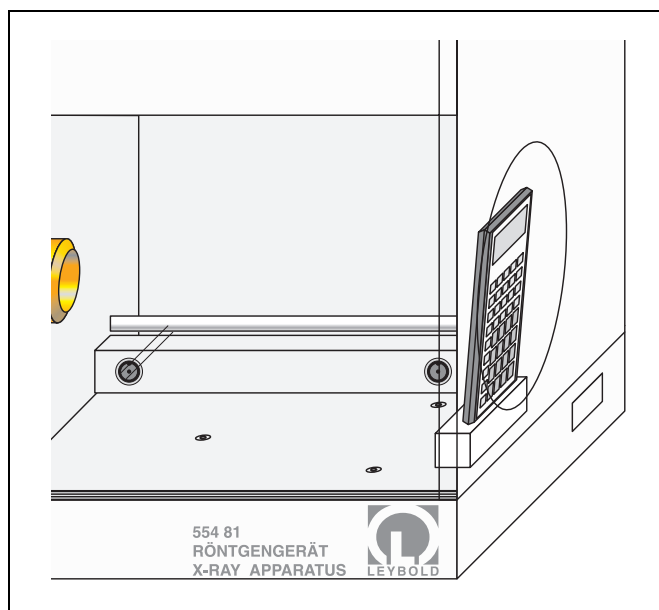|	
1 X-ray apparatus	554 811
or	
1 X-ray apparatus	554 812

Additionally required:

1 Object for transillumination, e.g. pocket calculator with plastic housing

Any flat, opaque object with an internal structure and made primarily of plastic and metal parts is suitable.

Setup

–   Remove the collimator from the experiment chamber, as well as the goniometer or any other assemblies.
–   Remove the protective cover of the luminous screen.

Fig. 1   Experiment setup for demonstrating fluorescence of a luminous screen due to x-ray radiation

Safety notes

The x-ray apparatus fulfills all regulations governing an x-ray apparatus and fully protected device for instructional use and is type approved for school use in Germany (NW 807/97 Rö).

The built-in protection and screening measures reduce the local dose rate outside of the x-ray apparatus to less than 1 μSv/h, a value which is on the order of magnitude of the natural background radiation.

■   Before putting the x-ray apparatus into operation inspect it for damage and to make sure that the high voltage is shut off when the sliding doors are opened (see Instruction Sheet for x-ray apparatus).
■   Keep the x-ray apparatus secure from access by unauthorized persons.

Do not allow the anode of the x-ray tube Mo to overheat.

■   When switching on the x-ray apparatus, check to make sure that the ventilator in the tube chamber is turning.

Carrying out the experiment

Note:
Carry out the experiments in a darkened room.

a) Brightness of the luminous screen:

–   Close the lead glass sliding door, set the tube high voltage $U = 35$ kV and switch on the apparatus with the hv on/off key.
–   Increase the emission current I continuously from 0 to 1.00 mA and observe the brightness of the luminous screen.

b) Varying the emission current I:

–   Place the transillumination object, e.g. pocket calculator, in the experiment chamber as close as possible in front of the luminous screen.
–   Set the emission current $I = 1.00$ mA, the tube high voltage $U = 35$ kV and switch on the unit with the hv on/off key.
–   Reduce the emission current I in steps and observe the change on the luminous screen.

c) Varying the tube high voltage U:

–   Set the emission current $I = 1.00$ mA.
–   Reduce the tube high voltage in steps and observe the change on the luminous screen.

Atomic and Nuclear Physics

X-ray physics
Physics of the atomic shell

*Bragg reflectio*n: diffraction of x-rays at a monocrystal

Objects of the experiment

■ To investigate Bragg reflection at an NaCl monocrystal using the characteristic x-ray radiation of molybdenum.

■ To determine the wavelength for the characteristic K_α and K_β x-ray radiation of molybdenum.

■ To confirm Bragg's law of reflection.

■ To verify the wave nature of x-rays.
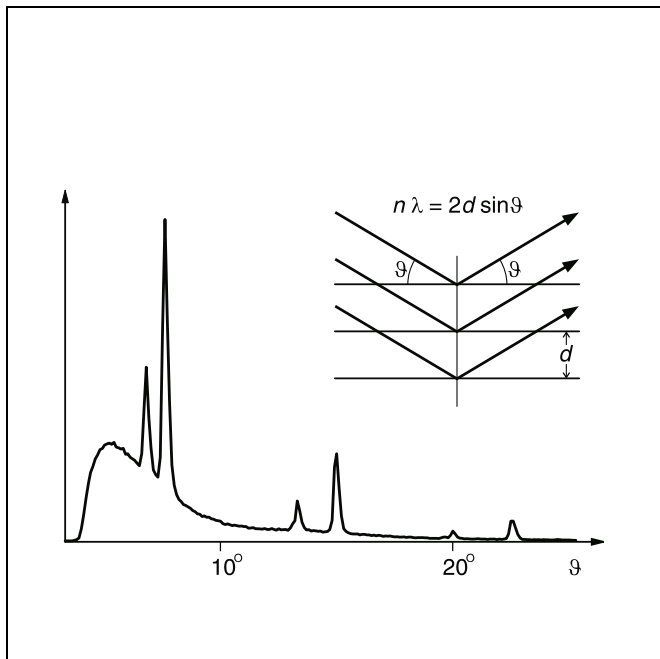
Principles

In 1913, *H. W.* and *W. L. Bragg* realized that the regular arrangement of atoms and/or ions in a crystal can be understood as an array of lattice elements on parallel lattice planes. When we expose such a crystal to parallel x-rays, additionally assuming that these have a wave nature, then each element in a lattice plane acts as a "scattering point", at which a spherical wavelet forms. According to *Huygens,* these spherical wavelets are superposed to create a "reflected" wavefront. In this model, the wavelength λ remains unchanged with respect to the "incident" wave front, and the radiation directions which are perpendicular to the two wave fronts fulfill the condition "angle of incidence = angle of reflection".

Constructive interference arises in the rays reflected at the individual lattice planes when their path differences Δ are integral multiples of the wavelength λ.

$$\Delta = n \cdot \lambda \text{ with } n = 1, 2, 3, \dots \quad\quad\quad (I)$$

As Fig. 1 shows for two adjacent lattice planes with the spacing *d,* we can say for the path differences Δ_1 and Δ_2 of the incident and reflected rays with the angle ϑ:

$$\Delta_1 = \Delta_2 = d \cdot \sin \vartheta$$

so that the total path difference is

$$\Delta = 2 \cdot d \cdot \sin \vartheta. \quad\quad\quad (II)$$

(I) and (II) give us Bragg's law of reflection:

$$n \cdot \lambda = 2 \cdot d \cdot \sin \vartheta \quad\quad\quad (III)$$

The angle ϑ is known as the glancing angle.

In this experiment, we verify Bragg's law of reflection by investigating the diffraction of x-rays at an NaCl monocrystal in which the lattice planes are parallel to the cubic surfaces of the unit cells of the crystal. The lattice spacing *d* of the cubic

Apparatus

1 X-ray apparatus 554 811

1 End-window counter
  for α, β, γ and x-ray radiation 559 01

additionally required:

1 PC with Windows 9x or Windows NT

face-centered NaCl crystal is half the lattice constant a_0. We can thus say [1]

$2 \cdot d = a_0 = 564.02$ pm

The measurements are conducted using the built-in goniometer of the x-ray apparatus (554 811). The x-rays are detected using a GM counter tube (end-window counter) which is swiveled in tandem with the NaCl crystal in a 2_ coupling with respect to the incident light; this means that the counter tube always advances by an angle which is twice that of the crystal (cf. Fig. 2).

The x-ray radiation consists of the bremsstrahlung continuum and several sharply defined lines which correspond to the characteristic x-ray radiation of the Mo anode and which originate in the K_α and K_β transitions of the molybdenum atoms. This characteristic radiation is particularly suitable for investigating Bragg's law. Its properties are known from the literature [2] and summarized in table 1. Table 2 shows the corresponding glancing angles at which the diffraction maxima of the characteristic radiation are to be expected for scattering at an NaCl monocrystal (d = 282.01 pm) up to the third diffraction order.

Safety notes

The x-ray apparatus fulfills all German regulations governing an x-ray apparatus and fully protected device for instructional use and is type approved for school use in Germany (NW 807/97 Rö).

The built-in protection and screening measures reduce the local dose rate outside of the x-ray apparatus to less than 1 μSv/h, a value which is on the order of magnitude of the natural background radiation.

■ Before putting the x-ray apparatus into operation, inspect it for damage and check to make sure that the high voltage shuts off when the sliding doors are opened (see Instruction Sheet of x-ray apparatus).
■ Keep the x-ray apparatus secure from access by unauthorized persons.

Do not allow the anode of the x-ray tube Mo to overheat.

■ When switching on the x-ray apparatus, check to make sure that the ventilator in the tube chamber is turning.

The goniometer is positioned solely by electric stepper motors.

■ Do not block the target arm and sensor arm of the goniometer and do not use force to move them.
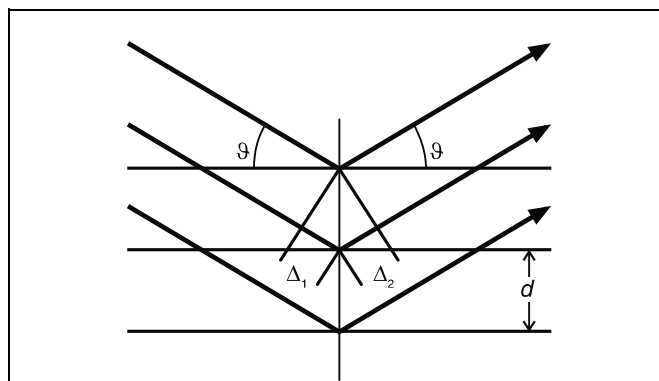

Fig. 1　Diagram of the reflection of x-rays at the lattice planes of a monocrystal.
Δ_1, Δ_2: path differences,
ϑ: glancing angle,
d: spacing of lattice planes

Table 1: Energy E, frequency ν and wavelength λ of the characteristic x-ray radiation of molybdenum (weighted mean values [1])

	$\dfrac{E}{\text{keV}}$	$\dfrac{\nu}{\text{EHz}}$	$\dfrac{\lambda}{\text{pm}}$
K_α	17.443	4.2264	71.080
K_β	19.651	4.8287	63.095

keV = 10^3 eV, EHz = 10^{18} Hz, pm = 10^{-12} m

Table 2: Glancing angle ϑ of the characteristic x-ray radiation of molybdenum for diffraction at an NaCl monocrystal up to the third order

n	$\vartheta(K_\alpha)$	$\vartheta(K_\beta)$
1	7.24°	6.42°
2	14.60°	12.93°
3	22.21°	19.61°

Fig. 2　Diagram showing the principle of diffraction of x-rays at a monocrystal and 2ϑ coupling between counter-tube angle and scattering angle (glancing angle)
1 collimator, **2** monocrystal, **3** counter tube
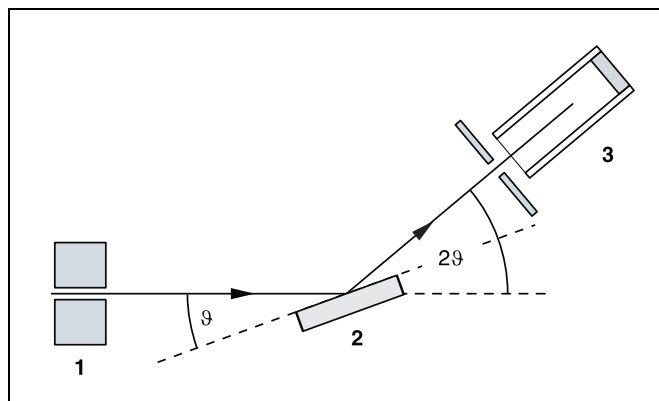
General remarks

In principle, you can conduct measurements in both manual scan and autoscan modes of the x-ray apparatus (see the Instruction Sheet of the x-ray apparatus). You can record the measured values manually by reading the values from the display field and writing them in a table, using a chart recorder or via a PC.

The fastest and most convenient measurement is in autoscan mode with simultaneous registration of measured values and subsequent evaluation on a Windows 9x/NT PC. This type of measurement is described in your Instruction Sheet.

The data is transmitted to the PC via the RS–232 serial interface on the x-ray apparatus. The software "X-ray Apparatus", supplied with the device, enables you to record, display and evaluate the data stream supplied by the x-ray apparatus. The program contains detailed online help which you can access by pressing F1. Please refer to the Instruction Sheet of the x-ray apparatus for details on installing the software.

The Instruction Sheet also describes recording data under Windows 3.1.

Setup

Setting up the Bragg configuration:

Fig. 3 shows some important details of the experiment setup. Specifically, you need to carry out the following steps (see also Instruction Sheet of x-ray apparatus):

– Mount the collimator in the collimator mount **(a)** (note the guide groove).
– Attach the goniometer to the guide rods **(d)** in such a way that the distance s_1 between the slit diaphragm of the collimator and the target arm is approx. 5 cm. Connect the ribbon cable **(c)** for controlling the goniometer.
– Remove the cap of the end-window counter, insert the end-window counter in the sensor seat **(e)** and connect the counter tube lead to the socket marked GM-Tube.

Fig. 3   Experiment setup in Bragg configuration

– Adjust the sensor seat **(b)** until the distance s_2 between the target arm and the slit diaphragm of the sensor seat is approx. 6 cm.
– Attach the target holder with target stage **(f)**.
– Loosen knurled screw **(g)**, lay the NaCl crystal flat on the target stage, carefully raise the stage as far at it will go and then tighten the knurled screw with care (press against the screw lightly to prevent it from stripping).
– Adjust the zero position of the goniometer measuring system as necessary (see Instruction Sheet of x-ray apparatus).

Notes:

NaCl crystals are hygroscopic and fragile. Store the crystals in a dry place. Avoid mechanical stresses on the crystal; handle the crystal by the short faces only.

If the counting rate is too low, you can reduce the distance s_2 between the target and the sensor somewhat. However, this distance must not be too small, as otherwise the angular resolution of the goniometer is no longer great enough to separate the characteristic K_α and K_β lines.

Preparing a PC-based measurement:

– Connect the RS–232 output to the serial interface on the PC (usually COM1 or COM2) using the 9-pin V.24 cable (included with the x-ray apparatus).
– If you have not already done so, install the software "X-ray Apparatus" under Windows 9x/NT (see Instruction Sheet of x-ray apparatus) and select the desired language.

Carrying out the experiment

– Start the program "X-ray Apparatus", check to make sure that the x-ray apparatus is properly connected and delete any existing measurement data by clicking the button [□] or pressing F4.
– Set the x-ray high voltage U = 35.0 kV, emission current I = 1.00 mA, measuring time per angular step Δt = 10 s and angular step width $\Delta\beta$ = 0.1°.
– Press the COUPLED key on the device to enable 2ϑ coupling of the target and sensor; set the lower limit value of the target angle to 2° and the upper limit to 25°.
– Press the SCAN key to start the measurement and data transmission to the PC.
– When the measurement is finished, save the measurement series to a file under a suitable name using the button [▣] or F2.
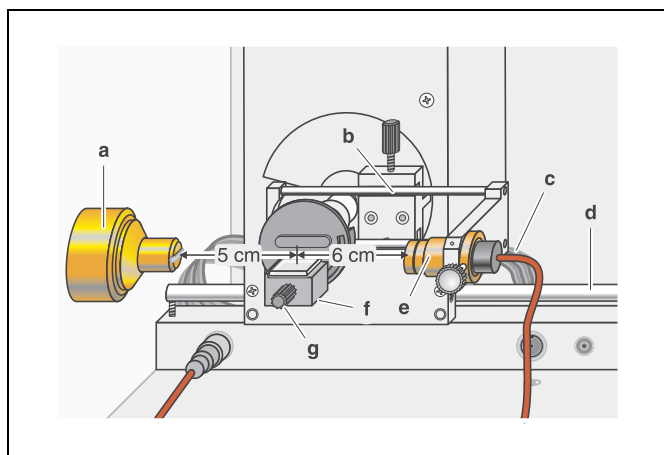
Measuring example

Fig. 4 shows the measured diffraction spectrum.
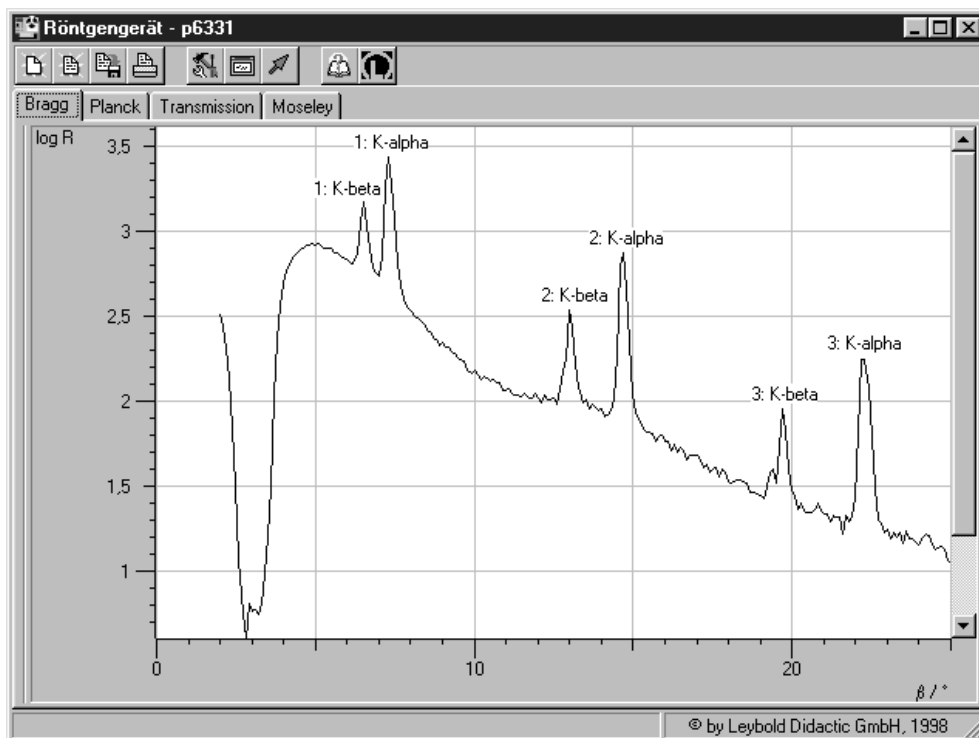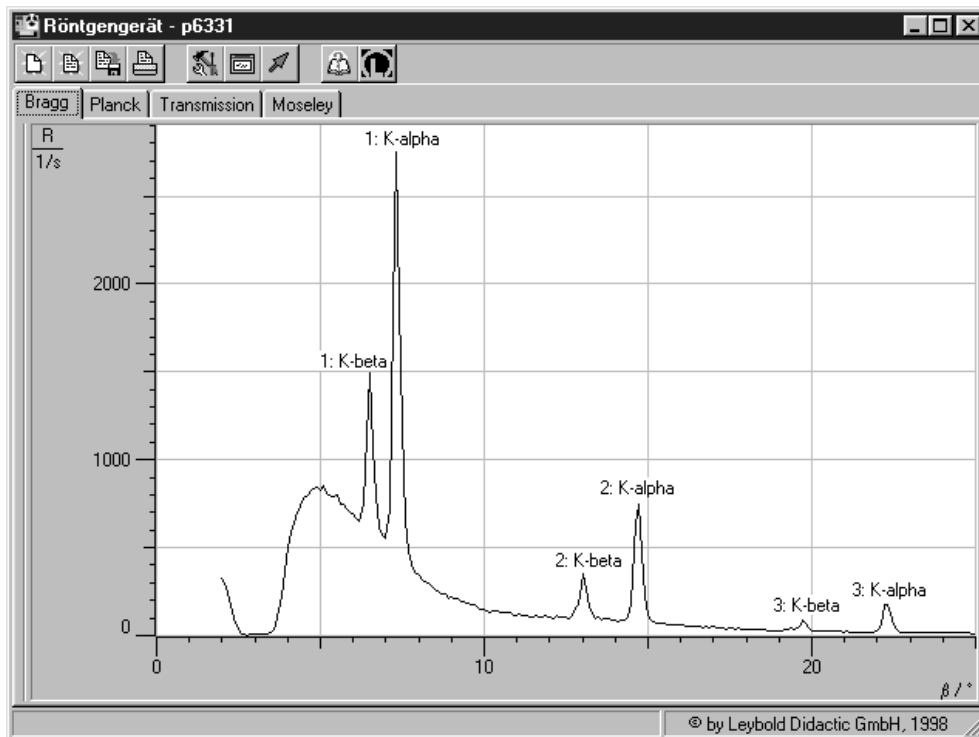
Fig. 4   Diffraction spectrum of x-ray radiation for *Bragg* reflection to the third order
at an NaCl monocrystal
Top: linear representation of counting rate *R*
Bottom: logarithmic representation of counting rate *R*
Parameters of x-ray tube: *U* = 35 kV and *I* = 1 mA

Evaluation

– Access the evaluation functions of the software "X-ray Apparatus" by clicking the right-hand mouse button and select the command "Calculate Peak Center".

– Using the left mouse button, mark the "entire width" of the peaks; if desired, insert the calculated peak center β and the peak width σ in the diagram with Alt+T and note the center as the glancing angle in the measurement table (see tables 3 and 4).

– Save your measurements and evaluations to a suitably named file with the button 🖼 or by pressing F2.

– Using the glancing angle ϑ and the lattice plane spacing d = 282.01 pm, calculate the wavelength λ using Bragg's law of reflection (IV) (see tables 3 and 4).

– Find the mean values for the individual diffraction orders of the measured wavelengths (see table 5).

Table 3: Measured glancing angles of the Mo K_α line and the calculated wavelengths λ for the first through third diffraction orders

n	$\vartheta(K_\alpha)$	$\dfrac{\lambda(K_\alpha)}{pm}$
1	7.24°	71.08
2	14.60°	71.09
3	22.20°	71.04

Table 4: Measured glancing angles of the Mo K_β line and the calculated wavelengths λ for the first through third diffraction orders

n	$\vartheta(K_\beta)$	$\dfrac{\lambda(K_\beta)}{pm}$
1	6.42°	63.07
2	12.94°	63.15
3	19.58°	63.01

Table 5: Mean value and literature value [2] for the characteristic wavelength λ

	$\dfrac{\lambda(K_\alpha)}{pm}$	$\dfrac{\lambda(K_\beta)}{pm}$
Mean value	71.07	63.08
Literature value	71.08	63.09

Results

The close agreement of the experimentally determined wavelengths for the characteristic lines with the literature values in table 5 verify the validity of Bragg's law. This simultaneously confirms the wave nature of x-rays, as this property was assumed in the process of deducing this law.

Additional information

The characteristic K_α and K_β lines actually consist of multiple, adjacent discrete lines, which can be observed separately at higher diffraction orders (see Physics Leaflet P 6.3.3.4). Table 1 shows the weighted mean values of the respective individual lines from this substructure.

Literature

[1] Handbook of Chemistry and Physics, 52nd Edition (1971–72), The Chemical Rubber Company, Cleveland, Ohio, USA.

[2] C. M. Lederer and V. S. Shirley, Table of Isotopes, 7th Edition, 1978, John Wiley & Sons, Inc., New York, USA.

Atomic and nuclear physics

X-ray physics
Physics of the atomic shell

Investigating the energy spectrum of an x-ray tube as a function of the high voltage and the emission current

Objects of the experiment

■ To recorde the energy spectra of an x-ray tube with Mo anode by means of Bragg reflection of the x-radiation at an NaCl crystal in the first diffraction order.

■ To understande the energy spectra as a superpositioning of the continuum of bremsstrahlung radiation and the lines of the characteristic x-ray radiation of the anode material.

■ To investigate how the bremsstrahlung radiation and the characteristic radiation depend on the high voltage and the emission current.

Principles

X-rays are created when fast-moving electrons are rapidly decelerated in matter. According to the laws of classical electrodynamics, this deceleration gives rise to electromagnetic radiation which is mainly radiated perpendicular to the direction of acceleration for energies below 50 keV, i.e. in this case perpendicular to the direction of the electrons striking the anode. For historical reasons, this x-ray component is referred to as "bremsstrahlung" after the German word for the deceleration process by which it occurs. The bremsstrahlung radiation has a continuous spectrum which extends to a certain maximum frequency ν_{max} or a minimum wavelength λ_{min}.

If the energy of the electrons exceeds a critical value, the characteristic x-radiation is generated, which appears in the spectrum as individual lines in addition to the continuous bremsstrahlung spectrum. These lines are generated when high-energy electrons penetrate deep into the atomic shells of the anode material and eject electrons from the innermost

orbitals by collision. The gaps created in this process are filled by electrons from the outer orbitals under emission of x-rays. The resulting x-radiation is characteristic of that anode material and is roughly comparable to the optical line spectrum of a material in a gaseous or vapor state. Solid bodies also emit individual, sharply defined lines in the x-ray range; unlike the visible light excited in the outer orbitals of the electron shell, their position is virtually independent of the chemical situation of the emitting atoms or the aggregate state of the material.

Fig. 1 serves to illustrate the nomenclature adopted for the orbital model of the atomic shell for the lines of the characteristic x-radiation: the individual orbitals are characterized by a particular binding energy and are designated from the innermost to the outermost with the letters K, L, M, N, etc. Electrons can move between the orbitals in accordance with the laws of quantum mechanics; these transitions entail either the absorption or emission of radiation, depending on the direction. For example, radiation from transitions to the K-orbital occur as a series of sequential lines designated K_α, K_β, K_γ, etc. Starting from K_α, the energy of the transitions increases and the corresponding wavelength decreases.

This experiment records the energy spectrum of an x-ray tube with a molybdenum anode. A goniometer with an NaCl crystal and a Geiger-Müller counter tube in the Bragg configuration together comprise the spectrometer. The crystal and counter tube are pivoted with respect to the incident x-ray beam in 2ϑ coupling (cf. Fig. 2).

Fig. 1 Simplified term diagram of an atom and definition of the K, L and M series of the characteristic x-ray radiation
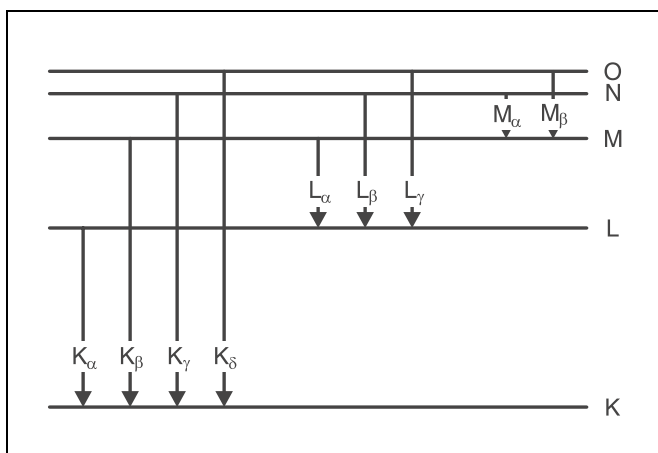
Apparatus

1 X-ray apparatus 554 811

1 End-window counter
  for α, β, γ and x-ray radiation 559 01

additionally required:
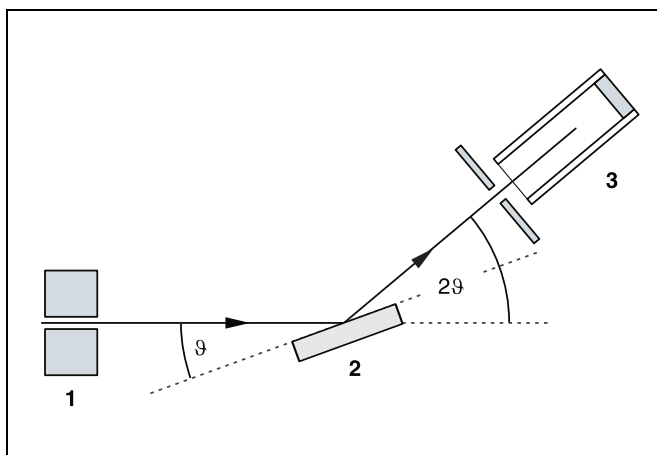
1 PC with Windows 95/98 or Windows NT

Fig. 2   Schematic diagram of diffraction of x-rays at a monocrystal
and 2ϑ coupling between counter-tube angle and scatter-
ing angle (glancing angle)
1 collimator, **2** monocrystal, **3** counter tube

In accordance with Bragg's law of reflection, the scattering
angle ϑ in the first order of diffraction corresponds to the
wavelength

$$\lambda = 2 \cdot d \cdot \sin \vartheta \qquad (I).$$
$d = 282.01$ pm: lattice plane spacing of NaCl

Together with the relationships valid for electromagnetic radia-
tion

$$\nu = \frac{c}{\lambda} \qquad (II)$$
ν: frequency, c: velocity of light

and

$$E = h \cdot \nu \qquad (III)$$
E: energy, h: Planck's constant

equation (I) gives us the energy of the x-radiation. The
spectrometer thus provides the wavelength, frequency or
energy spectrum of the radiation, depending on the selected
representation mode.

This experiment investigates the effect of the tube high voltage
U and the emission current I on the energy spectrum of the
x-ray tube. The high voltage U is applied as the accelerating
voltage for the electrons between the cathode and the anode
(see Fig. 3). The emission current I, i.e. the current flowing
between the anode and the cathode, can be controlled by
changing the heating voltage U_K of the cathode.

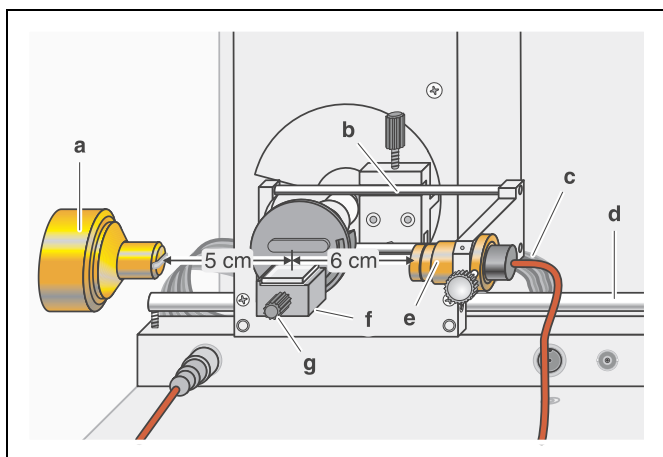Fig. 3   Schematic diagram showing the structure of the x-ray tube
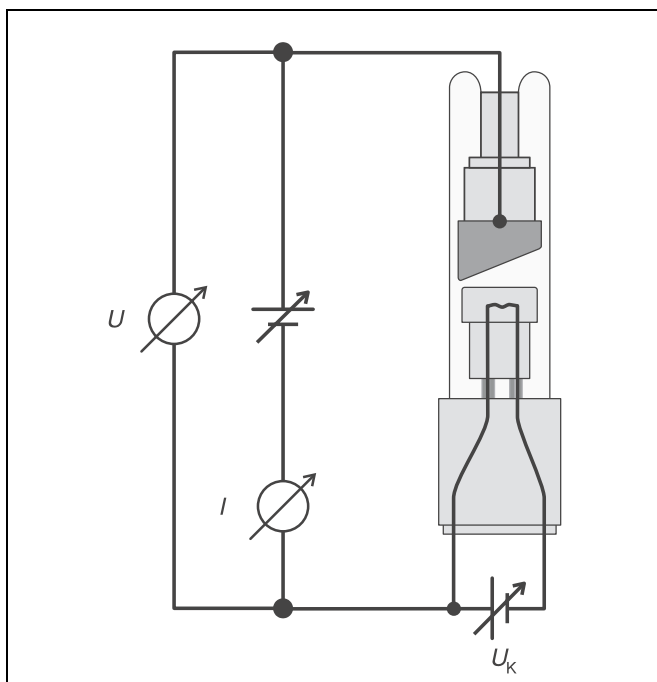
Fig. 4 Experiment setup for investigating the energy spectrum of an x-ray tube

Setup

Setup in Bragg configuration:

Fig. 4 shows some important details of the experiment setup. To set up the experiment, proceed as follows (see also the Instruction Sheet for the x-ray apparatus):

– Mount the collimator in collimator mount **(a)** (note the guide groove).

– Attach the goniometer to guide rods **(d)** so that the distance s_1 between the slit diaphragm of the collimator and the target arm is approx. 5 cm. Connect ribbon cable **(c)** for controlling the goniometer.

– Remove the protective cap of the end-window counter, place the end-window counter in sensor seat **(e)** and connect the counter tube cable to the socket marked GM TUBE.

– By moving sensor holder **(b)**, set the distance s_2 between the target arm and the slit diaphragm of the sensor receptor to approx. 6 cm.

– Mount target holder **(f)** with target stage.

– Loosen knurled screw **(g)**, place the NaCl crystal flat on the target stage, carefully raise the target stage with crystal all the way to the stop and gently tighten the knurled screw (prevent skewing of the crystal by applying a slight pressure).

– If necessary, adjust the zero position of the goniometer (see Instruction Sheet for x-ray apparatus).

Notes:

NaCl crystals are hygroscopic and extremely fragile. Store the crystals in a dry place; avoid mechanical stresses on the crystal; handle the crystal by the short faces only.

If the counting rate is too low, you can reduce the distance s_2 between the target and the sensor somewhat. However, the distance should not be too small, as otherwise the angular resolution of the goniometer is no longer sufficient to separate the characteristic K_α and K_β lines.

Preparing the PC-based measurement:

– Connect the RS–232 output to the serial interface on your PC (usually COM1 or COM2) using the 9-pin V.24 cable (supplied with x-ray apparatus).

– If necessary, install the software "X-ray Apparatus" under Windows 95/98/NT (see Instruction Sheet for x-ray apparatus) and select the desired language.

Carrying out the experiment

a) Varying the tube high voltage:

– Start the software "X-ray Apparatus", check to make sure that the apparatus is connected correctly, and clear any existing measurement data using the button ⬚ or the F4 key.

– Set the emission current I = 1.00 mA, the measuring time per angular step Δt = 10 s and the angular step width $\Delta\beta$ = 0.1°.

– Press the COUPLED key to activate 2ϑ coupling of target and sensor and set the lower limit of the target angle to 2.5° and the upper limit to 12.5°.

– Set the tube high voltage U = 15 kV and start measuring and data transmission to the PC by pressing the SCAN key.

– Conduct additional measurement series using the tube high voltages U = 20 kV, 25 kV, 30 kV and 35 kV.

To show the wavelength-dependency, open the "Settings" dialog with the button ⬚ or F5 and enter the lattice plane spacing for NaCl.

Save the measurement series under an appropriate name by pressing the button ⬚ or the F2 key.

b) Varying the emission current:

Clear existing measurement data using the button ⬚ or the F4 key and set the tube high voltage to U = 35 kV.

– Set the emission current I = 0.40 mA and start measuring and data transmission to the PC by pressing the SCAN key.

– Record additional measurement series using the emission currents I = 0.60 mA, 0.80 mA and 1.00 mA.

– To show the wavelength-dependency, open the "Settings" dialog with the button ⬚ or F5 and enter the lattice plane spacing for NaCl.

– Save the measurement series under an appropriate name by pressing the button ⬚ or the F2 key.

Measuring example
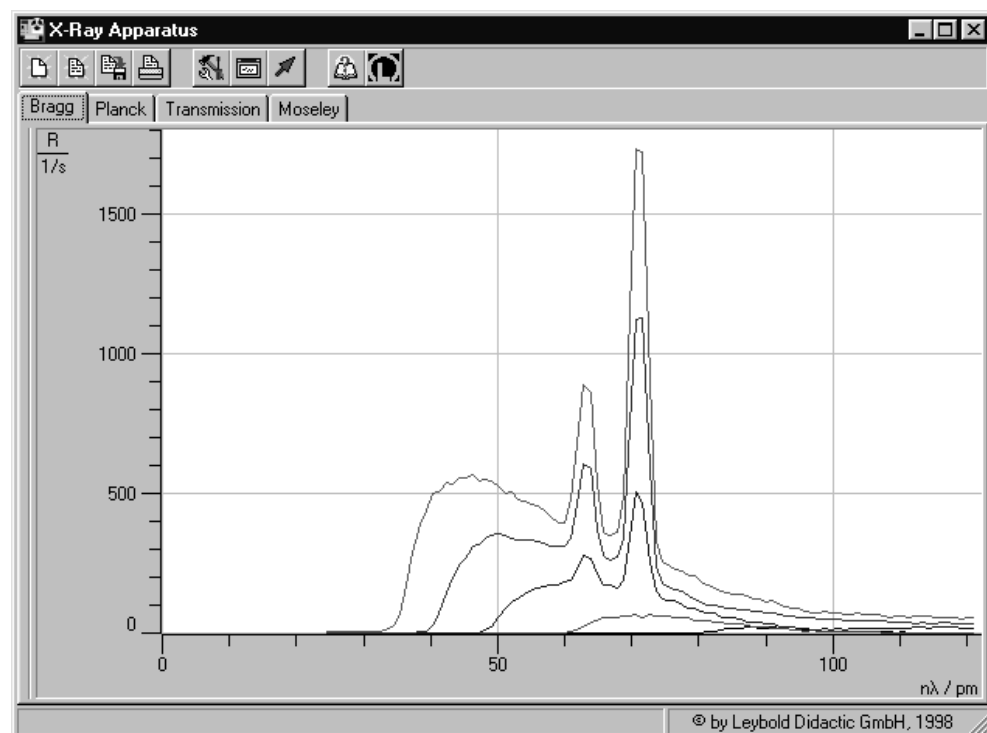
a) Varying the tube high voltage:

Fig. 5   Spectra of x-ray tube Mo for tube high voltages $U =$ 15 kV (bottom), 20 kV, 25 kV, 30 kV, 35 kV (top);
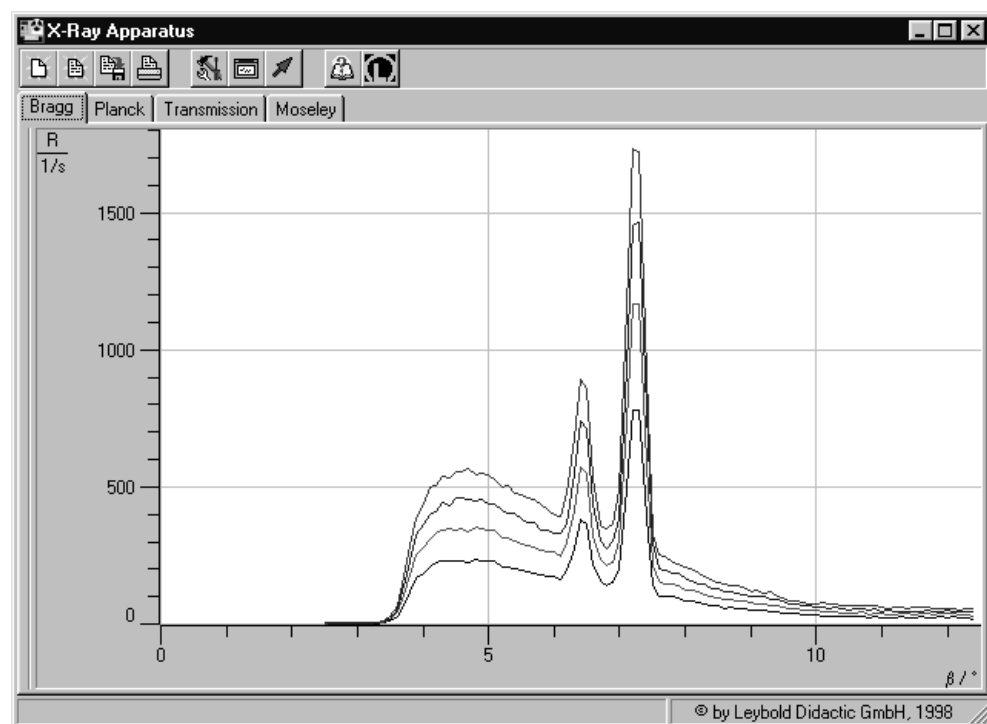
b) Varying the emission current:

Fig. 6   Spectra of x-ray tube Mo for emission currents $I =$ 0.4 mA (bottom), 0.6 mA, 0.8 mA, 1.0 mA (top); x-ray high voltage $U =$ 35 kV.

Evaluation

a) Varying the tube high voltage:

– Load the saved measurement series.
– Place the cursor in each diagram, click the right mouse button to access the evaluation functions of the software "X-ray Apparatus" and, for each curve, select "Calculate Peak Center" and mark the "full width" of the peak with the left mouse button.
– Write down the peak centers in a measuring table (see table 1) and calculate the mean values.

Tab. 1: Wavelengths of the characteristic radiation of molybdenum determined from the spectra under variation of the tube high voltage U

$\dfrac{U}{kV}$	$\dfrac{\lambda(K_\alpha)}{pm}$	$\dfrac{\lambda(K_\beta)}{pm}$
25	71.04	62.13
30	71.09	63.14
35	71.04	63.10

Mean values:

$\lambda(K_\alpha)$ = 71.06 pm, $\lambda(K_\beta)$ = 63.12 pm

Literature values [1] for comparison:

$\lambda(K_\alpha)$ = 71.080 pm, $\lambda(K_\beta)$ = 63.095 pm

b) Varying the emission current:

– Load the saved measurement series.
– Place the cursor in each diagram, click the right mouse button to access the evaluation functions of the software "X-ray Apparatus" and, for each curve, select "Calculate Peak Center" and mark the "full width" of the peak with the left mouse button.
– Write down the peak centers in a measuring table (see table 2) and calculate the mean values.
– Now select the menu command "Display Coordinates", find the maxima $R(K_\alpha)$ and $R(K_\beta)$ of the characteristic lines, and determine the maximum of the continuum of bremsstrahlung radiation R_C and write it down (see table 3) and display it in the graph (see Fig. 7).

Fig. 7   Counting rates as a function of the emission current
Circles: K_α-line
Squares: K_β-line
Triangles: bremsstrahlung continuum
Lines: straight lines through origin
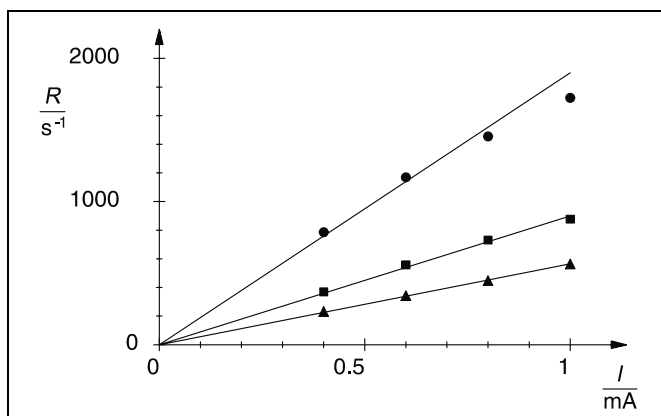
Tab. 2: Wavelengths of the characteristic radiation of molybdenum determined from the spectra under variation of the emission current I

$\dfrac{I}{mA}$	$\dfrac{\lambda(K_\alpha)}{pm}$	$\dfrac{\lambda(K_\beta)}{pm}$
0.4	71.09	63.15
0.6	71.05	63.15
0.8	71.08	63.15
1.0	71.04	63.10

Mean values:

$\lambda(K_\alpha)$ = 71.07 pm, $\lambda(K_\beta)$ = 63.14 pm

Tab. 3: Counting-rate maxima of the characteristic lines and the bremsstrahlung continuum as a function of the emission current I

$\dfrac{I}{mA}$	$\dfrac{R(K_\alpha)}{s^{-1}}$	$\dfrac{R(K_\beta)}{s^{-1}}$	$\dfrac{R_C}{s^{-1}}$
0.4	786	369	232
0.6	1169	558	343
0.8	1455	731	448
1.0	1724	877	564

Results

a) Varying the tube high voltage:

Fig. 5 clearly shows how the continuum of bremsstrahlung changes as the tube high voltage U increases. The intensity of the radiation increases, as the electrons generate more x-ray quanta on deceleration as the energy increases. The limit wavelength λ_{min} is shifted to smaller values, i. e. higher-energy, "harder" radiation is generated. For quantitative investigation of the relationship between the limit wavelength and the tube voltage see experiment P6.3.3.3.

A minimum energy of the electrons is required to excite the characteristic energy. The K_α and K_β lines thus only become apparent above U = 20 kV. Their intensity increases with the tube high voltage. However, the tube high voltage has no effect on the positions of the characteristic lines (see table 1).

b) Varying the emission current:

As we can see from Fig. 6, the emission current I has no effect on the shape of the x-ray spectrum. The positions of the characteristic lines remain unchanged (see table 2). However, the intensity of the bremsstrahlung spectrum and the characteristic lines decreases proportionally with the emission current (see table 3 and Fig. 7). Deviations from this proportionality at counting rates above 1000 s^{-1} are due to dead-time effects in counting-rate measurements.

Literature

[1] C. M. Lederer and V. S. Shirley, Table of Isotopes, 7th Edition, 1978, John Wiley & Sons, Inc., New York, USA.

Atomic and nuclear physics

X-ray physics
Physics of the atomic shell

Fine structure of the characteristic x-radiation of a molybdenum anode

Objects of the experiment

■ Investigating the fine structure of the characteristic x-radiation of molybdenum by means of Bragg reflection at an NaCl monocrystal in the fifth diffraction order.

■ Identifying the characteristic K_α, K_β and K_γ lines.

■ Resolving the fine structure of the K_α line as a line doublet and determining the wavelength interval $\Delta\lambda$ within the doublet.

Principles

On closer examination, the characteristic K_α and K_β lines of the x-radiation prove to be line doublets. The two doublets can be resolved by means of Bragg reflection at an NaCl monocrystal when measured in a higher diffraction order. However, they differ in their physical nature.

The K_β doublet consists of the pure K_β line, i.e. transitions of excited atoms from the M-shell to the K-shell, and the K_γ line, i.e. transitions from the N-shell to the K-shell. The wavelength interval $\Delta\lambda$ between the two lines is just 1.2 pm (see table 1), so that they can only be resolved at a high resolution.

Table 1: Transition energies E, wavelengths λ and relative components of the characteristic K_α, K_β and K_γ lines of molybdenum (weighted mean values according to [1])

	$\dfrac{E}{\text{keV}}$	$\dfrac{\lambda}{\text{pm}}$	Relative proportion
K_α	17.44	71.08	1.000
K_β	19.60	63.26	0.170
K_γ	19.97	62.09	0.027
Doublet $K_\beta + K_\gamma$	19.65	63.09	

The fine structure of the K_α line arises from the fine structure of the L-shell, and thus ultimately from the spin-orbit characteristic of the electrons. The L-shell actually consists of three sub-shells, designated L_I, L_{II} and L_{III} in x-ray spectroscopy. The transitions from these sub-shells to the K-shell with emission of an x-ray is subject to the selection rules
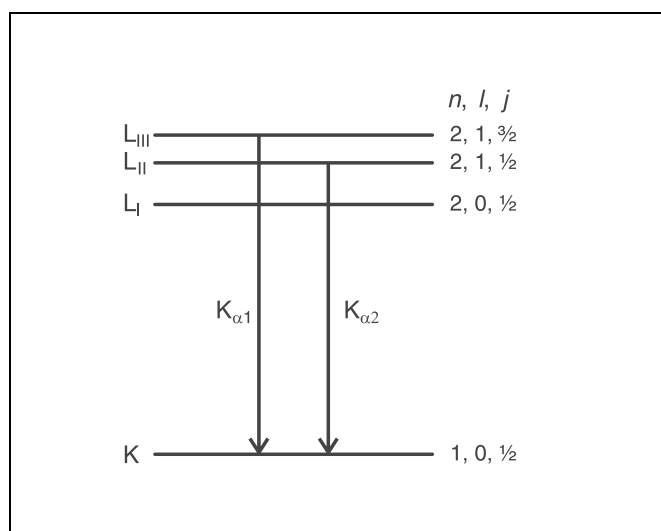
$$\Delta l = \pm 1, \ \Delta j = 0, \pm 1 \tag{I}$$

for the change of the orbital angular momentum l and the total angular momentum j on transition. Thus, two transitions from the L-shell to the K-shell are permitted, designated $K_{\alpha1}$ and $K_{\alpha2}$ (see Fig. 1). Table 2 shows the values generally found in the literature for molybdenum. According to these, the wavelength interval within the K_α doublet is $\Delta\lambda = 0.43$ pm.

Fig. 1   Diagram of fine structure of the characteristic line K_α

Table 2: Wavelengths λ (calculated from literature specifications [1] for transition energies) and relative proportions of K_α radiation of molybdenum

Line	$\dfrac{\lambda}{\text{pm}}$	Relative proportion
$K_{\alpha1}$	70.93	1.000
$K_{\alpha2}$	71.36	0.525

Apparatus

1 X-ray apparatus 554 811

1 End-window counter
for α, β, γ and x-ray radiation 559 01

additionally required:

1 PC with Windows 9x/NT

The object of the experiment is to resolve this fine structure by means of Bragg reflection at an NaCl monocrystal at higher diffraction orders.

According to Bragg's law of reflection, the following relationship exists between the wavelength λ of the incident characteristic radiation and the glancing angle ϑ at which we may expect an intensity maximum:

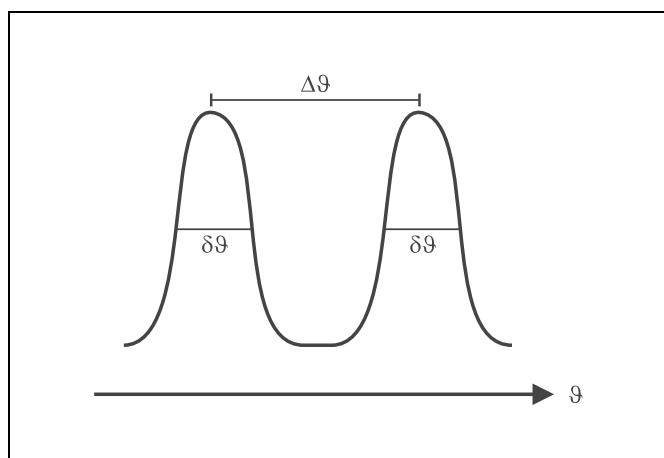$$n \cdot \lambda = 2 \cdot d \cdot \sin\vartheta \qquad\qquad\qquad\qquad (II)$$
n: diffraction order,
$d = 282.01$ pm: lattice plane spacing of NaCl

Fig. 2   Definition of the angular width $\delta\vartheta$ and the angular spacing $\Delta\vartheta$ of two intensity maxima.
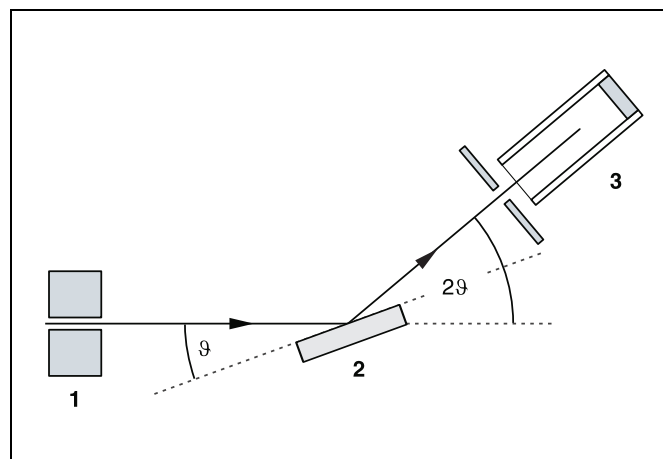

Fig. 3   Diagram showing the diffraction of x-rays at a monocrystal **1** collimator, **2** monocrystal, **3** counter tube

Safety notes

The x-ray apparatus fulfills all regulations governing an x-ray apparatus and fully protected device for instructional use and is type approved for school use in Germany (NW 807/97 Rö).

The built-in protection and screening measures reduce the local dose rate outside of the x-ray apparatus to less than 1 μSv/h, a value which is on the order of magnitude of the natural background radiation.

- Before putting the x-ray apparatus into operation inspect it for damage and to make sure that the high voltage is shut off when the sliding doors are opened (see Instruction Sheet for x-ray apparatus).
- Keep the x-ray apparatus secure from access by unauthorized persons.

Do not allow the anode of the x-ray tube Mo to overheat.

- When switching on the x-ray apparatus, check to make sure that the ventilator in the tube chamber is turning.

The goniometer is positioned solely by electric stepper motors.

- Do not block the target arm and sensor arm of the goniometer and do not use force to move them.

The wavelength interval $\Delta\lambda$ of two lines thus corresponds to the angular spacing

$$\Delta\vartheta = \frac{n \cdot \Delta\lambda}{2 \cdot d \cdot \cos\vartheta} \qquad\qquad\qquad\qquad (III),$$

which increases with the diffraction order. It is important to distinguish between the angular spacing $\Delta\vartheta$ and the angular width $\delta\vartheta$ of an intensity maximum. This latter should be smaller than the angular spacing so that the two lines can be observed separately (see Fig. 2). The angular width is determined by the opening slit of the counter tube (see Fig. 3), its distance from the crystal and the divergence of the incident x-ray beam, and remains constant even for higher diffraction orders. Thus, the K_α doublet can be resolved in the diffraction order $n = 5$.

Setup

Setup in Bragg configuration:

Fig. 4 shows some important details of the experiment setup. To set up the experiment, proceed as follows (see also the Instruction Sheet for the x-ray apparatus):

– Mount the collimator in the collimator mount **(a)** (note the guide groove).
– Attach the goniometer to guide rods **(d)** so that the distance s_1 between the slit diaphragm of the collimator and the target arm is approx. 5 cm. Connect ribbon cable **(c)** for controlling the goniometer.
– Remove the protective cap of the end-window counter, place the end-window counter in sensor seat **(e)** and connect the counter tube cable to the socket marked GM TUBE.
– By moving the sensor holder **(b)**, set the distance s_2 between the target arm and the slit diaphragm of the sensor seat to approx. 6 cm.
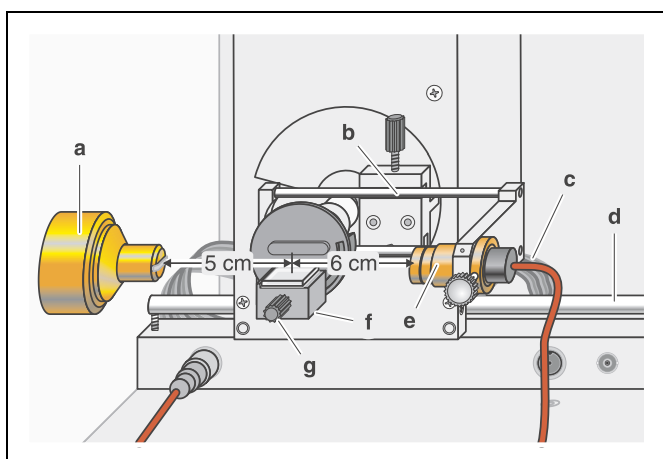

Fig. 4   Experiment setup in Bragg configuration

– Mount the target holder **(f)** with target stage.
– Loosen knurled screw **(g)**, place the NaCl crystal flat on the target stage, carefully raise the target stage with crystal all the way to the stop and gently tighten the knurled screw (prevent skewing of the crystal by applying a slight pressure).
– If necessary, adjust the mechanical zero position of the goniometer (see Instruction Sheet for x-ray apparatus).

Notes:

NaCl crystals are hygroscopic and extremely fragile. Store the crystals in a dry place; avoid mechanical stresses on the crystal; handle the crystal by the short faces only.

If the counting rate is too low, you can reduce the distance s_2 between the target and the sensor somewhat. However, the distance should not be too small, as otherwise the angular resolution of the goniometer is no longer sufficient.

Preparing the PC-based measurement:

– Connect the RS–232 output and the serial interface on your PC (usually COM1 or COM2) using the 9-pin V.24 cable (supplied with x-ray apparatus).
– If necessary, install the software "X-ray Apparatus" under Windows 9x/NT (see Instruction Sheet for x-ray apparatus) and select the desired language.

Carrying out the experiment

– Start the software "X-ray Apparatus", check to make sure that the apparatus is connected correctly, and clear any existing measurement data using the button 🗋 or the F4 key.
– Set the tube high voltage U = 35 kV, the emission current I = 1.00 mA and the angular step width $\Delta\beta$ = 0.1°.
– Press the COUPLED key for 2ϑ coupling of target and sensor.

a) First order of diffraction:

– To record the first diffraction order, set the lower limit of the target angle to 5.5° and the upper limit to 8.0°, and set the measuring time per angular step to Δt = 10 s.
– Start measurement and data transfer to the PC by pressing the SCAN key.
– When the measurement is finished, open the "Settings" dialog with the button 🔣 or F5 and enter the lattice plane spacing for NaCl to show the wavelength-dependency of the counting rate.
– Save the measurement series under a suitable name using the button 🔣 or by pressing F2.

b) Fifth order of diffraction:

– To record the fifth diffraction order, set the lower limit of the target angle to 32.5° and the upper limit to 40.5°, and
– Set the measuring time per angular step to Δt = 400 s.

Note: Due to the low counting rate to be expected, you need to set a relatively long measuring time to obtain a satisfactory statistical accuracy. In this setting, the total measuring time is 9 h.

– Start measurement and data transfer to the PC by pressing the SCAN key.
– When the measurement is finished, open the "Settings" dialog with the button 🔣 or F5 and enter the lattice plane spacing for NaCl to show the wavelength-dependency of the counting rate.
– Save the measurement series under a suitable name using the button 🔣 or by pressing F2.

Measuring example

Fig. 5 shows the diffraction spectrum measured in the first order, and Fig. 6 shows the spectrum for the fifth order of diffraction.

a) First order of diffraction:

Fig. 5   Diffraction spectrum of x-rays in Bragg reflection in the first order at an NaCl monocrystal
Parameters: U = 35 kV, I = 1 mA, Δt = 10 s

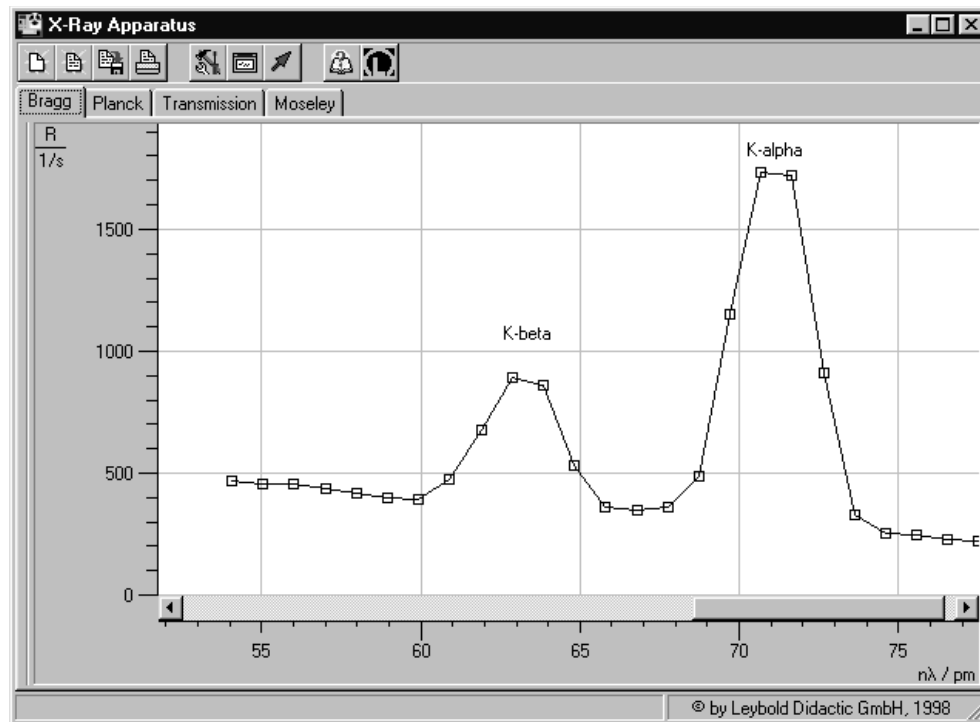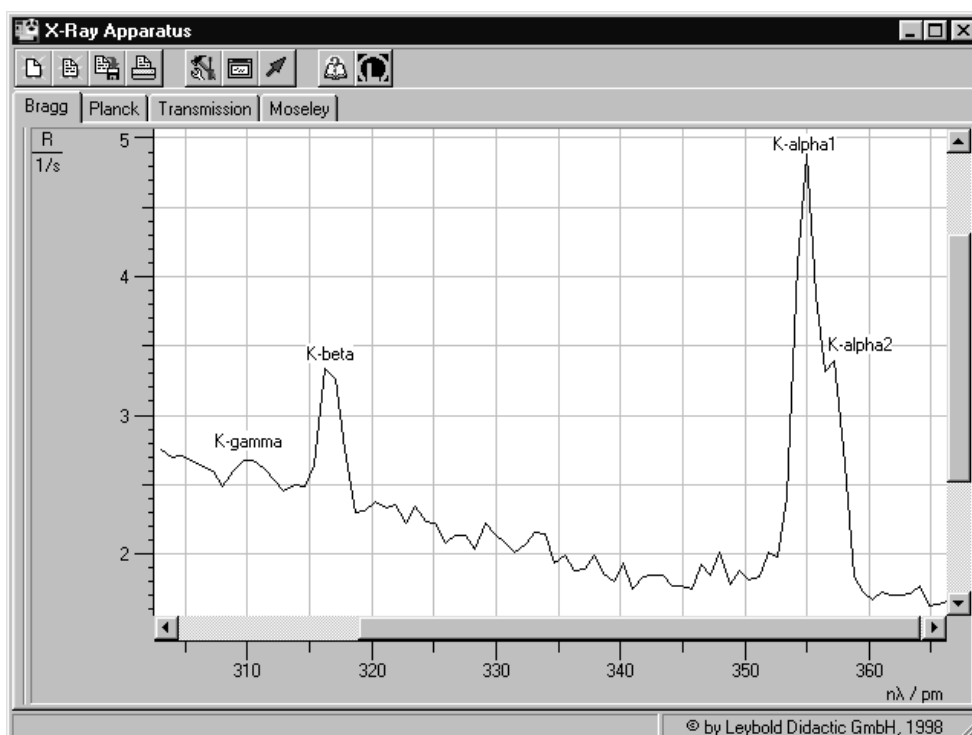### b) Fifth order of diffraction:

Fig. 6   Diffraction spectrum of x-rays in Bragg reflection in the fifth order at an NaCl monocrystal
Parameters: U = 35 kV, I = 1 mA, Δt = 400 s

Evaluation

– In the diagram, click the right mouse button to access the evaluation functions of the software "X-ray Apparatus" and select the command "Display Coordinates".

– Drag the mouse pointer across the peaks and read the corresponding $n \cdot \lambda$ values in the bottom left corner of the window.

a) First order of diffraction:

Table 3: Measuring results for the first diffraction order and literature value for the characteristic wavelengths (cf. table 1)

Line doublet	Measurement result $\dfrac{\lambda}{pm}$	Literature value $\dfrac{\lambda}{pm}$
K_α	71.0	71.08
$K_\beta + K_\gamma$	63.1	63.09

b) Fifth order of diffraction:

Table 4: Measuring results for the fifth diffraction order and literature value for the characteristic wavelengths (cf. tables 1 and 2)

Lines	Measurement result $\dfrac{5 \cdot \lambda}{pm}$	$\dfrac{\lambda}{pm}$	Literature value $\dfrac{\lambda}{pm}$
$K_{\alpha 1}$	355	71.0	70.93
$K_{\alpha 2}$	357	71.4	71.36
K_β	316.7	63.34	63.26
K_γ	310.3	62.06	62.09

Splitting of doublet K_α:

$\Delta\lambda = 0.4$ pm   Literature value: $\Delta\lambda = 0.43$ pm

Splitting of doublet $K_\beta + K_\gamma$:

$\Delta\lambda = 1.28$ pm   Literature value: $\Delta\lambda = 1.17$ pm

Results

The characteristic K_α und K_β lines we observe in the first diffraction order split into doublets. We can observe this split in the fifth diffraction order.

The fine structure of the K_α doublet is a consequence of the fine structure of the L-shell. The K_β doublet is composed of the pure K_β line and the K_γ line.

Additional information

Strictly speaking, the K_β and K_γ lines also show a fine structure due to the fine structure of shells M and N. However, this split is so slight that we cannot observe it with the means at hand. Table 1 shows the weighted mean values of the respective individual lines from this substructure.

Literature

[1] C. M. Lederer and V. S. Shirley, Table of Isotopes, 7th Edition, 1978, John Wiley & Sons, Inc., New York, USA.
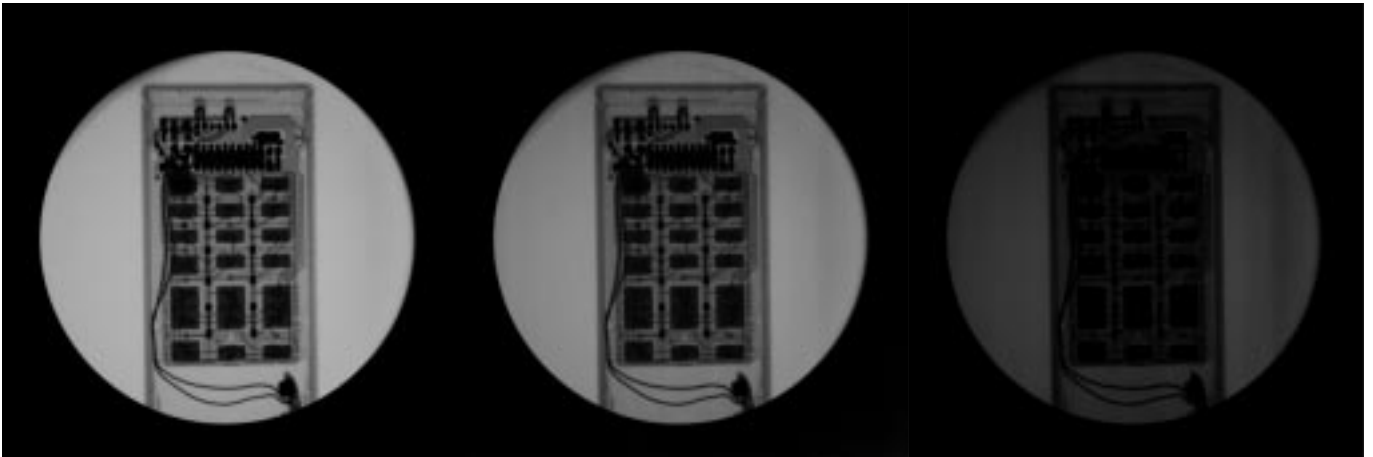
Fig. 2   Luminous-screen image of a pocket calculator
(photographed using a digital camera) at maximum tube
high voltages and different emission currents.
I = 1.0 mA, I = 0.7 mA and I = 0.4 mA

Measuring example

a) Brightness of the luminous screen:

The luminous screen becomes brighter as the emission current
rises.

b) Varying the emission current I:

Fig. 2 shows the relationship between the luminous screen and
the emission current I.

c) Varying the tube high voltage U:

Fig. 3 shows the relationship between the luminous screen and
the tube high voltage U.

Fig. 3   Luminous-screen image of a pocket calculator
(photographed using a digital camera) at maximum emis-
sion currents and different tube high voltages.
U = 35 kV, U = 31 kV and U = 27 kV
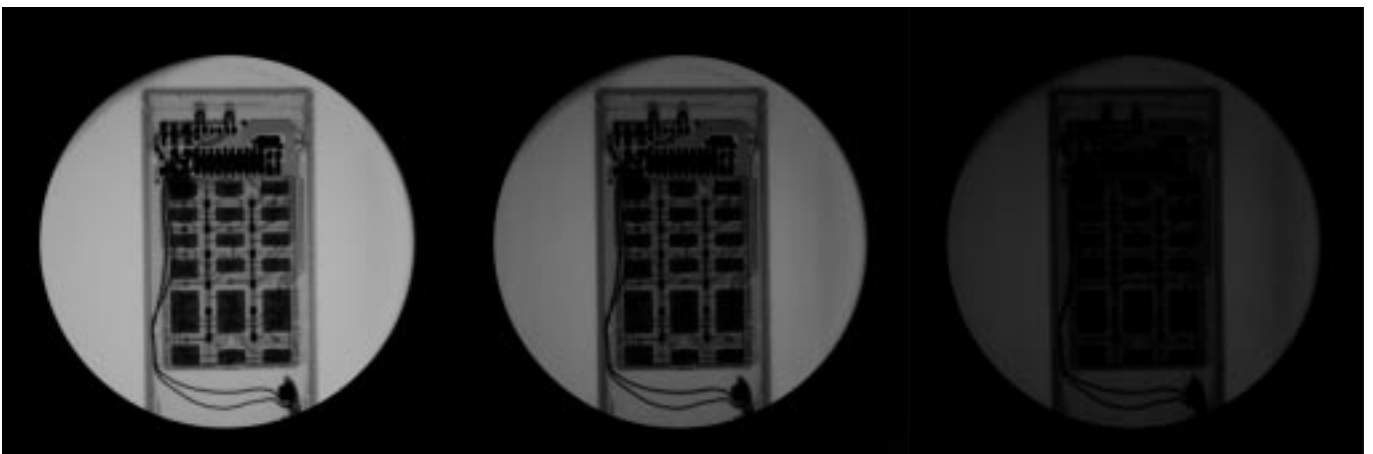
Evaluation

When no object is in the beam path, the luminous screen
fluoresces more brightly as the emission current rises, because
the intensity of the x-radiation increases.

The brightness of the luminous screen is reduced behind the
transilluminated object, because the object attenuates the
x-rays. Objects that are thicker or have greater attenuation
characteristics show up on the luminous screen as darker
features. However, the brightness of the image as a whole
increases with the emission current.

An increase in the tube high voltage generally results in greater
image contrast, as the x-rays are harder (a greater proportion
of high-energy x-rays). At the same time, the brightness in-
creases, because the intensity of the x-rays also increases (see
P6.3.3.2).

Results

The luminous screen shows a relatively sharp image of the
internal structure of the transilluminated object. This explains
the great importance of x-rays in diagnostic medicine and
non-destructive materials testing.

Atomic and nuclear physics

X-ray physics
Detection of x-rays

**LD
Physics
Leaflets**

P6.3.1.4

Determining
the ion dose rate of the x-ray tube
with molybdenum anode

Objects of the experiment

■ To introduce and to explanate the terms ion dose (exposure dose) and ion dose rate for quantifying the action of x-rays.

■ To determine the ion dose rate in an air-filled plate capacitor by measuring the ionization current.

Principles

Dosimetry is the quantitative measurement of the effects that x-rays cause when passing through matter and which can be used to detect x-rays. Dosimetry is thus important for medical and technical applications as well as in radiation protection. It does not represent a measurement of the actual intensity of the x-radiation. Such a determination would require e.g. calorimetric measurements in which the entire x-radiation is absorbed and converted into heat. However, with suitable calibration, measurements of dose and time can be used as a measure of the radiation intensity.

Dose and dose rate:

In terms of radiation, the dose can be defined on the basis of both the ionizing action and the energy absorption of the x-rays when they pass through matter. The first case is the measure of the ion dose (also called the exposure dose) and the second the absorbed dose.

The ion dose (exposure dose)

$$J = \frac{dQ}{dm} \qquad (I)$$

is the quotient of the charge dQ generated in air by charge carriers of one sign due to irradiation, and the mass dm of the irradiated volume element. Its derived SI unit is the coulomb per kilogram (C kg^{-1}): 1 C kg^{-1} = 1 As kg^{-1}

The absorbed dose

$$K = \frac{dW}{dm} \qquad (II)$$

is the quotient of the energy dW absorbed by the irradiated material and the mass dm of the irradiated volume element. Its derived SI unit is the gray (Gy): 1 Gy = 1 J kg^{-1}

Fig. 1 Diagram of beam path in plate capacitor, for calculating the irradiated volume V

0708-Ste
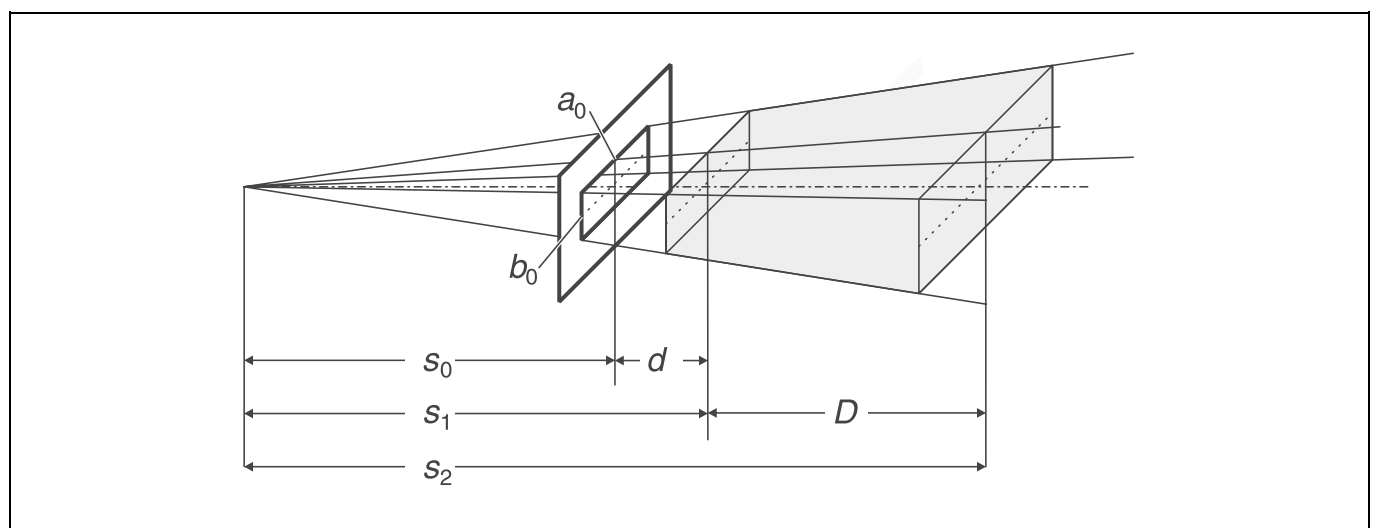
Apparatus

1 X-ray apparatus	554 811
or	
1 X-ray apparatus	554 812
1 Plate capacitor x-ray	554 840
1 Power supply 450 V DC	522 27
1 Electrometer amplifier	532 14
1 STE resistor 1 GΩ, 0.5 W	577 02
1 Voltmeter, U ≤ 300 V DC, input resistance ≥ 10 MΩ . . . . e.g.	531 100
1 Voltmeter, U ≤ 10 V DC . . . . e.g.	531 100
1 Screened cable BNC/4 mm	575 24
Connecting leads	

The effective intensity of the x-rays is defined as the quotient of dose and time. The ion dose rate is defined as

$$j = \frac{dJ}{dt} \tag{III},$$

measured in A kg^{-1}, and the absorbed dose rate is defined as

$$k = \frac{dK}{dt} \tag{IV}$$

measured in Gy s^{-1} = W kg^{-1}.

Determining the ion dose rate:

The ion dose rate can be measured in an air-filled plate capacitor by measuring the saturation value of the ionization current I_C (see experiment P6.3.1.3). This is determined as

$$I_C = \frac{dQ}{dt};$$

using (I) and (II), this gives us:

$$j = \frac{dI_C}{dm} \tag{V}$$

As x-rays diverge as they propagate and are attenuated in air, the ion dose rate j is a location-dependent quantity, and would require a great deal of effort to measure. It is easier to measure the mean ion dose rate

$$<j> = \frac{I_C}{m}, \tag{VI}$$

for which we need to determine the total ionization current I_C and the mass

$$m = \rho \cdot V \tag{VII}$$

of the total irradiated volume V.

The density ρ of air is calculated as

$$\rho = \rho_0 \cdot \frac{T_0}{T} \cdot \frac{p}{p_0} \tag{VIII}$$

with $\rho_0 = 1.293$ kg m^{-3} , $T_0 = 273$ K and $p_0 = 1013$ hPa

from the temperature T and barometric pressure p in the experiment chamber. The volume V can be calculated with the aid of Fig. 1.

Calculating the irradiated volume *V*:

In Fig. 1, the focal spot of the x-ray tube is presumed to closely approximate a point. The rectangular diaphragm in front of the plate capacitor shapes the radiation cone of the x-ray tube into a beam which penetrates the volume V of air to be calculated.

The distance between the focal spot and the rectangular diaphragm is $s_0 = 15.5$ cm. The dimensions of the diaphragm are $a_0 = 4.5$ cm and $b_0 = 0.6$ cm. The x-rays propagate in a straight line, and thus illuminate at any given distance s from the focal spot a rectangle behind the diaphragm with the dimensions

$$a(s) = \frac{s}{s_0} \cdot a_0 \text{ and } b(s) = \frac{s}{s_0} \cdot b_0 \tag{IX}.$$

The irradiated volume of air in the plate capacitor is thus equivalent to the integral

$$V = \int_{s_1}^{s_2} a(s) \cdot b(s) \cdot ds \tag{X}.$$

with the integral limits

$$s_1 = s_0 + d \text{ and } s_2 = s_0 + d + D \tag{XI}$$

$d = 2.5$ cm: distance from diaphragm to plate capacitor
$D = 16.0$ cm: length of plate capacitor.

This gives us

$$V = \frac{1}{3} \cdot \frac{a_0 \cdot b_0}{s_0^2} \cdot \left(s_2^3 - s_1^3\right)$$

and thus

$$V = a_0 \cdot b_0 \cdot D \cdot \left(\frac{s_2^2 + s_2 s_1 + s_1^2}{s_0^2}\right) = 125 \text{ cm}^3 \tag{XII}.$$
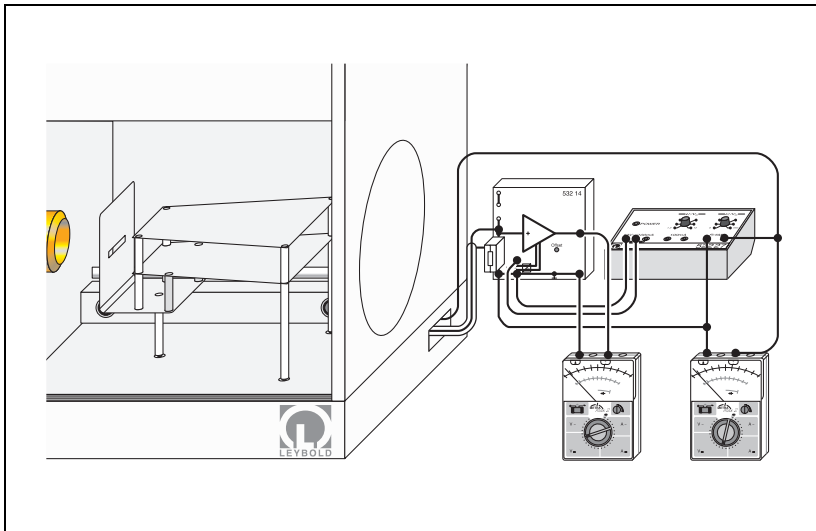
Fig. 2 Experiment setup for measuring the ionization current in a plate capacitor
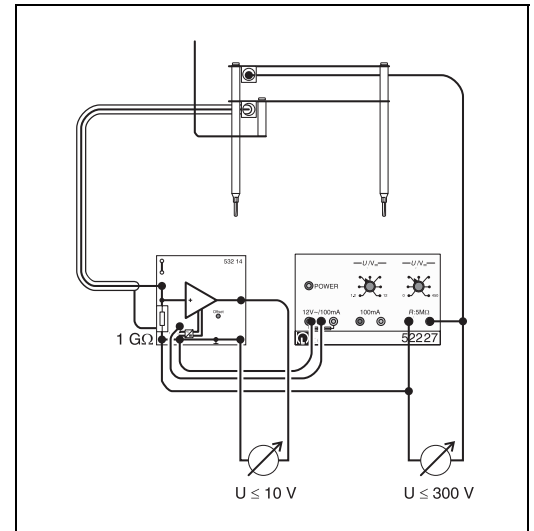
Fig. 3 Connecting the plate capacitor and the electrometer amplifier for determining the ionization current

Setup

Set up the experiment as shown in Fig. 2. Fig. 3 shows the electrical connections of the plate capacitor and the electrometer amplifier for determining the ionization current.

Mechanical setup:

— If necessary, demount the collimator of the x-ray apparatus and remove any experiment equipment from the chamber of the x-ray apparatus.

— Connect the adapter cable BNC/4 mm to the bottom capacitor plate (BNC socket) with the BNC plug and connect the connecting lead to the top capacitor plate (safety socket) of the plate capacitor x-ray.

— Lift the plate capacitor into the experiment chamber of the x-ray apparatus and insert the mounting plugs in the mounting sockets. Check to make sure that the capacitor plates are aligned parallel to the base plate of the x-ray apparatus, and correct as necessary.

— Feed the two cables into the free channel until they reappear on the right side of the x-ray apparatus

Electrical assembly:

— Connect the connecting lead to the positive pole of the 450 V DC power supply and connect the adapter cable BNC/4 mm to the electrometer amplifier fitted with the 1 GΩ resistor.

— Ground the electrometer amplifier to the negative terminal of the 450 V DC amplifier.

— Connect a voltmeter to measure the capacitor voltage U_C and the output voltage of the electrometer amplifier U_E.

— Plug in the x-ray apparatus to the mains power and switch it on.

Carrying out the experiment

— Determine the temperature ϑ and the barometric pressure p in the experiment chamber and use these to calculate the irradiated mass m according to equations (VII) and (VIII).

a) Saturation ionization current I_C as a function of the emission current I:

— Set the tube high voltage to U = 35 kV.

— Set the capacitor voltage $U_C \geq$ 140 V, so that the saturation value of the ionization current I_C is reached.

To record a measurement series, increase the emission current I in steps from 0 mA to 1 mA and determine the ionization current I_C for each step from the voltage U_E at the output of the electrometer amplifier:

$$I_C = \frac{U_E}{1 \text{ G}\Omega}$$

— Write down your measuring results and the calculated mean ion dose rate.

b) Saturation ionization current I_C as a function of the tube high voltage U:

— Set the emission current I = 1.0 mA.

— Set the capacitor voltage U$C \geq$ 140 V.

Increase the tube high voltage U in steps from 5 kV to 35 kV and determine the corresponding ionization current I_C.

— Write down your measuring results and the calculated mean ion dose rate.

Measuring example and evaluation

T = 303 K and p = 1017 hPa:

From equation (VIII) we can calculate ρ = 1.17 kg m^{-3}

and from (VII) and (XII) m = 0.147 10^{-3} kg

Thus, in accordance with (VI) the mean ion dose rate is

$$\frac{<j>}{\mu A \cdot kg^{-1}} = \frac{I_C}{nA} \cdot \frac{1}{0.147 \text{ kg}}$$

a) Measurements as a function of the emission current *I*:

Tab. 1: Saturation value of the ionization current I_C and the mean ion dose rate $< j >$ as a function of the emission current *I* of the x-ray tube, tube high voltage *U* = 35 kV.

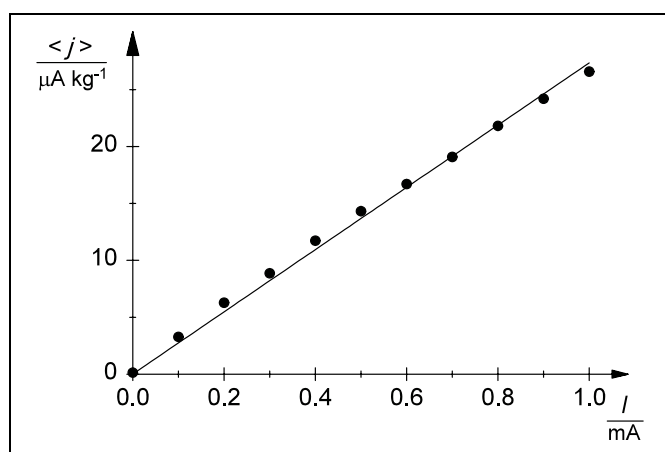| $\dfrac{I}{\text{mA}}$	$\dfrac{I_C}{\text{nA}}$	$\dfrac{< j >}{\mu\text{A} \cdot \text{kg}^{-1}}$
0.0	0.02	0.14
0.1	0.48	3.27
0.2	0.92	6.27
0.3	1.30	8.86
0.4	1.72	11.7
0.5	2.10	14.3
0.6	2.45	16.7
0.7	2.80	19.1
0.8	3.20	21.8
0.9	3.55	24.2
1.0	3.90	26.6

Fig. 4   Mean ion dose rate $< j >$ as a function of the emission current *I* of the x-ray tube, *U* = 35 kV

b) Saturation ionization current I_C as a function of the tube high voltage *U*:

Tab. 2: Saturation value of ionization current I_C and mean ion dose rate $< j >$ as a function of the tube high voltage *U*, emission current *I* = 1.0 mA

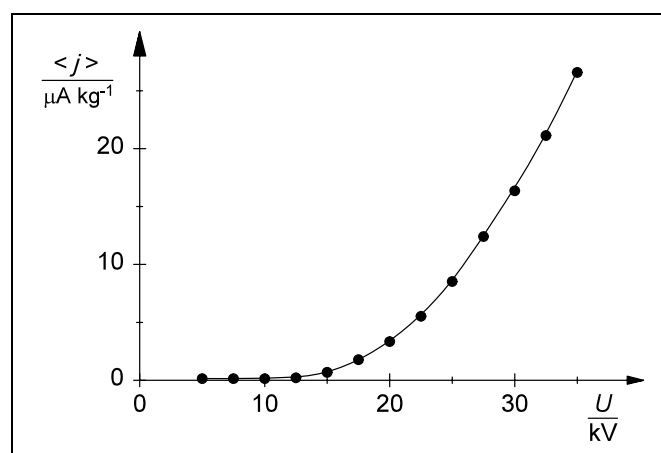| $\dfrac{U}{\text{kV}}$	$\dfrac{I_C}{\text{nA}}$	$\dfrac{< j >}{\mu\text{A} \cdot \text{kg}^{-1}}$
5.0	0.02	0.14
7.5	0.02	0.14
10.0	0.02	0.14
12.5	0.03	0.20
15.0	0.10	0.68
17.5	0.26	1.77
20.0	0.49	3.34
22.5	0.81	5.52
25.0	1.25	8.52
27.5	1.82	12.4
30.0	2.40	16.4
32.5	3.10	21.1
35.0	3.90	26.6

Fig. 5   Mean ion dose rate $< j >$ as a function of the tube high voltage, *I* = 1.0 mA

Results

At the maximum operating parameters of the x-ray tube (*U* = 35 kV, *I* = 1 mA), the mean ion dose rate in the plate capacitor is

$< j >$ = 26.6 μA kg^{-1}.

Additional information

In addition to the ion dose and the absorbed dose, the dose equivalent *D* is a further important quantity. It is measured in sieverts (Sv): 1 Sv = 1 J kg^{-1}.

A radiation with a specific dose equivalent has the same biological effect on tissues as hard x-rays generated with a voltage of 200 kV and having the corresponding absorbed dose. In x-ray and γ radiation, the absorbed dose *K* and the dose equivalent *D* are identical when *K* is measured in Gy and *D* in Sv. The conversion factor for the ion dose *J* is: 1 Sv $\triangleq$ 0.0308 As kg^{-1}.

The mean ion dose rate of 26.6 A kg^{-1} in the plate capacitor thus corresponds to a dose equivalent rate of 864 μSv s^{-1} resp. 3.11 Sv h^{-1}.

For comparison: in the measurements for type approval of the x-ray apparatus, a dose equivalent rate of over 10 Sv h^{-1} was measured in the radiation cone of the x-ray tube.

Solid-state physics

Properties of crystals
X-ray structural analysis

Laue diagrams: investigating the lattice structure of monocrystals

Objects of the experiment

■ Evaluating the *Laue* diagrams of an NaCl and an LiF monocrystal.

■ Investigating the symmetry and lattice structure of both crystals.
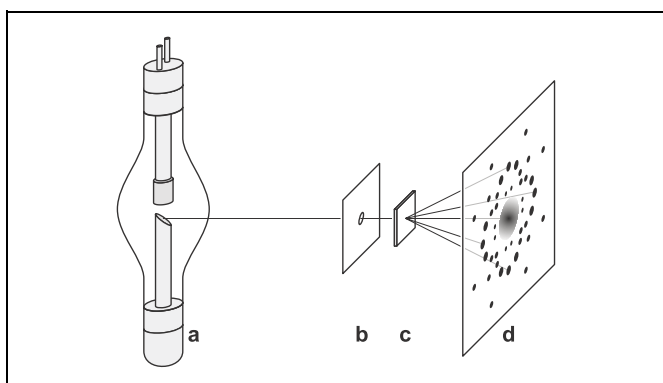
Principles

Fig. 1 Scheme of the setup for taking a *Laue* diagram of a mono-crystal
- **a** X-ray tube
- **b** Collimator
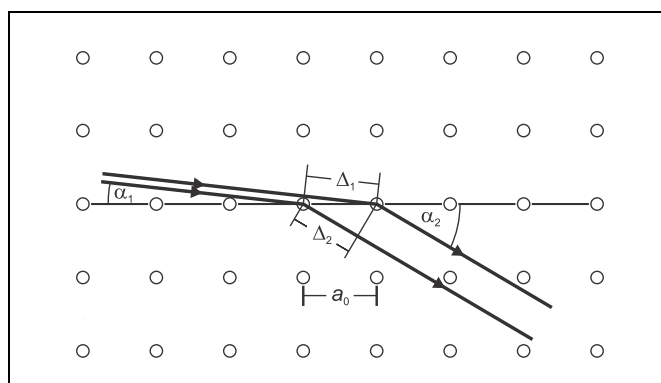- **c** Crystal
- **d** X-ray film

Fig. 2 Two-dimensional representation for calculating the difference of path $\Delta = \Delta_1 - \Delta_2$ between two neighbouring X-rays which are diffracted at a row of points in a cubic crystal.

In 1912, *Max von Laue* proposed to provide evidence for the supposed wave character of X-rays by diffraction at crystals. *Friedrich* and *Knipping* took up his proposal and exposed a crystal to a collimated ray from an X-ray tube. On a photographic plate behind the crystal they observed – as expected – discrete reflections. For the first time they also confirmed the spatial lattice structure of crystalline substances with this experiment.

Laue condition:

In his interpretation of these findings, *von Laue* considered the crystal to be a lattice built up of three groups of one-dimensional equidistant rows of points. When an X-ray is diffracted at a row of points,

$$\Delta = \Delta_1 - \Delta_2 = a_0 \cdot \cos \alpha_1 - a_0 \cdot \cos \alpha_2 \qquad (I)$$

a_0: distance between the points
α_1: angle between the incoming X-ray and the row of points
α_2: angle between the diffracted X-ray and the row of points

is the difference of path of partial rays scattered at two neighbouring points (lattice elements, see Fig. 2). There is construc-tive interference between the partial rays if Δ in an integer multiple of the wavelength λ. This condition has to be fulfilled in all three spatial directions.

In a cubic crystal, the rows of points associated with the three spatial directions are all perpendicular to each other the dis-tance a_0 between the points always being the same. The *Laue* condition for constructive interference therefore reads:

$$a_0 \cdot \cos \alpha_1 - a_0 \cdot \cos \alpha_2 = h \cdot \lambda$$
$$a_0 \cdot \cos \beta_1 - a_0 \cdot \cos \beta_2 = k \cdot \lambda$$
$$a_0 \cdot \cos \gamma_1 - a_0 \cdot \cos \gamma_2 = l \cdot \lambda \qquad (II)$$

with integer values of h, k, l

Here α_1, β_1 and γ_1 are the angles between the incoming ray and the rows of points whereas α_2, β_2 and γ_2 are the angles between the diffracted ray and the rows of points. The quanti-ties h, k, l are called *Laue* or extended *Miller* indices. As they are small integer numbers, the *Laue* condition cannot be fulfilled for arbitrary wavelengths λ, but only for particular ("appropriate") ones.

Apparatus

1 X-ray apparatus	554 811
or	
1 X-ray apparatus	554 812
1 X-ray film holder	554 838
1 filmpack 2 (X-ray film)	554 892
1 LiF crystal for Laue diagrams	554 87
1 NaCl crystal for Laue diagrams	554 88
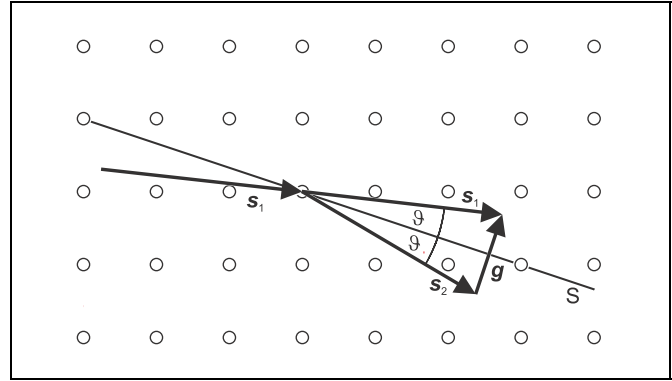
Fig. 3   Geometric connection between the unit vectors s_1 and s_2 and the vector $\boldsymbol{g} = \lambda \boldsymbol{G}$.

The unit vectors

$$\boldsymbol{s}_1 = \left(\cos \alpha_1, \cos \beta_1, \cos \gamma_1 \right)$$

and

$$\boldsymbol{s}_2 = \left(\cos \alpha_2, \cos \beta_2, \cos \gamma_2 \right) \tag{III}$$

are frequently introduced. They point in the direction of the incoming X-ray and the outgoing X-ray, respectively. The *Laue* condition (II) then takes the form

$$\boldsymbol{s}_1 - \boldsymbol{s}_2 = \lambda \cdot \boldsymbol{G} \text{ with } \boldsymbol{G} = (h, k, l) \cdot \frac{1}{a_0} \tag{IV}$$

$\boldsymbol{G}$ is called the vector of the reciprocal lattice. The *Laue* condition is fulfilled if h, k and l are integers.

Bragg condition:

As $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are unit vectors, they have equal magnitudes. Therefore the vector $\boldsymbol{G}$ is perpendicular to the bisectrix S

between the incoming and the diffracted X-ray (see Fig. 3). From this

$$\lambda \cdot | \boldsymbol{G} | = | \boldsymbol{s}_1 - \boldsymbol{s}_2 | = 2 \cdot \sin \vartheta$$

follows and after inserting the magnitude of $\boldsymbol{G}$

$$\lambda = 2 \cdot \sin \vartheta \cdot \frac{a_0}{\sqrt{h^2 + k^2 + l^2}} \tag{V}$$

Eq. (V) is identical with *Bragg*'s law if the spacing of the lattice planes is

$$d = \frac{a_0}{\sqrt{h^2 + k^2 + l^2}} \tag{VI}$$

From *Bragg*'s point of view the crystal lattice thus consists of a set of lattice planes that have the spacing d (see Fig. 4 and experiment P6.3.3.1). These lattice planes are parallel to the bisectrix S and perpendicular to the vector $\boldsymbol{G}$ of the reciprocal lattice.

The conditional equation of the set of lattice planes in the co-ordinate system spanned by the crystal axes reads

$$x \cdot h + y \cdot k + z \cdot l = m \cdot a_0 \tag{VII}$$
m: running number in a set of lattice planes

h^{-1}, k^{-1} and l^{-1} are the axis sections of the first lattice plane ($m = 1$) measured in units of the lattice constant (see Fig. 5). As the indices h, k, l represent the set of lattice planes uniquely, the set is assigned the symbol (h k l).

Fig. 4   Two-dimensional representation of *Bragg* reflection of X-rays at a set of lattice planes in a cubic crystal. The lattice planes are parallel to the bisectrix S between the incoming and the diffracted X-ray.

Fig. 5 Two-dimensional representation of the set of lattice planes (1 3 0) in a cubic crystal.

Crystals with NaCl structure:

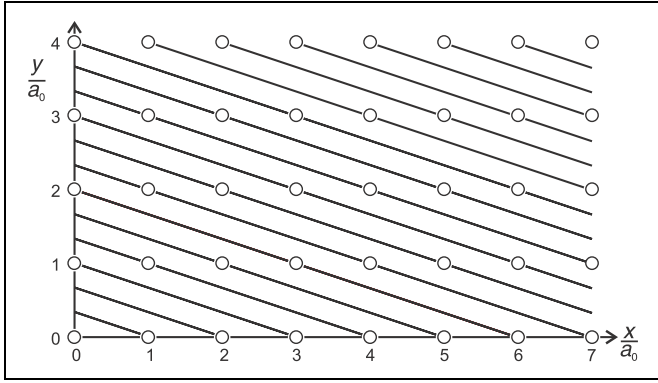In the case of crystals with NaCl structure, the condition for constructive interference turns out to be more complicated than in simple cubic crystals because alkali atoms (e.g. Na) and halogenide atoms (e.g. Cl) take turns in a cubic lattice. The spatial lattice is no longer built up of rows of points with the distance a_0, but it is a series of cubic unit cells with an edge length a_0 (see Fig. 6). Every unit cell contains four alkali atoms with the co-ordinates

$$\boldsymbol{r}_1 = (0,0,0),\ \boldsymbol{r}_2 = \left(\frac{a_0}{2}, \frac{a_0}{2}, 0\right), \boldsymbol{r}_3 = \left(\frac{a_0}{2}, 0, \frac{a_0}{2}\right), \boldsymbol{r}_4 = \left(0, \frac{a_0}{2}, \frac{a_0}{2}\right)$$

and four halogenide atoms with the co-ordinates

$$\boldsymbol{r}_5 = \left(\frac{a_0}{2}, 0, 0\right), \boldsymbol{r}_6 = \left(0, \frac{a_0}{2}, 0\right), \boldsymbol{r}_7 = \left(0, 0, \frac{a_0}{2}\right), \boldsymbol{r}_8 = \left(\frac{a_0}{2}, \frac{a_0}{2}, \frac{a_0}{2}\right)$$

At each atom of the unit cell the incoming X-ray is scattered, whereby the amplitudes of the scattered partial waves depend on the atomic number of the atom. The differences of path Δ_i of the partial waves can be calculated from the co-ordinates $\boldsymbol{r}_i$ of the atoms:

$$\Delta_i = \left(\boldsymbol{s}_1 - \boldsymbol{s}_2\right) \cdot \boldsymbol{r}_i \qquad\qquad (VIII).$$

The partial waves scattered at the alkali atoms A and the halogenide atoms H interfere to form a common wave that is

"scattered at the unit cell". The amplitude of this wave has the form

$$A = A_A + A_H \qquad\qquad (IX)$$

with

$$A_A = f_A \left(\cos\left(\frac{2\pi}{\lambda}\Delta_1\right) + \cos\left(\frac{2\pi}{\lambda}\Delta_2\right) + \cos\left(\frac{2\pi}{\lambda}\Delta_3\right) + \cos\left(\frac{2\pi}{\lambda}\Delta_4\right)\right)$$

and

$$A_H = f_H \cdot \left(\cos\frac{2\pi}{\lambda}\Delta_5 + \cos\frac{2\pi}{\lambda}\Delta_6 + \cos\frac{2\pi}{\lambda}\Delta_7 + \cos\frac{2\pi}{\lambda}\Delta_8\right)$$

All waves that start from the unit cells interfere constructively if the *Laue* condition (IV) is fulfilled. By inserting (IV) and (VIII) in (IX) one obtains

$$A_A = f_A \cdot (1 + \cos((h + k) \cdot \pi) + \cos((h + l) \cdot \pi) + \cos((k + l) \cdot \pi))$$

and

$$A_H = f_H \cdot (\cos(h \cdot \pi) + \cos(k \cdot \pi) + \cos(l \cdot \pi) + \cos((h+k+l) \cdot \pi)).$$

A short calculation shows that

$$A = \begin{cases} 4 \cdot f_A + 4 \cdot f_H, & \text{if } h, k \text{ and } l \text{ even} \\ 4 \cdot f_A - 4 \cdot f_H, & \text{if } h, k \text{ and } l \text{ odd} \\ 0, & \text{if } h, k \text{ and } l \text{ mixed} \end{cases} \qquad (X)$$

The amplitudes A of the waves starting from the unit cells thus only are different form zero if all indices h, k, l are even or if they are all odd.

Evaluating a *Laue* diagram:

The object of the evaluation of a *Laue* diagram is to assign the set of lattice planes that causes the scattering to one of the reflections observed on the X-ray film. For this the co-ordinate system is chosen so that its origin O corresponds to the space point of the incoming X-ray on the X-ray film. The X-ray film is perpendicular to the ray, i.e., it lies in the x-y-plane (see Fig. 7). The orientation of the z-axis is opposite to the propagation direction of the X-ray. The X-ray penetrates the flat crystal at the point K; its undiffracted part impinges on the X-ray film at the point O. The part of the X-ray which is scattered at K and which fulfils the *Laue* condition (II) leaves the crystal with an
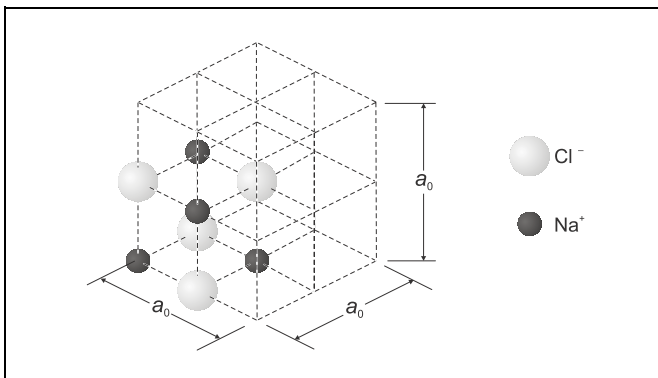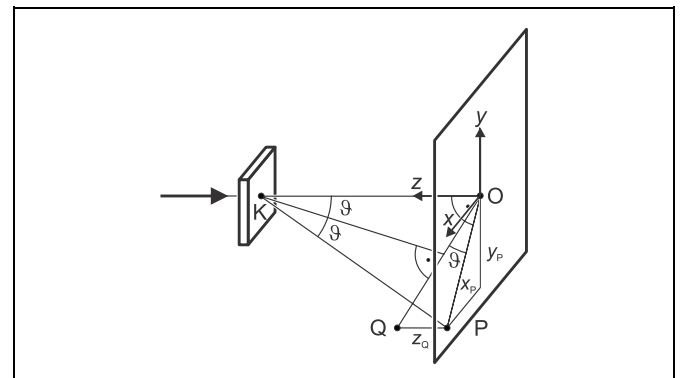
Fig. 6 Unit cell of an NaCl crystal

Fig. 7 Geometrical description of an X-ray that is diffracted at a point K of the crystal and that penetrates the film plane in the point P

angle 2ϑ relative to the direction of the primary ray and impinges on the X-ray film at the point P = $(x_P, y_P, 0)$. Therefore:

$$\tan 2\vartheta = \frac{\sqrt{x_P^2 + y_P^2}}{L} \tag{XI}$$

L: distance between crystal and X-ray film

The direction of the set of lattice planes (h k l), which leads to the reflection, is given by the bisectrix of the angle 2ϑ (see Fig. 3). The angle between the perpendicular on the bisectrix which passes O and the straight line OP is ϑ. This perpendicular intersects a parallel to the z-axis through P in the point Q. The vector **OQ** has the co-ordinates (x_Q, y_Q, z_Q) with

$$\tan \vartheta = \frac{z_Q}{\sqrt{x_Q^2 + y_Q^2}} \tag{XII}$$

and is parallel to the vector **G** of the reciprocal lattice. Because of $x_P = x_Q$, $y_P = y_Q$ and Eq. (XI),

$$z_Q = \sqrt{x_Q^2 + y_Q^2 + L^2} - L \tag{XIII}.$$

The crystals used in this experiment are cut parallel to the (1 0 0) plane. Their crystal axes thus coincide with the laboratory co-ordinate system. From the fact that the vectors **G** and **OQ** are parallel, it therefore follows that

$$h : k : l = x_Q : y_Q : z_Q \tag{XIV}$$

The indices h, k, l which are looked for therefore are the smallest unmixed triple of integers which fulfil Eq. (XIV). They allow all parameters of the diffraction that leads to the reflection to be calculated: the spacing of lattice planes d is obtained from Eq. (VI), the wavelength λ from Eq. (V) and the *Bragg* angle ϑ is, according to Eqs. (XII) and (XIV),

$$\vartheta = \arctan\left(\frac{l}{\sqrt{h^2 + k^2}}\right) \tag{XV}.$$

Setup and carrying out the experiment

The experimental setup is illustrated in Fig. 8.

– If necessary, remove the goniometer or the plate capacitor X-ray.

Remark:

NaCl and LiF crystals are hygroscopic and brittle:
keep the crystals in a place as dry as possible, avoid mechanical stress to the crystals, and only touch the front side of a crystal.

a) *Laue* diagram at NaCl:

– Carefully attach the NaCl crystal for Laue diagrams **(b)** to the pinhole diaphragm **(a)** (from the scope of supply of the X-ray film holder) with transparent adhesive tape.
– Attach the collimator, and cautiously turn it so that the outside edges of the crystal are aligned as horizontally (or vertically) as possible.
– Clamp the X-ray film **(c)** at the film holder so that it is centred, and see to it that the entire surface of the film is planar.
– Clamp the film holder onto the experiment rail, and mount the experiment rail in the experiment chamber of the X-ray apparatus.
– Make a 15 mm long spacer from paper board and shift the film holder so that the distance between the monocrystal and the film is 15 mm (by varying the distance between the crystal and the film the area covered in the diagram is changed).
– Set the tube high voltage U = 35 kV, the emission current I = 1.0 mA and $\Delta\beta$ = 0.0°.
– Select the measuring time Δt = 1800 s, and start the exposure timer with the key SCAN.

   If the exposure time is longer, the reflections near the centre are blurred by the unscattered X-rays; however structures which are farer away from the centre become discernable.

– When the exposure time is over, take the film holder with the experiment rail out of the experiment chamber.
– Remove the X-ray film from the holder, and develop it according to the instruction sheet for the X-ray film.

b) *Laue* diagram at LiF:

– Exchange the NaCl crystal with the LiF crystal, and align the LiF crystal.
– Clamp a new X-ray film in the film holder, and mount the experiment rail with the film holder once more.
– Shift the film holder so that the distance L between the monocrystal and the film is 11 mm.
– Select the measuring time Δt = 1200 s, and start the exposure timer with the key SCAN.
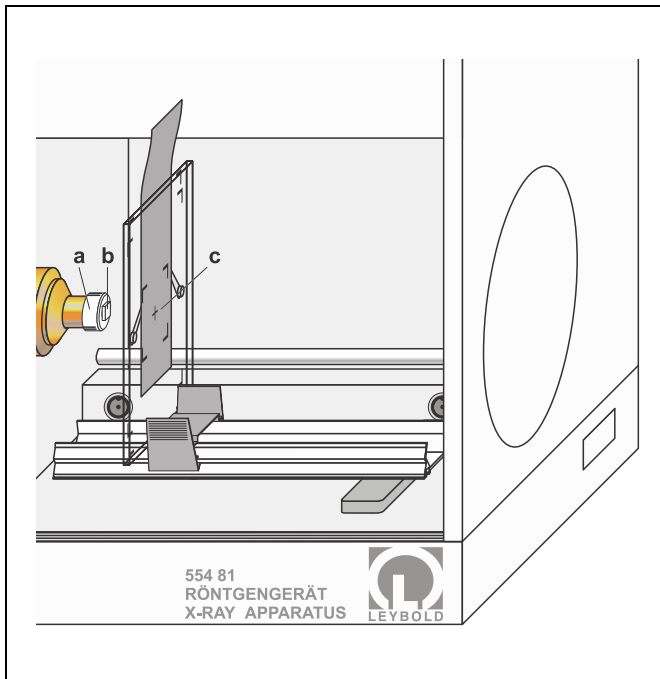– When the exposure time is over, take the X-ray film from the film holder and develop it.

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Fig. 8   Experimental setup for taking a *Laue* diagram at crystals

Measuring example

a) *Laue* diagram at NaCl:
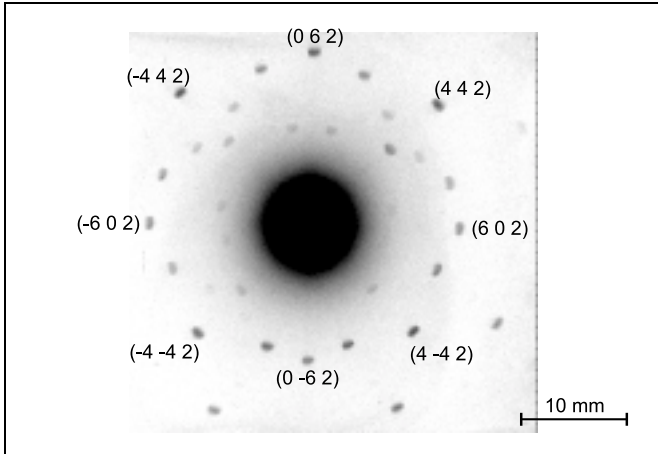
Fig. 9   *Laue* diagram at NaCl,
         $U = 35$ kV, $I = 1$ mA, $L = 15$ mm, $\Delta t = 1800$ s
         (for identifying the reflections refer to Table 1)

b) *Laue* diagram at LiF:

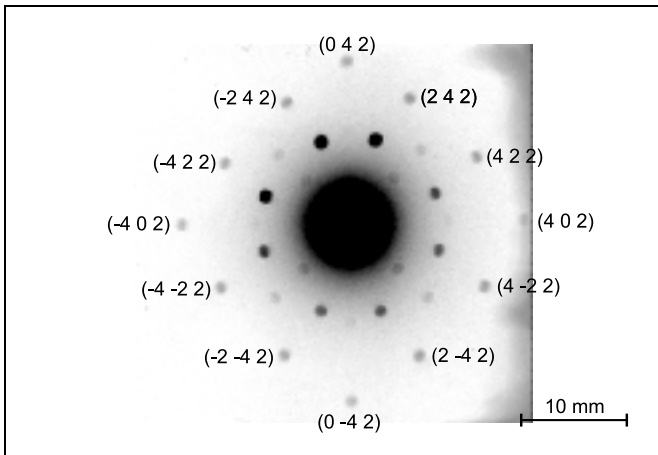Fig. 10   *Laue* diagram at LiF,
         $U = 35$ kV, $I = 1$ mA, $L = 11$ mm, $\Delta t = 1200$ s
         (for identifying the reflections refer to Table 3)

Evaluation

– Lay a piece of millimetre-square graph paper on the X-ray film, read the x_Q- and y_Q-co-ordinates of the reflections, and calculate the z_Q-co-ordinate according to Eq. (XIII).

– Identify the indices h, k and l according to Eq. (XIV).

– Calculate the spacing of the lattice planes d according to Eq. (VI), the Bragg angle ϑ according to Eq. (XV) and the wavelength λ according to Eq. (V).

– Now apply Eqs. (XI) and (XIV) to calculate the co-ordinates x_P and y_P or x_Q and y_Q, respectively, and compare them with the measured values.

a) *Laue* diagram at NaCl:

Tab. 1:   Coordinates and extended *Miller* indices of the reflections in the *Laue* diagram of NaCl (*: calculated)

	$\dfrac{x_Q}{mm}$	$\dfrac{y_Q}{mm}$	$\dfrac{z_Q}{mm}$ *	h	k	l	$\dfrac{x}{mm}$ *	$\dfrac{y}{mm}$ *
1	17.2	8.4	9,3	4	2	2	15.0	7.5
	−7.8	−15.2	7,7	−2	−4	2	−7.5	−15.0
	7.8	−15.2	7,7	2	−4	2	7.5	−15.0
	15.8	−8.0	8,2	4	−2	2	15.0	−7.5
2	12.6	−0.4	4,6	6	0	2	11.2	0.0
	0.2	14.5	5,9	0	6	2	0.0	11.2
	−13.2	−0.1	5,0	−6	0	2	−11.2	0.0
	0.0	−11.2	3,7	0	−6	2	0.0	−11.2
3	11.5	3.6	4,2	6	2	2	10.0	3.3
	4.2	12.4	4,9	2	6	2	3.3	10.0
	−4.3	13.0	5,3	−2	6	2	−3.3	10.0
	−12.2	4.0	4,7	−6	2	2	−10.0	3.3
	−11.2	−3.9	4,1	−6	−2	2	−10.0	−3.3
	−3.3	−10.2	3,4	−2	−6	2	−3.3	−10.0
	3.2	−10.0	3,3	2	−6	2	3.3	−10.0
	10.5	−3.9	3,7	6	−2	2	10.0	−3.3
4	9.0	9.2	4,8	4	4	2	8.6	8.6
	−11.0	11.0	6,6	−4	4	2	−8.6	8.6
	−9.0	−9.2	4,8	−4	−4	2	−8.6	−8.6
	9.0	−9.0	4,7	4	−4	2	8.6	−8.6
5	9.0	5.8	3,4	6	4	2	7.5	5.0
	6.3	9.2	3,7	4	6	2	5.0	7.5
	−6.5	9.8	4,1	−4	6	2	−5.0	7.5
	−9.5	6.2	3,8	−6	4	2	−7.5	5.0
	−8.2	−5.5	3,0	−6	−4	2	−7.5	−5.0
	−5.2	−8.0	2,8	−4	−6	2	−5.0	−7.5
6	6.4	6.2	2,4	3	3	1	5.3	5.3
	−6.8	6.8	2,8	−3	3	1	−5.3	5.3
	−5.8	−5.8	2,1	−3	−3	1	−5.3	−5.3
	5.3	−5.3	1,8	3	−3	1	5.3	−5.3
7	6.8	1.3	1,5	5	1	1	6.0	1.2
	1.8	7.8	2,0	1	5	1	1.2	6.0
	−1.2	8.0	2,0	−1	5	1	−1.2	6.0
	−7.2	1.2	1,7	−5	1	1	−6.0	1.2
	−7.0	−1.5	1,6	−5	−1	1	−6.0	−1.2

Tab. 2: Spacing of lattice planes d, *Bragg* angle ϑ and wavelength λ associated with the sets of lattice planes of NaCl, $a_0 = 564.02$ pm [1]

h	k	l	$\dfrac{d}{pm}$	ϑ	$\dfrac{\lambda}{pm}$
4	2	2	115.1	24.1°	94.0
6	0	2	89.2	18.4°	56.3
6	2	2	85.0	17.5°	51.1
4	4	2	94.0	19.5°	62.8
6	4	2	75.4	15.5°	40.3
3	3	1	129.4	13.3°	59.5
5	1	1	108.5	11.1°	41.8

b) *Laue* **diagram at LiF:**

Tab. 3: Co-ordinates and extended *Miller* indices of the reflections in the *Laue* diagram of LiF (*: calculated)

	$\dfrac{x_Q}{mm}$	$\dfrac{y_Q}{mm}$	$\dfrac{z_Q}{mm}$ *	h	k	l	$\dfrac{x}{mm}$ *	$\dfrac{y}{mm}$ *
1	14.2	−0.1	7.0	4	0	2	14.7	0.0
	0.2	13.3	6.3	0	4	2	00	14.7
	−14.2	0.0	7.0	−4	0	2	−14.7	0.0
	0.1	−15.2	7.8	0	−4	2	0.0	−14.7
2	10.5	5.0	5.0	4	2	2	11.0	5.5
	5.5	10.0	4.9	2	4	2	5.5	11.0
	−5.8	10.3	5.2	−2	4	2	−5.5	11.0
	−10.5	5.2	5.1	−4	2	2	−11.0	5.5
	−11.0	−5.8	5.6	−4	−2	2	−11.0	−5.5
	−5.6	−11.5	5.9	−2	−4	2	−5.5	−11.0
	5.8	−11.2	5.7	2	−4	2	5.5	−11.0
	11.0	−5.5	5.5	4	−2	2	11.0	−5.5
3	8.0	0.0	2.6	6	0	2	8.3	0.0
	−0.5	7.2	2.2	0	6	2	0.0	8.3
	−9.1	−0.3	3.3	−6	0	2	−8.3	0.0
	0.5	−8.0	2.6	0	−6	2	0.0	−8.3
4	7.2	2.0	2.3	6	2	2	7.3	2.4
	2.2	6.5	2.0	2	6	2	2.4	7.3
	−2.0	7.4	2.4	−2	6	2	−2.4	7.3
	−7.0	2.2	2.2	−6	2	2	−7.3	2.4
	−7.2	−2.3	2.4	6	−2	2	−7.3	−2.4
	−2.2	−7.8	2.7	2	−6	2	−2.4	−7.3
	2.7	−7.6	2.6	2	−6	2	2.4	−7.3
	7.2	−2.8	2.4	6	−2	2	7.3	−2.4
5	6.0	5.8	2.8	4	4	2	6.3	6.3
	−6.0	6.0	2.9	−4	4	2	−6.3	6.3
	−6.2	−6.3	3.1	−4	−4	2	−6.3	−6.3
	6.5	−6.5	3.3	4	−4	2	6.3	−6.3
6	4.0	3.5	1.2	3	3	1	3.9	3.9
	−3.5	3.6	1.1	−3	3	1	−3.9	3.9
	−3.8	−4.0	1.3	−3	−3	1	−3.9	−3.9
	4.2	−4.0	1.4	3	−3	1	3.9	−3.9

Tab. 4: Spacing of lattice planes d, *Bragg* angle ϑ and wavelength λ associated with the sets of lattice planes of LiF, a_0 = 402.80 pm [1]

h	k	l	$\dfrac{d}{pm}$	ϑ	$\dfrac{\lambda}{pm}$
4	0	2	90.1	26.6°	80.6
4	2	2	82.2	24.1°	67.1
6	0	2	63.7	18.4°	40.3
6	2	2	60.7	17.5°	36.5
4	4	2	67.1	19.5°	44.8
3	3	1	92.4	13.3°	42.5

Results

A *Laue* diagram is a diffraction photograph of a monocrystal taken with a continuous ("white") spectrum of X-rays. From the continuum of the X-rays only those wavelengths (cf. Tables 2 and 4) contribute to the diffraction pattern taken on a plane film which fulfil the *Bragg* condition for a particular set of lattice planes.

The symmetry of the *Laue* diagrams is in accordance with the cubic structure of the NaCl and the LiF crystal.

Literature

[1]Handbook of Chemistry and Physics, 52nd Edition (1971–72), The Chemical Rubber Company, Cleveland, Ohio, USA.

Addendum 1:

The larger film 554 896 enables the recording of larger images, which provide more resolution, but also require a bit more exposure time.

NaCl, 6000 s, d= 25 mm, 35 kV, 1 mA

LiF, 6000 s, d= 25 mm, 35 kV, 1 mA
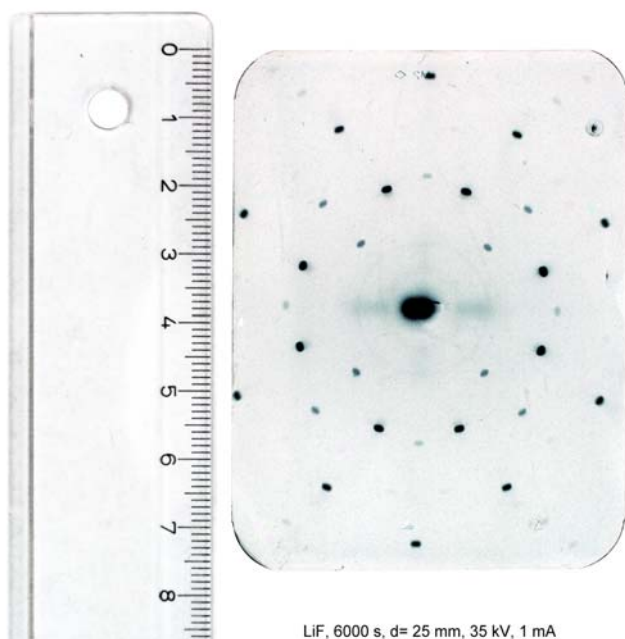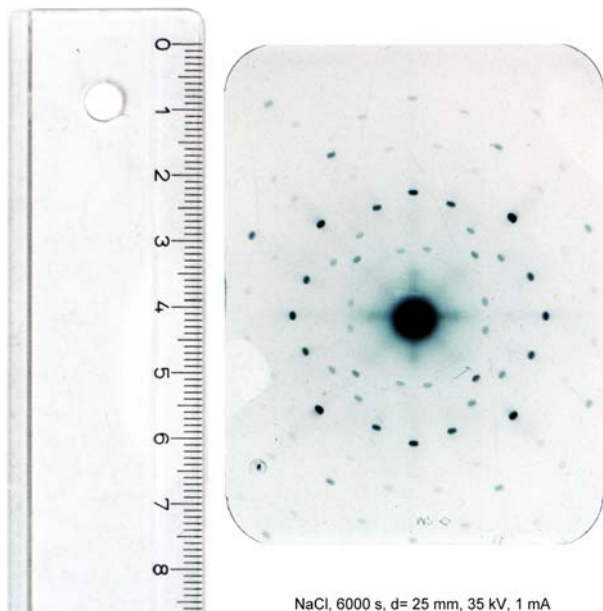
Hint: To reduce the black area in the middle, caused by the direct beam, glue a 3x3 mm piece of the lead foil from an already opened film sheet in front of the film during exposure.

Addendum 2:

The crystals 554 87 and 554 88 are usually delivered on a glass plate 25 x 25 x 1 mm. This plate is glass, not the crystal.