

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

Objects of the experiment

- Investigating the fine structure of the characteristic x-radiation of copper by means of Bragg reflection at an NaCl monocrystal in the third diffraction order.
- Investigating the fine structure of the characteristic x-radiation of copper by means of Bragg reflection at an KBr monocrystal in the fourth diffraction order.
- 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} line of the x-radiation of copper prove to be a line doublet. The doublet can be resolved by means of Bragg reflection at an NaCl or KBr monocrystal when measured in a higher diffraction order.

In contrast to the molybdenum spectrum there is no K_{γ} line in copper, as the N shell is not populated in the elements of this row in the periodic table.

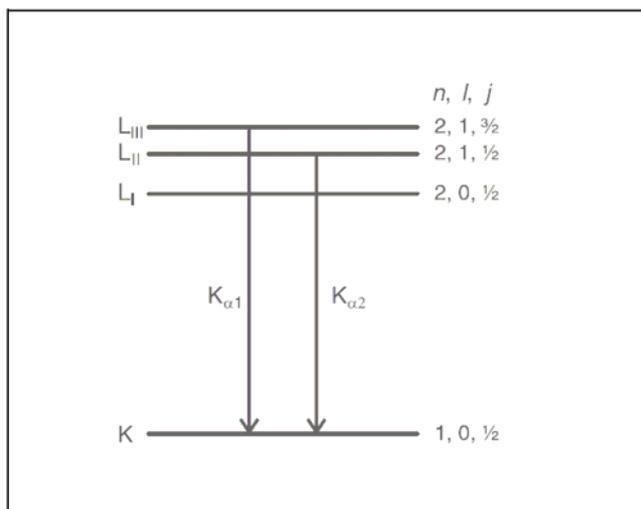
Table 1: Transition energies E and wavelengths λ of the characteristic K_{α} , K_{β} lines of copper (weighted mean values according to [1])

	$\frac{E}{\text{keV}}$	$\frac{\lambda}{\text{pm}}$
K_{α}	8,04	154,17
K_{β}	8,91	139,2

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

$$\Delta l = \pm 1, \Delta j = 0, \pm 1 \quad (I)$$

Fig. 1 Diagram of fine structure of the characteristic line K_{α}



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 $K_{\alpha 1}$ and $K_{\alpha 2}$ (see Fig. 1). Table 2 shows the values generally found in the literature for copper. According to these, the wavelength interval within the K_{α} doublet is $\Delta\lambda = 0.38$ pm.

Table 2: Wavelengths λ (calculated from literature specifications [1] for transition energies)

Line	$\frac{\lambda}{\text{pm}}$
$K_{\alpha 1}$	154.05
$K_{\alpha 2}$	154.43

Apparatus

1 X-ray apparatus	554 800
1 X-ray tube Cu	554 862
1 Goniometer	554 831
1 End-window counter for α , β , γ and x-ray radiation	559 01
suggested:	
1 KBr crystal	554 791
additionally required:	
1 PC with Windows 98/2000/XP/Vista	

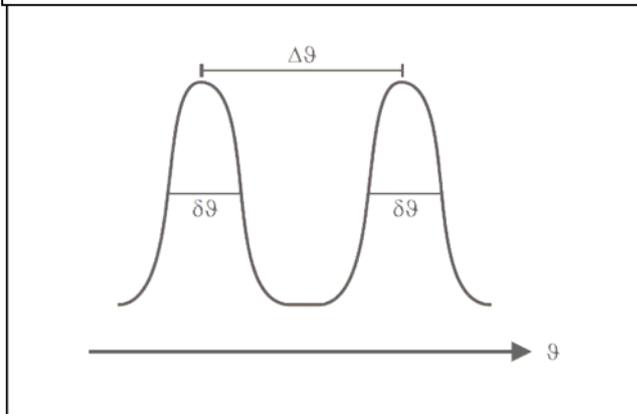


Fig. 2 Definition of the angular width $\delta\theta$ and the angular spacing $\Delta\theta$ of two intensity maxima.

The object of the experiment is to resolve this fine structure by means of Bragg reflection at an NaCl or a KBr 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:

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

n : diffraction order,

$d = 282.01$ pm: lattice plane spacing of NaCl

$d = 329.9$ pm: lattice plane spacing of KBr

Safety notes

The built-in protection and screening measures reduce the local dose rate outside of the X-ray apparatus to less than $1 \mu\text{Sv/h}$, a value which is on the order of magnitude of the natural background radiation. The high dose rate which is produced inside the device means that the operator must use special care when operating the X-ray apparatus.

The X-ray apparatus is intended for operation in dry rooms which are suitable for electrical operating equipment or installations, height 0 - 2000 m above sea level. When used as intended the X-ray apparatus is safe to operate.

- Keep the X-ray apparatus secure from access by unauthorized persons.
- Before putting the device into operation for the first time, check the rating plate (on rear of housing) to make sure that the mains voltage value given there agrees with the mains voltage at your location
- Inspect the housing and the control and display elements of the X-ray apparatus, particularly the lead glass panes and sliding doors as well as the lead glass tube surrounding the X-ray tube, carefully for damage before putting the device into operation.
- Before putting into operation, make sure that the Anode cable is securely plugged into the heatsink of the anode.

If any faults or defects are noted, do not put the X-ray apparatus into operation. Notify your local LD Didactic GmbH representative immediately.

- Do not put live animals inside the X-ray apparatus.

Do not allow the anode of the X-ray tube to overheat:

- When putting the X-ray apparatus into operation, check to make sure that the ventilator in the tube chamber is turning.

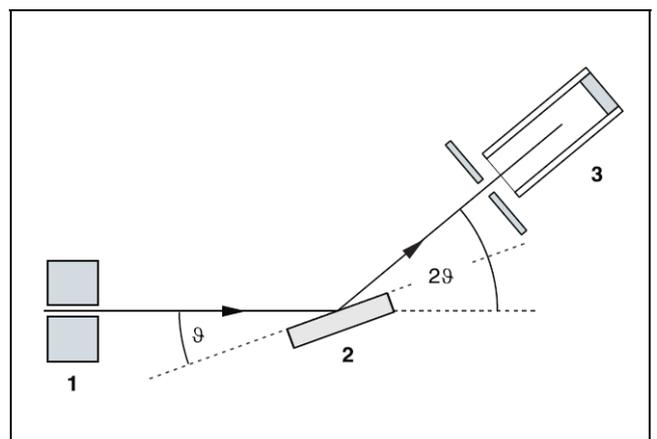


Fig. 3 Diagram showing the diffraction of x-rays at a monocrystal

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

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

which increases with the diffraction order. It is important to distinguish between the angular spacing $\Delta\theta$ and the angular width $\delta\theta$ 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 highest possible diffraction orders, for NaCl $n = 3$, for KBr $n = 4$. Observation at higher orders is not possible, as the reflection would be beyond 180° .

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.

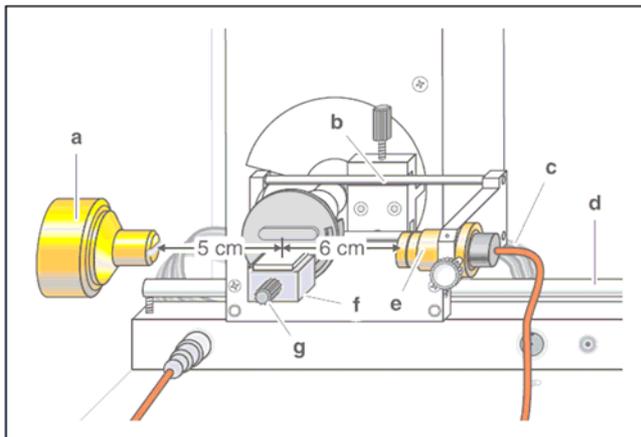


Fig. 4 Setting up the experiment in Bragg configuration

- 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 and KBr 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 USB output and the USB interface on your PC using the cable supplied with the x-ray apparatus.
- If necessary, install the software "X-ray Apparatus" under Windows (see Instruction Sheet for x-ray apparatus) and select the desired language.

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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 $\Delta\beta = 0.1^\circ$.
- Press the COUPLED key for 2 θ coupling of target and sensor.

Measurement with NaCl crystal

a) First order of diffraction:

- To record the first and second diffraction order, set the lower limit of the target angle to 2.5° and the upper limit to 40.0° , and set the measuring time per angular step to $\Delta t = 1$ 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) Third order of diffraction:

- To record the third diffraction order, set the lower limit of the target angle to 45° and the upper limit to 60°
- Set the measuring time per angular step to $\Delta t = 4$ s.

Note: Due to the lower counting rate to be expected, you need to set a modestly long measuring time to obtain a satisfactory statistical accuracy. In this setting, the total measuring time is 10 minutes.

- 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.

Measurement with KBr crystal

a) First order of diffraction:

- To record the first to third diffraction order, set the lower limit of the target angle to 2.5° and the upper limit to 50° , and set the measuring time per angular step to $\Delta t = 1$ 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 KBr 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) Fourth order of diffraction:

- To record the fourth diffraction order, set the lower limit of the target angle to 65° and the upper limit to 75° , and
- Set the measuring time per angular step to $\Delta t = 10$ 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 16 minutes.

- 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 KBr 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

a) First order of diffraction:

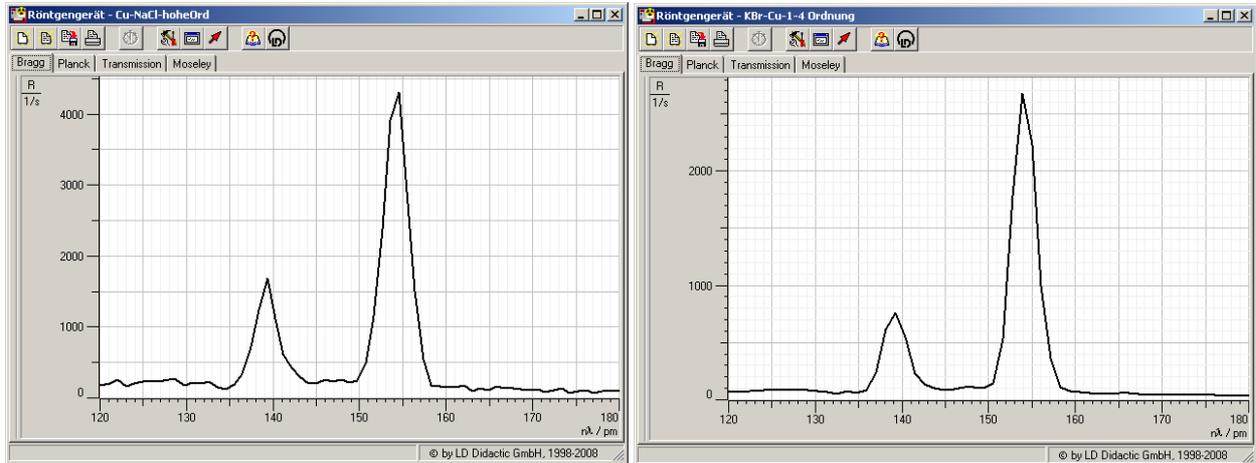


Fig. 5 Diffraction spectrum of x-rays in Bragg reflection in the first order at an NaCl (left) and KBr (right) monocrystal

b) High order of diffraction:

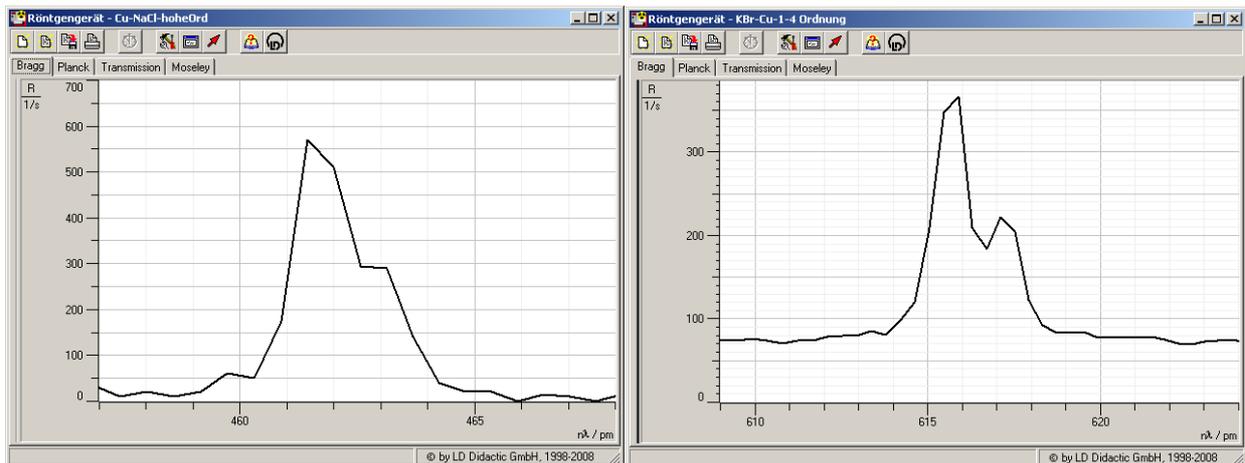


Fig. 6 Diffraction spectrum of x-rays in Bragg reflection in the third order at an NaCl monocrystal (left) and fourth order at an KBr monocrystal (right)

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)

	Measurement result NaCl	Measurement result KBr	Literature value
Line	$\frac{\lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$
K_{α}	139.21	139.12	139.2
K_{β}	154.5	154.17	154.3

b) Highest order of diffraction:

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

	Measurement result		Literature value
NaCl	$\frac{3 \cdot \lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$
$K_{\alpha 1}$	461.7	153.9	154.05
$K_{\alpha 2}$	463.2	154.4	154.43
KBr	$\frac{4 \cdot \lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$	$\frac{\lambda}{\text{pm}}$
$K_{\alpha 1}$	615.69	153.92	154.05
$K_{\alpha 2}$	617.32	154.33	154.43

Splitting of doublet K_{α} measured with NaCl

$$\Delta\lambda = 0.5 \text{ pm} \quad \text{Literature value: } \Delta\lambda = 0.38 \text{ pm}$$

Splitting of doublet K_{α} measured with KBr

$$\Delta\lambda = 0.41 \text{ pm} \quad \text{Literature value: } \Delta\lambda = 0.38 \text{ pm}$$

Results

The characteristic K_{α} line we observe in the first diffraction order splits into a doublet. We can observe this split in the highest possible diffraction order.

The fine structure of the K_{α} doublet is a consequence of the fine structure of the L-shell.

The different crystals used for measuring the splitting show a significant difference in resolution. The splitting is visible, but hard to measure exactly in the NaCl third order spectrum, but easily evaluate able in fourth order KBr. The fourth order NaCl spectrum would be better resolved than fourth order KBr, but it simply doesn't exist, as the Bragg equation can not be fulfilled.

Additional information

Strictly speaking, the K_{β} line also shows a fine structure due to the fine structure of shell M. However, this split is so slight that we cannot observe it with the means at hand.

Literature

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