# K alpha double splitting of molybdenum X-rays / fine structure





http://localhost:1337/c/5f6085a77e9d5b0003e1e745





## **General information**

### **Application**

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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.





#### Other information (2/2)

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The goal of this experiment is to get to investigate the monochromatic characteristic X-radiation of copper.

Learning





- 1. Analyse the intensity of the molybdenum X-radiation as a function of the Bragg angle and with the aid of a LiF monocrystal.
- Tasks
- 2. Determine the wavelengths and intensities of the  $K_{\alpha_1}$  and  $K_{\alpha_2}$  lines and compare your

values to the theoretical values.



#### **Theory (1/3)**

Figure 1 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  $^2\mathrm{S}_{1/2}$  term results. The same applies to the  $L_1$  shell. A missing p electron on the  $L_2$  or  $L_3$  shell results in  $^2\mathrm{P}_{1/2-3/2}$  or  $^2\mathrm{P}_{3/2}$  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  $K_\alpha$  lines, only the two lines  $K_{\alpha_1}$  and  $K_{\alpha_2}$  can be observed. Since the conditions  $^2\mathrm{P}_{1/2}$  and  $^2\mathrm{P}_{3/2}$  are fourfold and twofold degenerate, the intensities of the  $K_{\alpha_1}$  and  $K_{\alpha_2}$  lines have the ratio 4:2.

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Fig. 1: Energy-level-diagram of molybdenum (Z = 42)

**Theory (2/3)** 

When X-rays of the wavelength  $\lambda$  impinge on the lattice planes of a monocrystal under the glancing angle  $\theta$ , the rays that are reflected on the lattice planes interfere with each other in a constructive manner provided that their path difference corresponds to an integral multiple of the wavelength. This situation is explained by Bragg's law:

 $2d\sin(\theta) = n\lambda$  (1)

(d: interplanar spacing; n = 1, 2, 3,...)



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



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#### **Theory (3/3)**

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If the interplanar spacing d is known, the wavelength  $\lambda$  can be determined with the aid of the glancing angle  $\theta$ . The energy of the radiation then results from:

$$E = h \cdot f = rac{hc}{\lambda}$$
 (2)

Note:

The data of the energy-level diagram were taken from the "Handbook of Chemistry and Physics", CRC Press Inc., Florida. Planck's constant h =  $6.6256 \cdot 10^{-34} Js$ 

Velocity of light c =  $2.9979 \cdot 10^8 \frac{m}{s}$ 

Interplanar spacing LiF (200) d =  $2.014 \cdot 10^{-10} \mathrm{m}$ 

Equivalent 1 eV =  $1.6021 \cdot 10^{-19}$ J



#### 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 Mo tube	09057-61	1
4	XRC 4.0 X-ray characteristics upgrade set	09135-88	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 1 mm into the beam outlet of the tube plug-in unit.

**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.

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#### Procedure (1/3)

- 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.

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Fig. 5: Connection of the computer

#### **Procedure (2/3)**



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XR4.0 X-ray I	Boniometer		Instruction manual	
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Mode	1:2 coupling mode	Detector angle	8.0 *	
Crystal	LF (100); d=201,4 pm	Crystal start angle	4.0	
Absorber	No absorber	Crystal stop angle	(d5.0 *	
		Crystal increment	0,1 * *	
	Calibrate	Integration ime	2,0 • •	
OK.	1	Cancel	Help	

Fig /: Settings of the goniometer (LiF crystal)

- Click the experiment chamber (see the red marking in Figure 6) to change the parameters for the experiment. Select the parameters as shown in Figure 7 for the LiF crystal.
- 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. 8.
- 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.

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Tube informationen	
XR4.0 X-ray Plug-in W tube	Instruction manual
Order number 09057-80	www.phywe.com
Tube adjustments	
Tube voltage	35,0 • kV
Emission current	1.0 mA
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Fig 8: Voltage and current settings



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<ul> <li>Start the measurement by clicking the red circle: Void you ke to Select the first item and confirm by clicking OK. The measured values will now be transferred directly to the "measure" software.</li> <li>At the end of this manual, you will find a brief introduction to the evaluation of the resulting spectra.</li> </ul> Overview of the goniometer and X-ray unit settings: <ul> <li>1:2 coupling mode</li> <li>Gate time 30 - 60 s; angle step width 0.1°</li> <li>Scanning range 44° - 64° and 61° - 63° (LiF monocrystal)</li> <li>Anode voltage U<sub>A</sub> = 35 kV; anode curren I<sub>A</sub> = 1 mA</li> </ul>	rocedure (3/3)		ЭН	YWE
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## **Evaluation**

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#### Task 1

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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.

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  $\theta$ .



Fig. 9: X-ray spectrum of molybdenum; LiF monocrystal as the analyser

#### Task 1 (part 2)

Table 1 shows the values of the glancing angles  $\theta$  that were determined based on Figure 9 as well as the values of the wavelengths  $\lambda$  of the characteristic X-ray line of molybdenum that were calculated with the aid of equation (1).

For comparison, table 2 shows the  $\lambda$  values that were calculated with the aid of equation (2) and based on the energy values of Figure 1. In Figure 9, the splitting of the  $K_{\alpha}$  doublet becomes just about visible as of the fourth-order interference (n = 4). For the analysis of the X-ray spectrum see also P2540205.

	$\vartheta(K_a)/^{\circ}$	$\vartheta(K_{\beta})/^{\circ}$	$\lambda(K_a)/pm$	$\lambda(K_{\beta})/pm$
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  $K_{\alpha}$  and  $K_{\beta}$  lines calculated with the aid of the experimental values

$\lambda(K_{\alpha l})/pm$	$\lambda(K_{\alpha 2})/pm$	$\lambda(K_{eta})/pm$
71.36	70.93	63.29

Table 2: Wavelengths of the  ${\bf K}_\alpha$  and  ${\bf K}_\beta$  lines calculated with the aid of the energy values (see Fig. 1)

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#### Task 2

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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  $I(K_{\alpha_1})/I(K_{\alpha_2}) \approx 1.8$ .



Fig. 10: Splitting of the  $K_{\alpha_1}$  and  $K_{\alpha_2}$  lines of molybdenum (n = 4)

#### Task 2 (part 2) **PHYWE** Mean value θ д λ n = 4 n = 5 $K_{a1}$ 30 44.8 61.8 70.84 $K_{\alpha 2}$ 45.1 62.45 71.22 25 20 61.4 61,6 61,8 62.2 Table 3 Fig. 11: Splitting of the $K_{\alpha_1}$ and $K_{\alpha_2}$ lines of molybdenum (n = 5)



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#### Note

#### "measure" software

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

- Click the button 🕂 "Mark" and select the area for the peak determination.
- Click the button <sup>▲</sup> "Peak analysis".
- The window "Peak analysis" appears (see Fig. 12). Then, click "Calculate". If not all of the desired peaks (or too many of them) are calculated, readjust the error tolerance accordingly.
- $\circ\;$  Select "Visualise results" in order to display the peak data directly in the spectrum.



Fig. 12: Automatic peak analysis with "measure"

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