K and L absorption edges of X-rays / Moseley's law and the Rydberg constant

Physics | Modern Physics | Production & use of X-rays

Difficulty level	Group size	Preparation time	Execution time
hard	2	45+ minutes	45+ minutes

This content can also be found online at:

http://localhost:1337/c/5f6089387e9d5b0003e1e770

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General information

Application

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Setup

Most applications of X rays are based on their ability to pass through matter. Since this ability is dependent on the density of the matter, imaging of the interior of objects and even peaple becomes possible. This has wide usage in fields such as medicine or security.

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Other information (1/2)

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Prior knowledge

The prior knowledge for this experiment is found in the Theory section.

Main principle

Samples of various thicknesses are irradiated with the polychromatic X-rays of a copper X-ray tube. The radiation that passes through the samples is analysed with the aid of a monocrystal. The Rydberg constant is calculated based on the glancing angles of the absorption edges. This experiment is included in the “XRS 4.0 X-ray structural analysis” upgrade set.

Other information (2/2)

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Learning objective

The goal of this experiment is to get to investigate the X-radation profil of copper while using K and L edge absorption.

Tasks

1. Analyse the copper X-radiation with the aid of a LiF monocrystal and as a function of the Bragg angle without and with several K edge absorption samples as absorbers. Determine the K absorption edges of different absorbers based on the spectra.
2. Calculate the Rydberg constant and the screening constant based on the energy values of the K absorption edges.
3. Proceed as described for task 1, but this time with various samples for L edge absorption.
4. Calculate the Rydberg constant based on the energy values of the L absorption edges.

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Safety Instructions

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When handling chemicals, you should wear suitable protective gloves, safety goggles, and suitable clothing. Please refer to the appendix for detailed safety instructions.

Theory (1/4)

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When X-rays interact with matter, they lose energy due to Compton scattering, pair production, and photoelectric effects. The respective strength of these three effects depends on the energy of the radiation. In the range of energy that is available during this experiment, the photoelectric effect plays the most important role. Figure 1 shows the schematic course of the transmission T as a function of the radiation energy E. The cause of the irregularity that is known as “edge absorption” is the photoelectric effect.

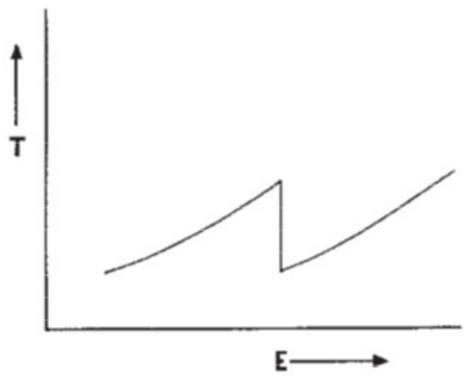

Fig. 1: Schematic course of the transmission T as a function of the energy E in the area of an absorption edge

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Theory (2/4)

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The following is valid for the binding energy E_n of an electron on a shell with the principal quantum number n:

$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2}(Z-\sigma)^2$ where (n = 1, 2, 3, ...) (1)

With the introduction of the Rydberg constant R:

$R = \frac{m_e e^4}{8\epsilon_0^2 h^2} = 3.2898 \cdot 10^{15}\ s^{-1}$ (2)

equation (1) becomes:

$E_n = R \cdot h(Z-\sigma)^2 \frac{1}{n^2}$ (3)

Electron mass : $m_e = 9.1091 \cdot 10^{-31}\ kg$

Elementary charge: $e = 1.6021 \cdot 10^{-19}\ As$

Plank's constant: $h = 6.6256 \cdot 10^{-34}\ Js$

Dielectric constant: $\epsilon_0 = 8.8544 \cdot 10^{-12}\ F/m$

Atomic number: Z

Screening constant: σ

For electrons on the K shell (n = 1), the screening constant is σ ~= 1.

Theory (3/4)

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Calculation of the energy based on the glancing angles:
Using the Bragg equation

$2d\sin(\theta) = n\lambda$ (4) (d: interplanar spacing; n = 1, 2, 3,...)

(LiF(200) interplanar spacing d = 201.4 pm)

with n = 1 and together with the energy equation

$E = h \cdot f = \frac{h \cdot c}{\lambda}$ (5)

we finally obtain the energy (n = 1) based on the glancing angles of the absorption edges:

$E = \frac{h \cdot c}{2d\ \sin(\theta)}$ (6)

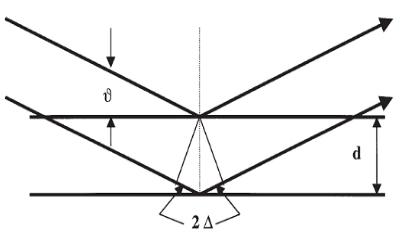

Fig. 2: Bragg scattering on a pair of lattice planes

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Theory (4/4)

Table 1 shows the θ values of the absorption edges of various absorbers that were taken from Figure 8. Equation (6) was used to calculate the energy values E_K of the associated K shells. For comparison, the corresponding literature values are also provided.
Equation (3) is converted in order to calculate the Rydberg constant R.

$$Z = \frac{1}{\sqrt{R \cdot h}} \cdot \sqrt{E + \sigma} \text{ (with n = 1)} \qquad (7)$$

	Z	θ [°]	E_K (exp.) [keV]	E_K (lit.) [keV]
Zn	30	18.6	9.65	9.66
Ge	32	16.1	11.10	11.10
Se	34	14.0	12.72	12.66
Br	35	13.2	13.48	13.47
Rb	37	11.6	15.31	15.20
Sr	38	11.0	16.13	16.10
Ag	47	6.8	25.99	25.51

Table 1: K edge energies

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Equipment

Position	Material	Item No.	Quantity
1	XR 4.0 expert unit, 35 kV	09057-99	1
2	XR 4.0 X-ray goniometer	09057-10	1
3	XR4 X-ray Plug-in Cu tube	09057-51	1
4	XR 4.0 X-ray structural analysis upgrade set	09145-88	1
5	XR 4.0 X-ray Chemical set for edge absorption	09056-07	1
6	Silver nitrate, cryst. 25 g	30222-04	1

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Setup and Procedure

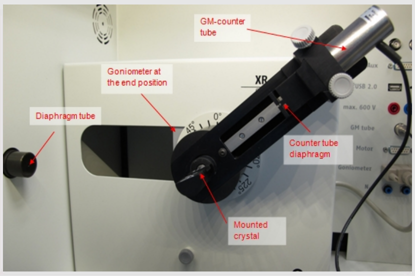
Setup

Connect the goniometer and the Geiger-Müller counter tube to their respective sockets in the experiment chamber (see the red markings in Fig. 3). The goniometer block with the analyser crystal should be located at the end position on the right-hand side. Fasten the Geiger-Müller counter tube with its holder to the back stop of the guide rails. Do not forget to install the diaphragm in front of the counter tube (see Fig. 4). Insert a diaphragm tube with a diameter of 2 mm (without an absorber) or 5 mm (with an absorber) into the beam outlet of the tube plug-in unit for the collimation of the X-ray beam.

For calibration: Make sure, that the correct crystal is entered in the goniometer parameters. Then, select “Menu”, “Goniometer”, “Autocalibration”. The device now determines the optimal positions of the crystal and the goniometer to each other and then the positions of the peaks.

← Fig. 3: Connectors in the experiment chamber

↓ Fig. 4: Set-up of the goniometer



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Procedure (1/4)

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- Connect the X-ray unit via the USB cable to the USB port of your computer (the correct port of the X-ray unit is marked in Figure 5).
- Start the “measure” program. A virtual X-ray unit will be displayed on the screen.
- You can control the X-ray unit by clicking the various features on and under the virtual X-ray unit. Alternatively, you can also change the parameters at the real X-ray unit. The program will automatically adopt the settings.

Fig. 5: Connection of the computer

Procedure (2/4)

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Fig. 6: Part of the user interface of the software

- Click the experiment chamber (see the red marking in Figure 6) to change the parameters for the experiment. Select the settings as shown in the overview for the various experiments.
  Glancing angle θ = 5°-26°. For the recording without any absorber, use the diaphragm tube with a diameter of 2 mm. If an absorber is used, use the diaphragm tube with a diameter of 5 mm.
- If you click the X-ray tube (see the red marking in Figure 6), you can change the voltage and current of the X-ray tube. Select the parameters as shown in Fig. 7.

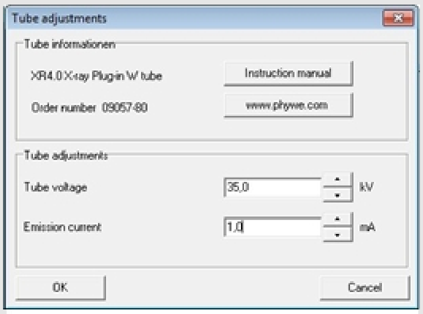

Fig 7: Voltage and current settings

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Procedure (3/4)

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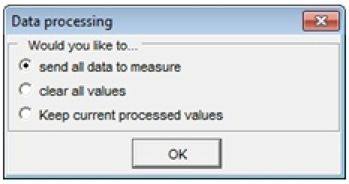
- Start the measurement by clicking the red circle: 

- After the measurement, the following window appears:



- Select the first item and confirm by clicking OK. The measured values will now be transferred directly to the “measure” software.
- At the end of this manual, you will find a brief introduction to the evaluation of the resulting spectra.

Procedure (4/4)

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Overview of the goniometer and X-ray unit settings:

- 1:2 coupling mode
- scanning range: 4°-21°
- angle step width 0.1°
- Anode voltage U_A = 35 kV; anode curren I_A = 1 mA

Recording without an absorber

- Gate time 2 s

Recording with a K edge absorber

- Gate time 3 s

Recording with a L edge absorber

- Gate time 6 s

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Evaluation

Task 1

Analyse the copper X-radiation with the aid of a LiF monocrystal and as a function of the Bragg angle without and with several K edge absorption samples as absorbers. Determine the K bsorption edges of different absorbers based on the spectra.

Figure 8 shows the intensity I of the copper X-radiation as a function of the Bragg angle θ up to the characteristic K_β line. The top curve shows the spectrum without any absorber. All of the other curves were recorded with an additional absorber sample. The higher atomic number of the absorber is, the more the absorption edge is shifted towards smaller glancing angles.

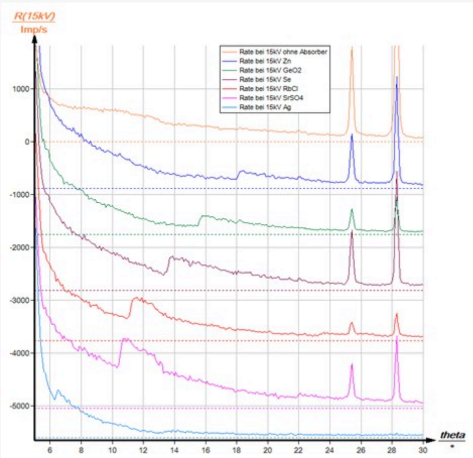

Fig. 8: X-ray spectra of copper without any absorber (top curve) and with the absorption edges of various elements

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Task 1

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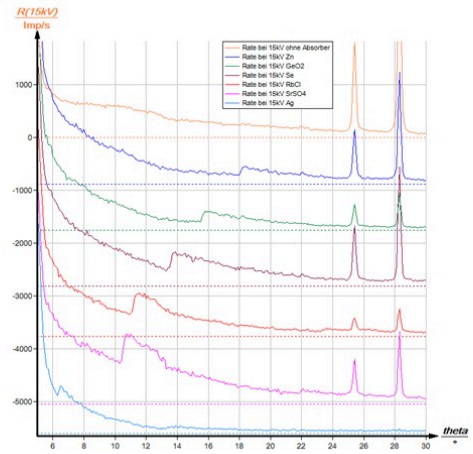

Fig. 8: X-ray spectra of copper without any absorber (top curve) and with the absorption edges of various elements

Task 2

Calculate the Rydberg constant and the screening constant based on the energy values of the K absorption edges.

With the aid of equation (6), the edge absorption energy values can be obtained. Figure 9 shows the function $\mathrm{Z} = \mathrm{f}\left(\sqrt{\mathrm{E_K}}\right)$ based on the energy values $\mathrm{E_K}$ (exp.) of table 1.
Based on the equation of the straight line $\mathrm{a} = \frac{1}{\sqrt{\mathrm{R \cdot h}}}$ the following follows for the Rydberg constant:

$$\mathrm{R} = \frac{1}{\mathrm{h}} \cdot \frac{|\Delta(\sqrt{\mathrm{E}})|^2}{(\Delta \mathrm{Z})^2} \qquad (8)$$

With the value for R and the $\mathrm{E_K}$ (exp.) values of table 1, equation (3) leads to $\sigma(\mathrm{K}) = (3.5 \pm 0.1)$ as the mean value of the screening constant.

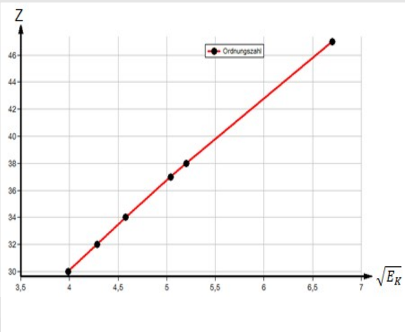

Fig. 9: Moseley line of the K edge absorption to determine the Rydberg constant.

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Task 3

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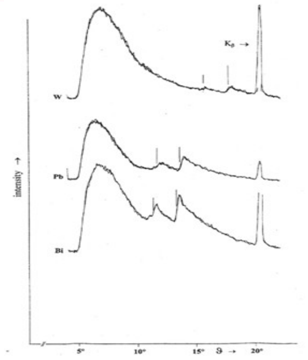

Fig. 10: X-ray spectrum of copper with the L absorption edges of various elements

Proceed as described for task 1, but this time with various samples for L edge absorption.

Figure 10 shows bremsspectrum with the absorption edges of elements of a higher atomic number. However, although three edges of the three L shells can be expected in theory, only two can be seen. A separation of the absorption edges of the $\mathrm{L_2}$ and $\mathrm{L_3}$ sub-shells is not possible.

Task 4

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Calculate the Rydberg constant based on the energy values of the L absorption edges.

Table 2 shows the results concerning the L edge absorption. The literature value $\mathrm{E_{L_{1,2}}}$ that is given for comparison has been calculated by taking the mean of the corresponding $\mathrm{L_1}$ and $\mathrm{L_2}$ values.
An evaluation with the aid of equation (1) does not make any sense in this case, since – apart from the Coulomb interaction – other interactive processes must also be taken into account. Nevertheless, equation (1) is helpful in giving a rough idea of the screening of the electrons on L shells. According to (3) and with n = 2 plus the experimental energy values in table 2, the following results:

$$\sigma(\mathrm{K}) << \sigma(\mathrm{L_{1,2}}) < 15 < \sigma(\mathrm{L_3}) < 20$$

The growth of the screening constant underlines the decreasing influence of the nuclear potential on the electrons on the outer shells.

Figure 11 shows the linear course of the function $\mathrm{Z = f}\left(\sqrt{\mathrm{E_K}}\right)$ for $\mathrm{L_{1,2}}$ and $\mathrm{L_3}$ (9).

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Task 4 (part 2)

	W (Z = 74)	Hg (Z = 80)	Pb (Z = 82)	Bi (Z = 83)
$\theta(L_{1,2})$	15.5	12.4	11.6	11.2
$E_{L_{1,2}}$ (exp)	11.52	14.33	15.31	15.85
$E_{L_{1,2}}$ (lit)	11.82	14.52	15.53	16.05
$\theta(L_3)$	17.6	14.5	13.6	13.2
E_{L_3} (exp)	10.20	12.29	13.09	13.48
E_{L_3} (lit)	10.21	12.28	13.04	13.42

Table 2: L edge energies

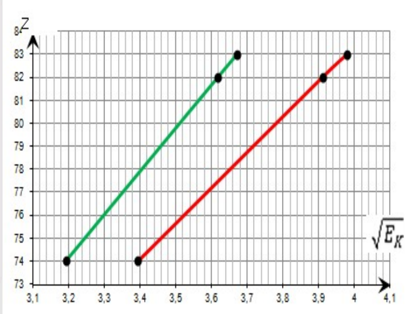

Fig. 11: Moseley lines for the L edge absorption

Note

"measure" software

First convert the glancing angles (crystal angle = x-axis) of the spectra into the corresponding energy values. To do so, proceed as follows: “Analysis”, “X-ray spectroscopy”, “Convert x-axis”, and “Energy (n = 1)”. Moseley lines can be obtained from the converted spectra (Imp/s = f(E/keV) as follows: K" id="MathJax-Element-3-Frame" role="presentation" style="position: relative;" tabindex="0">K

- Click “Analysis”, “X-ray spectroscopy”, and “Moseley straight line”. The window “Moseley straight line” appears. It offers K and L edge absorption. Then, select the middle of the absorption edge as a narrow band with the aid of the marker and click “Accept value”. If necessary, the area of the absorption edge can be zoomed with the aid of the zoom function. If the absorber and its atomic number were entered into the start window, the corresponding pair values for the edge energy and atomic number are displayed. The latter can also be entered later into the additional window “Moseley straight line”. In order to generate the straight line, click “Generate Moseley line”. The Rydberg constant can be determined by clicking “Analysis”, “X-ray spectroscopy”, and “Determine Rydberg constant”. With “Display options”, “Channels”, and “Symbol”, the measuring points of the Moseley line can be displayed if desired.

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Appendix

Security Information (1/7)

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Hazard symbol, signal word	Hazard statements	Precautionary statements
Rubidium chloride (RbCl)		
-	--	--
Germanium(IV) oxide (GeO_2)		
	H302: Harmful if swallowed H332: Harmful if inhaled	--

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Security Information (2/7)

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Hazard symbol, signal word	Hazard statements	Precautionary statements
Silver (I) chloride (AgCl)		
	H400: Very toxic to aquatic life	P273: Avoid release to the environment.
Zinc		
-	--	--

Security Information (3/7)

PHYWE

Hazard symbol, signal word	Hazard statements	Precautionary statements
Selenium		
 	H301: Toxic if swalloed H331 Toxic if inhaled H373: Causes damage to organs through prolonged or repeated exposure H413: May cause long lasting harmful effects to aquatic life	--.

Security Information (4/7)

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Hazard symbol, signal word	Hazard statements	Precautionary statements
Potassium bromide (KBr)		
	H315: Causes skin irritation H319: Causes serious eye irritation H335: May cause respiratory irritation	P261: Avoid breathing dust/fume/gas/mist/vapours/spray. P305 + P351 + P338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. .
Strontium sulphate ($SrSO_4$)		
-	--	--

Security Information (5/7)

PHYWE

Hazard symbol, signal word	Hazard statements	Precautionary statements
Lead (IV) oxide (PbO_2)		
	H272: May intensify fire; oxidiser H302: Harmful if swallowed H332: Harmful if inhaled H360: May damage fertility or the unborn child H373: Causes damage to organs through prolonged or repeated exposure H410: Very toxic to aquatic life with long lasting effects	P201: Obtain special instructions before use. P220: Keep/Store away from clothing/…/combustible materials. P273: Avoid release to the environment. P308 + P313: IF exposed or concerned: Get medical advice/attention.

Security Information (6/7)

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Hazard symbol, signal word	Hazard statements	Precautionary statements
Tungsten(IV) oxide (WO_2)		
	H335: May cause respiratory irritation	--

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