K_α doublet splitting of molybdenum X-rays / fine structure 5.4.07-00

What you can learn about ...

- ➔ Characteristic X-ray radiation
- ➔ Energy levels
- ➔ Selection rules
- ➔ The Bragg equation
- ➔ Energy term symbols

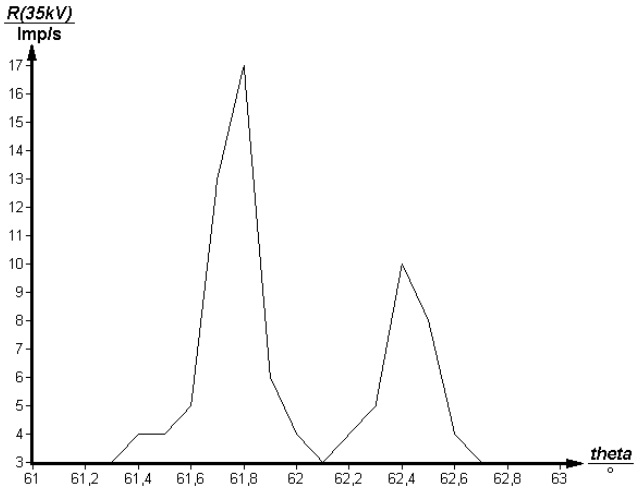
Principle:

The polychromatic molybdenum X-ray spectrum is to analyzed by means of a monocrystal. The energy of the characteristic lines is to be determined from the positions of the glancing angles at various orders of diffraction. The separation of the K_α doublet in higher order diffraction is to be examined.

What you need:

X-ray basic unit, 35 kV	09058.99	1
Goniometer for X-ray unit, 35 kV	09058.10	1
Plug-in module with Mo X-ray tube	09058.60	1
Counter tube, type B	09005.00	1
Lithium fluoride crystal, mounted	09056.05	1
Recording equipment:		
XYt recorder	11416.97	1
Connecting cable, *l* = 100 cm, red	07363.01	2
Connecting cable, *l* = 100 cm, blue	07363.04	2
or		
Software X-ray unit, 35 kV	14407.61	1
RS232 data cable	14602.00	1
PC, Windows® 95 or higher		

Complete Equipment Set, Manual on CD-ROM included
K_α doublet splitting of molybdenum X-rays / fine structure P2540700



X-ray spectrum of molybdenum; separation of the $K_{\alpha1}$ and $K_{\alpha2}$ lines in 5th order diffraction.

Tasks:

1. The intensity of the X-rays emitted by the molybdenum anode at maximum anode voltage is to be recorded as a function of the Bragg angle, using an LiF monocrystal as analyzer.
2. The wavelengths and ratio of the intensities of the two K_α lines are to be determined in high order diffraction, and a comparison made with the theoretical predictions.

Kα doublet splitting of molybdenum X-rays / fine structure

LEP 5.4.07 -00

Related topics
Characteristic X-ray radiation, energy levels, selection rules, the Bragg equation, energy term symbols.

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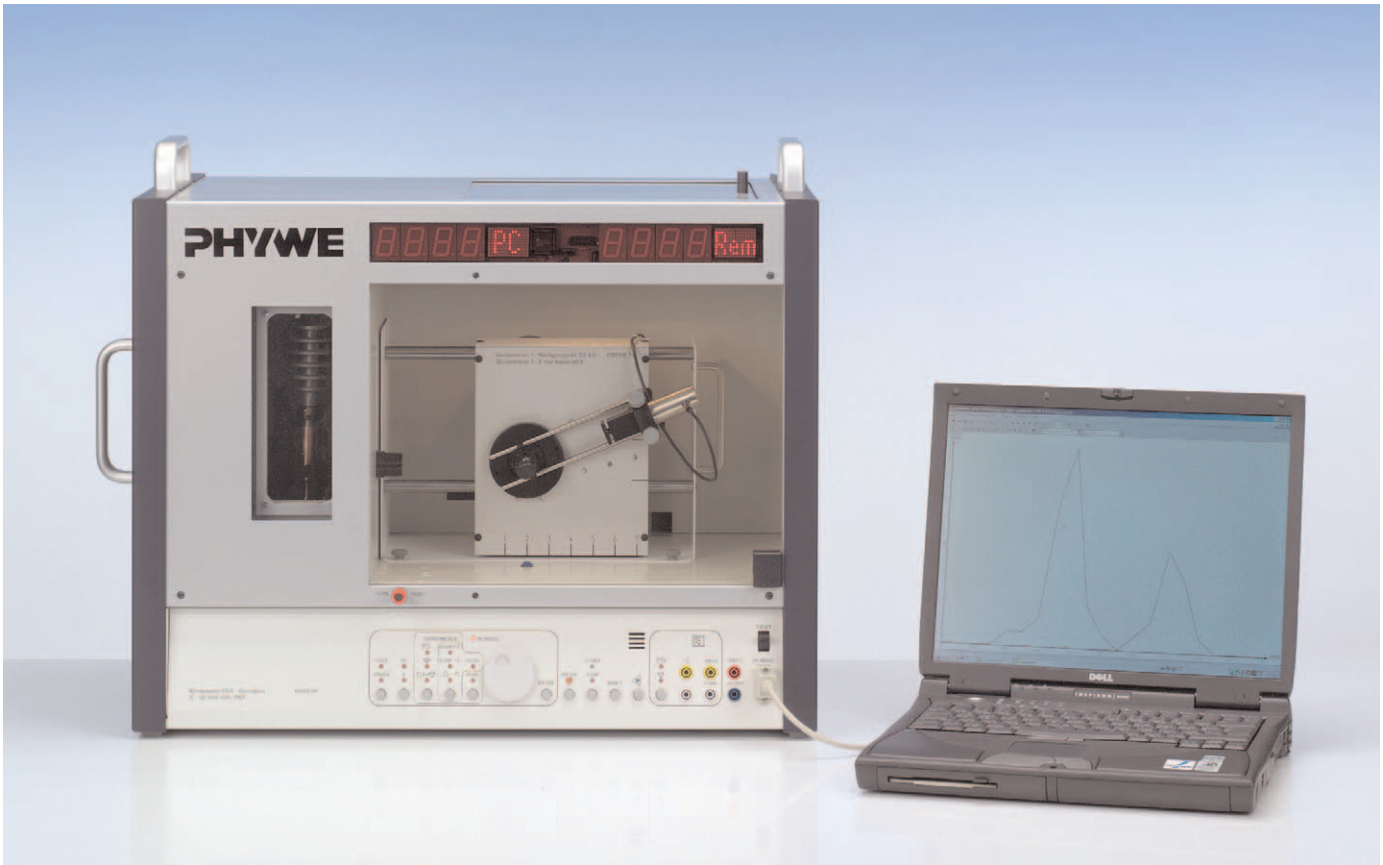
Set-up and procedure
Set up the experiment as shown in Fig. 1. Fix the diaphragm tube with 1 mm diameter aperture in the X-ray outlet tube. With the X-ray unit switched off, connect the goniometer and the counter tube to the appropriate sockets in the base plate of the experimenting area. Set the goniometer block to the middle position and the counter tube to the right stop.

The following settings are recommended for the recording of a complete spectrum (Fig. 3):
— Anode voltage U_A = 35 kV; Anode current I_A = 1 mA
— Gate time 3 s; Coupling mode; Analog output for crystal angle
— Auto mode; Starting and stopping angles 4° and 65°; Angle step width 0.1°

When an XY recorder is to be used, connect the Y axis with the analog output for the intensity, and the X axis with the analog output for the angular position.
For a determination of the separation of the $K_{\alpha1}$ and $K_{\alpha2}$ lines (Fig. 4), make the following changes to the settings: Scanning range 44°-46° for n = 4 and 61°-63° for n = 5; gate time 30 s.
In this case, increase the sensitivity for each of the axes when a recorder is used.

Fig. 1: Experimental set-up



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Theory and evaluation

The X-ray term scheme of molybdenum (Z = 42) is shown in Fig. 2.

When an electron is displaced from the K shell of the atom, it leaves a vacancy which is re-filled by an electron from one of the shells of higher energy. The difference in the energies of the levels concerned is emitted in the form of an X-ray. When an s electron is missing from the K shell, an $^2S_{1/2}$ term results. The same is true of the L_1 shell. A missing p electron in the L_2 or L_3 shell results in the term $^2P_{1/2}$ or $^2P_{3/2}$. Quantum mechanics selection rules for radiation transitions only allow transitions for which $\Delta l = \pm 1$. The transition L —> K is so forbidden, and is indeed not to be observed. Instead of 3 K_α lines, only the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines are to be observed. As conditions with j = 3/2 and j = 1/2 are fourfold or twofold degenerate, the intensities of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines behave as 4:2.

Fig. 3 shows a molybdenum X-ray spectrum analyzed with an LiF monocrystal. The wavelengths λ of the characteristic Mo X-ray lines can be calculated from the corresponding glancing angles ϑ by use of the Bragg equation (1).

$$2d \sin \vartheta = n\lambda \qquad (1)$$

(where n = 1, 2, 3, ...; d = interplanar spacing of the LiF crystal)

The wavelengths can also be calculated from the differences in the energy values in the term scheme (Fig. 2) using (2):

$$E = h \cdot f = \frac{h \cdot c}{\lambda} \qquad (2)$$

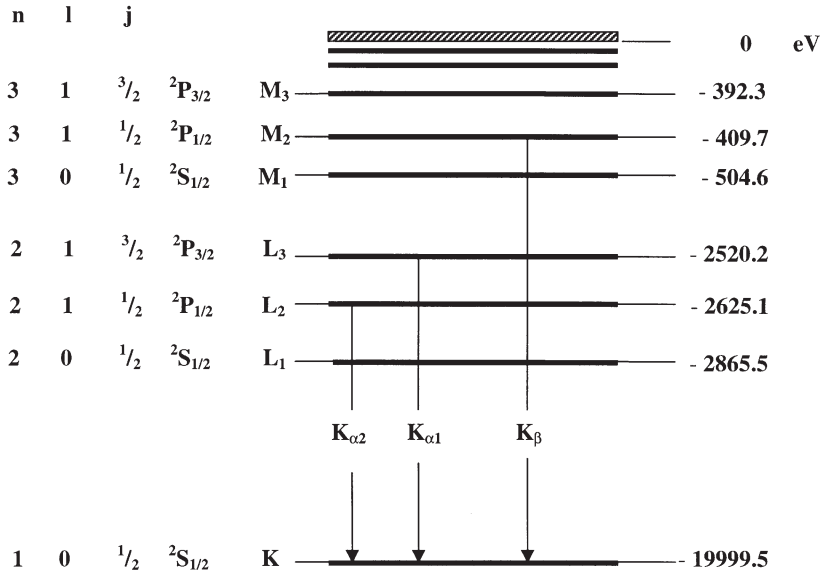
Planck's constant	h	=	$6.6256 \cdot 10^{-34}$ Js
Velocity of light	c	=	$2.9979 \cdot 10^{8}$ m/s
Lattice constant LiF (100)	d	=	$2.014 \cdot 10^{-10}$ m

The splitting of the K_α doublet can already be seen in Fig. 3 from the 4th order of diffraction.

The Table lists the experimentally determined glancing angles and the wavelengths which were calculated using (1), whereby the mean value is given for each of the K_α radiation lines. The values calculated using (2) are also given for comparison.

There is some indication of a separation of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines in Fig. 3. This separation becomes very distinct when an analysis of the spectrum in the region of the 4th and 5th order of diffraction is carried out with measured value recording conditions of 30 s / 0.1° (Figs. 4a and 4b). When a recorder is used, then the sensitivity of the two inputs must be increased.

Fig. 2: Energy levels of molybdenum



Table

d (LiF) = 201.4 pm	From experimental results				From energy levels		
	$\vartheta(K_\alpha)$/°	$\vartheta(K_\beta)$/°	$\lambda(K_\alpha)$/pm	$\lambda(K_\beta)$/pm	$\lambda(K_{\alpha 1})$/pm	$\lambda(K_{\alpha 2})$/pm	$\lambda(K_\beta)$/pm
n = 1	10.2	9.1	71.3	63.7			
n = 2	20.7	18.3	71.2	63.2			
n = 3	32.0	28.2	71.2	63.4			
n = 4	45.0	–	71.2	–			
n = 5	62.1	–	71.2	–			
			71.2_2	63.4_3	71.36	70.93	63.29

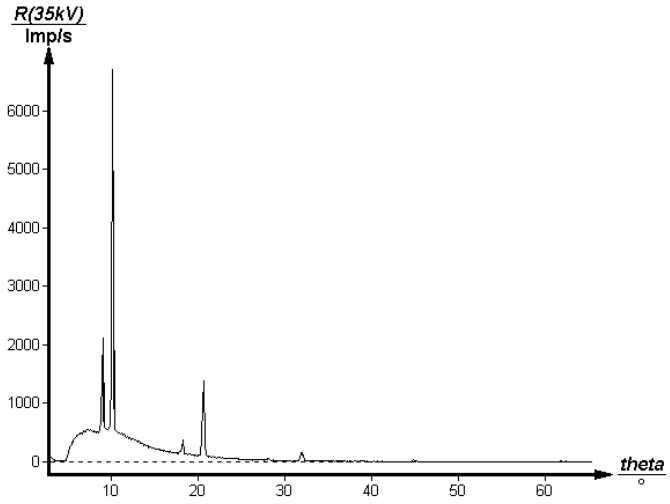


Fig. 3: X-ray spectrum of molybdenum; LiF-monocrystal as analyzer

The major lines are at the glancing angles ϑ ($K_{\alpha 1}$) = 44.80° and ϑ ($K_{\alpha 2}$) = 45.14° for n = 4 and ϑ ($K_{\alpha 1}$) = 61.77° and ϑ ($K_{\alpha 2}$) = 62.43° for n = 5. From these, we obtain the wavelengths λ ($K_{\alpha 1}$) = 70.97 pm and λ ($K_{\alpha 2}$) = 71.40 pm. The difference in the wavelengths of these two lines is therefore $\Delta\lambda$ = 0.43 pm which corresponds satisfactorily with the theoretical value.
As a first approximation, the intensity of a line is given by the peak height. The ratio of the intensities of the two lines is therefore $I(K_{\alpha 1})/I(K_{\alpha 2})$ ~ 1.8 and corresponds approximately to the value expected theoretically.

Fig. 4: X-ray spectrum of molybdenum;
4a: separation of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines in 4th order diffraction

4b: separation of the $K_{\alpha 1}$ and $K_{\alpha 2}$ lines in 5th order diffraction