Splitting of the characteristic K-alpha doublet radiation of molybdenum (Item No.: P2540701)

Curricular Relevance



Characteristic X-radiation, energy levels, selection rules for X-radiation, energy term symbols, Bragg's law

Overview

Short description

Principle

The X-radiation that is generated by an X-ray tube with a molybdenum anode is selected as a function of the Bragg angle with the aid of a monocrystal, and registered with a Geiger-Müller counter tube. The resulting X-ray lines are used to determine the separation of the lines of the K_{α} doublet as well as their respective intensities.

This experiment is included in the "XRC 4.0 X-ray characteristics" upgrade set.



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Equipment

Position No.	Material	Order No.	Quantity
1	XR 4.0 expert unit, X-ray unit, 35 kV	09057-99	1
2	XR 4.0 X-ray goniometer	09057-10	1
3	XR 4.0 X-ray Plug-in Mo tube	09057-61	1
4	Geiger-Mueller counter tube, 15 mm (type B)	09005-00	1
5	XR 4.0 X-ray LiF crystal, mounted	09056-05	1
6	XR 4.0 Software measure X-ray	14414-61	1
7	Data cable USB, plug type A/B, 1.8 m	14608-00	1
8	XR 4.0 X-ray Diaphragm tube d = 1 mm	09057-01	1

Tasks

- 1. Analyse the intensity of the molybdenum X-radiation as a function of the Bragg angle and with the aid of a LiF monocrystal.
- 2. Determine the wavelengths and intensities of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines and compare your values to the theoretical values.

Set-up and procedure

Set-up

Connect the goniometer and the Geiger-Müller counter tube to their respective sockets in the experiment chamber (see the red markings in Fig. 2). 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. 3).

Insert a diaphragm tube with a diameter of $1\,mm$ 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: Set-up of the goniometer



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Note

Details concerning the operation of the X-ray unit and goniometer as well as information on how to handle the monocrystals can be found in the respective operating instructions.

Procedure

Connect the X-ray unit via USB cable to the USB port of your computer (the correct port of the X-ray unit is marked in Fig. 4).

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- Start the "measure" program. A virtual X-ray unit will be displayed on the screen (Fig. 5).
- 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.
- Click the experiment chamber to change the pa-rameters for the experiment. In the case of the entire spectrum, select the settings as shown in Figure 6. If you measure the section of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines, select the following scanning range: 44° 46° (n = 4) and 61° 63° (n = 5) and a gate time of 30 60 s.
- If you click the X-ray tube, you can change the voltage and current of the X-ray tube. Select the parameters as shown in Figure 6.

Start the measurement by clicking the red circle: Experiment Hill

After the measurement, the following window appea	ars: Data processing
	Would you like to Send all data to measure C clear all values C Keep current processed values
	ок

- 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 a short introduction to the evaluation of data using the program "measure" is given.

Note

Never expose the Geiger-Müller counter tube to the primary X-radiation for an extended period of time.

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Instruction ma	nual
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35,0	kV
1.0	mA
	35,0

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KH4.U A-ray (aoniometer		Instruction manual
Order No	09057-10		www.phywe.com
evice adjustm	ents		
Mode	1:2 coupling mode	 Detector angle 	8,0 ▲ °
Crystal	LiF (100); d=201,4 pm	 Crystal start angle 	4,0 × °
Absorber	No absorber	 Crystal stop angle 	[6\$5,0 <u>↓</u> °
		Crystal increment	0,1 × °
	Calibrate	Integration iime	2,0 × s
ΟΚ	-1	Cancel	Help

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Theory and evaluation

Theory

Figure 8 shows the energy-level-diagram of molybdenum (Z=42).

When an electron is removed from the K shell of an atom, the resulting hole is filled by an electron from a higher shell. The energy difference of the energy levels that are involved in this process can be converted into X-radiation. When an s electron is missing from the K shell, an ${}^{2}S_{1/2}$ term results. The same applies to the L_{1} shell. A missing p electron on the L_{2} or L_{3} shell results in ${}^{2}P_{1/2-3/2}$ or ${}^{2}P_{3/2}$ terms. Since quantum-mechanical selection rules only allow radiative transitions with $\Delta l = \pm 1$, the transition $L_{1} \rightarrow K$ is not allowed. Indeed, instead of three K_{α} lines, only the two lines $K_{\alpha 1}$ and $K_{\alpha 2}$ can be observed. Since the conditions ${}^{2}P_{3/2}$ and ${}^{2}P_{1/2}$ are fourfold and twofold degenerate, the intensities of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines have the ratio 4:2.



With the aid of Bragg's law (1), the glancing angles artheta of the characteristic lines can be used to determine their wavelengths:

 $2d\sinartheta=n\lambda$ (1) $(d= ext{ interplanar spacing (LiF)}=201.4\,pm;\,n=1,\,2,\,3,\ldots)$

For comparison, the wavelengths can also be calculated from the energy-level-diagram in Figure 8 with the aid of (2):

$E = h \cdot f = rac{h \cdot c}{\lambda}$	(2)
Planck's constant	h	$= 6.6256 \cdot 10^{-34} \ Js$
Velocity of light	с	$= 2.9979 \cdot 10^8 \; m/s$
Equivalent	1eV	$= 1.6021 \cdot 10^{-19} J$

Note

The data of the energy-level diagram were taken from the "Handbook of Chemistry and Physics", CRC Press Inc., Florida.

Evaluation

In the following section, the evaluation of the data is described based on example results. Your results may differ from the results given below.

Task 1: Analyse the intensity of the molybdenum X-radiation as a function of the Bragg angle and with the aid of a **LiF** monocrystal.



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Figure 9 shows the X-ray spectrum of molybdenum that was analysed with a **LIF** monocrystal. With the aid of Bragg's law (1), the wavelengths of the characteristic lines can be determined based on their glancing angles ϑ .

Table 1 shows the values of the glancing angles ϑ that were determined based on Figure 9 as well as the values of the wavelengths λ of the characteristic X-ray line of molybdenum that were calculated with the aid of equation (1). For comparison, table 2 shows the λ values that were calculated with the aid of equation (2) and based on the energy values of Figure 8. In Figure 9, the splitting of the K_{α} doublet becomes just about visible as of the fourth-order interference (n = 4). For the analysis of the X-ray spectrum see also P2540201.



5	$\vartheta(K_a)/^{\circ}$	$\vartheta(K_{\beta})/^{\circ}$	$\lambda(K_a)/pm$	$\lambda(K_{\beta})/pm$
n=1	10.4	9.2	71.3	63.7
n=2	20.9	18.5	71.2	63.2
n=3	32.2	28.4	71.2	63.4
n=4	45.1	-	71.2	-
			71.22	63.43

Table 1: Wavelengths of the K_lpha and K_eta lines calculated with the aid of the experimental values

$\lambda(K_{\alpha l})/pm$	$\lambda(K_{\alpha 2})/pm$	$\lambda(K_{\beta})/pm$
71.36	70.93	63.29
Table 2: Wavelen	aths of the K_{lpha} and $K_{ar{eta}}$	lines calculated with

Task 2: Determine the wavelengths and intensities of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines and compare your values to the theoretical values. Figures 10 and 11 show certain sections of the X-ray spectrum of molybdenum. The splitting of the K lines can be seen clearly. The associated values are given in table 3. The wavelength was determined with the aid of equation (1).

As a first approximation, the intensity of an X-ray line is determined by its maximum. As a result, Figures 10 and 11 lead to an intensity ratio of $I(K_{\alpha 1})/I(K_{\alpha 2}) \approx 1.8$.

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	$ \vartheta $	ϑ	Mean value
	n = 4	n = 5	λ
$K_{\alpha 1}$	44.8	61.8	70.84
$K_{\alpha 2}$	45.1	62.45	71.22
Table 3			

"measure" software

With the "measure" software, the peaks in the spectrum can be determined rather easily:

- Click the button + and select the area for the peak determination.
- Click the button [] "Peak analysis".
- The window "Peak analysis" appears (see Fig. 12).

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- Then, click "Calculate".
- If not all of the desired peaks (or too many of them) are calculated, readjust the error tolerance accordingly.
- Select "Visualise results" in order to display the peak data directly in the spectrum.



Refer to the Help of the "measure" software for additional, more detailed explanations concerning the program features.

