Atom and Nuclear Physics

X-ray Physics

Structure of x-ray spectrums

Physics Leaflets

P6.3.6.5

Fine structure of the characteristic x-ray radiation of a tungsten anode

Experiment Objectives

- Recording a tungsten anode's spectrum.
- Investigating the L series' structure.
- Determining the L shell's division.

Basic Information

During the operation of an X-ray tube, besides the bremsstrahlung continuum, the characteristic radiation is also emitted (see also for example LD Physics leaflet P6.3.3.2). In contrast to the bremsstrahlung, the characteristic radiation does not exhibit a continuous distribution of the radiation intensity over the spectrum; its spectrum consists of distinct lines.

The characteristic radiation appears when the electrons accelerated in the X-ray tube toward the anode knock other electrons out of the inner shell of the anode material's atoms, the latter having a smaller binding energy than the striking electrons. The atom ionized as such then has a vacancy (electron hole) in a previously complete subshell. This state with a hole in the otherwise complete atomic shell is, except for the sign, very similar to an atom with only one single electron, which is why precisely identifying the state can be done by reverting to the known atomic number from nuclear physics, such as $1S_{1/2}$, $2P_{3/2}$, or generally nL_j. Alternately, the shells in the X-ray spectroscopy are also designated by the letters K, L, M, etc. along with their division into subshells such as L1, L2, L3.

Each of these electron holes is filled with an electron from a higher shell of the atom, linked more weakly: e.g. the *L* shell can thus be filled if an electron from the *M* shell crosses over. Such a crossover is associated with the emission of a photon. The radiation exhibits only certain discrete photon energies, which corresponds to the energy difference of the levels concerned, and is characteristic to each chemical element.

A higher resolution of the X-ray spectrum reveals a division of all shells (apart from the K shell) into individual subshells. Responsibility for this lies on the one hand with the spin-orbit coupling, e.g. the division between orbitals like L2 ($2P_{1/2}$) and L3 ($2P_{3/2}$), and on the other hand with the nuclear charge's modified shielding by the electrons still remaining in orbitals with another probability distribution of the hole, such as L1 ($2S_{1/2}$). The division by spin-orbit coupling is also known from the optical spectroscopy, for example sodium's yellow lines D_1, D_2.

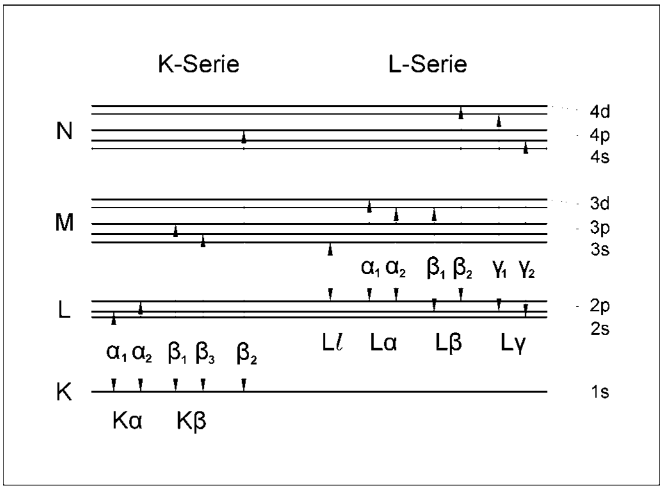

Figure 1: Simplified term diagram of an atom with a few characteristic X-ray lines from the K and L series.

There are two different nomenclature systems for the X-ray lines in use today; one is historic, from the Swedish physicist M. Siegbahn (e.g. $L\alpha_1$), and the other is systematic and recommended by IUPAC (e.g. L3-M5).

The characteristic X-ray lines' historic designations are composed by the electron shell's symbol (*K*, *L*, *M*, etc.) and the lower case Greek letters (α, β, γ, etc.) or a lower case Latin letter. Thus the designation $K\alpha$ line for the crossovers from the *L* shells to the *K* shell. A higher resolution reveals the division of the individual lines and labels these fine structure divisions with numbers corresponding to intensity.

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Further investigations then clarify the precise structure of the particular sublevels, which is represented in the following image.

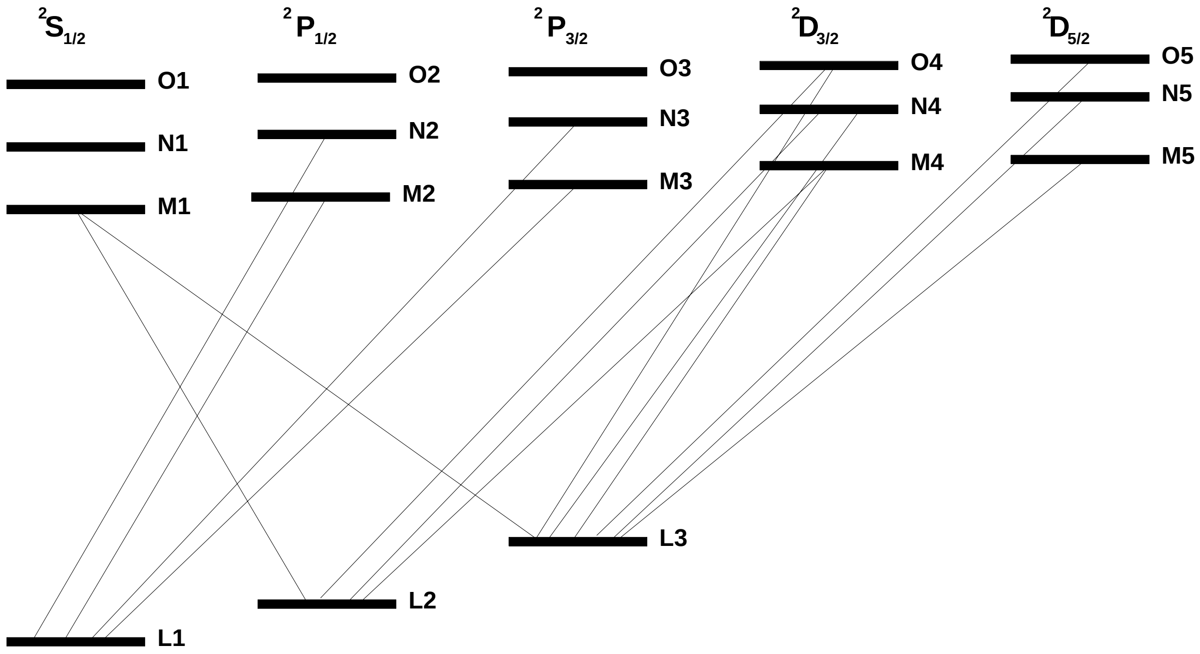

Figure 2: Detailed structure of the shells with crossovers allowed

	L1	L2	L3	M1	M2	M3	M4	M5	N1	N2	N3	N4	N5	O4, O5
L3				Ll			Lα2	Lα1	Lβ6			Lβ2	Lβ2	Lβ5
L2				Lν			Lβ1					Lγ1		Lγ6
L1					Lβ4	Lβ3				Lγ2	Lγ3			
K		Kα2	Kα1		Kβ3	Kβ1	Kβ5	Kβ5		Kβ2	Kβ2	Kβ4	Kβ4	

Table 1: List of the crossovers allowed and comparison of Siegbahn and IUPAC nomenclature

The K shell has the most deeply bound state, so $1S_{1/2}$, and does not split any further; the next-higher L shell is composed by three sublevels, named L1, L2, L3 in the X-ray spectroscopy and conforming to the $2S_{1/2}$, $2P_{1/2}$ and $2P_{3/2}$ states of the hole. The next-higher M shell is composed of 5 sublevels, since D orbitals can be taken here also.

The possible crossovers between the individual levels are represented in Table 1, for example an electron's crossover from level M5 (column) to L3 (row) emits an X-ray quantum with the difference of the two levels' binding energy, and this line is named L3-M5 according to the IUPAC notation and $L\alpha_1$ according to Siegbahn.

Only the allowed crossovers are labeled in Table 1; the selection rules prohibit any others. As in the optics, $\Delta L = \pm 1$, $\Delta j = 0, \pm 1$. An M1 ($2S_{1/2}$) - L1 ($3S_{1/2}$) crossover harms the first condition, and M5 to L2 would harm the second condition. As expected, both crossovers are not observed in the spectra.

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Apparatus

1 X-ray apparatus	554 800
1 X-ray tube W	554 864
1 LiF crystal for Bragg reflection	554 77
1 PC with Windows 98/NT or higher	

The X-ray apparatus fulfills the standards for the design of an educational X-ray device and of an inherent protection device, and it has a design approved under BfS 05/07 V/Sch RöV as an educational X-ray apparatus and inherent protection device.

The factory-provided safeguards and shielding installed reduce the dose rate outside the X-ray apparatus to below 1 μSv/h, a value that is in the magnitude of natural exposure to radiation.

■ Protect the X-ray apparatus from unauthorized access.

Overheating of the anode in the X-ray tube is to be avoided.

■ As the X-ray tube is powering up, check if the fan in the tubular space is turning.

The goniometer is moved solely by electric step motors.

■ Do not block the goniometer's target arm and sensor arm, or move them by force.

Setup

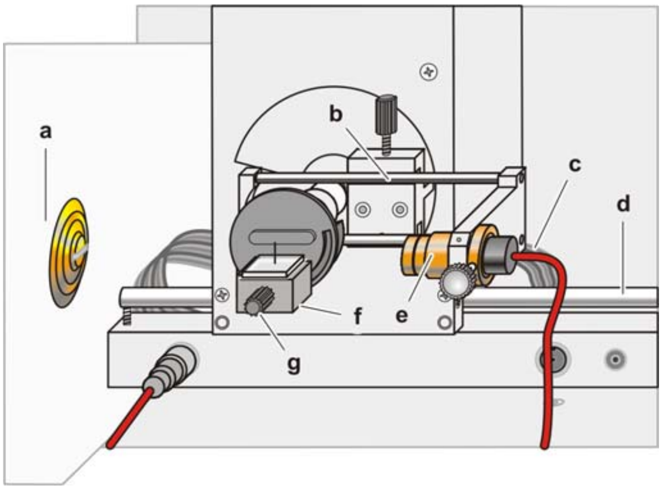

Figure 3: Setup of the goniometer

A few important details regarding the experiment setup are represented in Figure 3. The following detailed steps are required (see also the X-ray apparatus's operating manual):

- Assemble the X-ray apparatus with the tungsten X-ray tube.
- Install the collimator into the collimator receiver **(a)** (pay attention to the alignment pins).
- Attach the goniometer to the guiding rods **(d)** such that the separation s_1 between the collimator's slit diaphragm and the target arm measures about 6 cm. Fit the ribbon cable **(c)** for the goniometer controls.
- Remove the window counter tube's protective cap, insert the window counter tube into the sensor support **(e)** and connect the counter tube cable to the GM-TUBE socket.
- Set the separation s_2 between the target arm and the sensor support's slit diaphragm to about 6 cm by sliding the sensor fixing **(b)**.
- Fit the target support to the target table **(f)**.
- Loosen the knurled screw **(g)**, lay the Lif crystal for Bragg reflection on the target table, carefully raise the target table with the crystal to the stop and gently tighten the knurled screw (press lightly to avoid possible twisting).

Procedure

- Start the "X-ray apparatus" program, check that the apparatus is connected correctly and if necessary delete existing measured data with the button or the F4 key.
- Open the dialog window in the program with the button or the F5 key, and under Crystal, select "Crystal calibration," select the tungsten X-ray tube and the inserted crystal, to have the crystal calibrate automatically. The automatic adjustment begins after "Start search" is clicked and is completed after about 1 minute. The values are stored in the device after clicking "Adopt".
- Choose tube high voltage U = 35 kV, emission current I = 1.00 mA and angle increment $\Delta\beta$ = 0.1°.
- Press the COUPLED key for the 2ϑ coupling of target and sensor.

- Set the target angle's lower limit to 2.5° and the upper limit to 50.0°, and choose a measurement period per angle increment Δt = 2 sec.
- Start the measurement and data transmission to the PC with the SCAN key.
- Save the series of measurements under an appropriate file name with the button or the F2 key.

Measurement Example

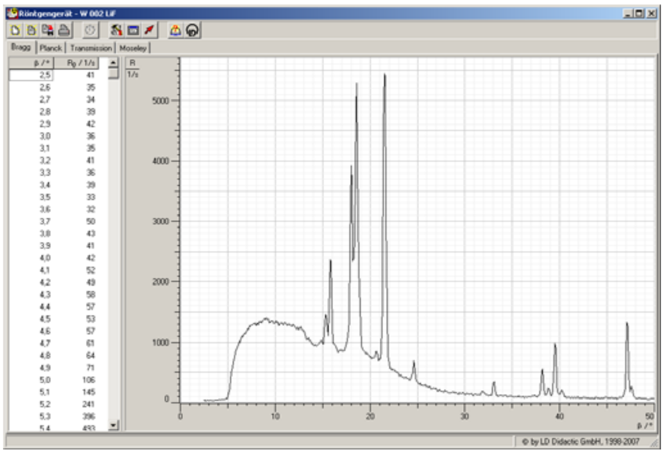

Figure 4: Tungsten tube's spectrum in angle representation

Figure 4 represents a typical spectrum of the tungsten anode. The continuum is recognizable here with a maximum under 10°, to which the characteristic lines are superimposed.

The Lγ, Lβ and Lα groups are recognizable between 15 and 22°, already showing a partial division. At angles about twice as big, the same lines appear in a second order with clearly improved resolution.

Higher Orders

If the correct settings for the crystal's lattice-plane spacing and the tube used are now chosen in the "X-ray apparatus" program under "Crystal," as represented in the following image,

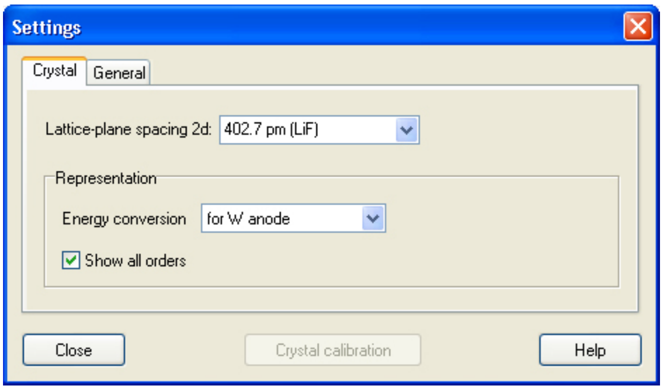

Figure 5: Selection for energy representation

and if "Show all orders" is then activated, then the measured angles Θ are converted into energy.

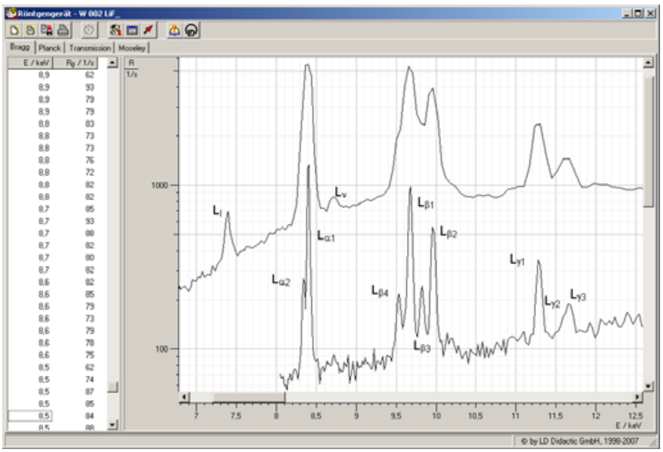

Figure 6: Energy representation with spectra in first and second order

The experiment works with fixed angle increments of 0.1 degrees, so the energy change dE/dΘ per reading point is not constant, but the higher the spectrum's order, the finer the angle increments.

From Bragg's law,

$\lambda = 2d \sin \Theta / n$

and

$E = hc/\lambda$

Thus

$E \sim n / \sin \Theta$

and

$dE/d\Theta \sim n \cos \Theta / \sin^2 \Theta$

The thickness of the individual characteristic lines is determined in the present experiment before the counter tube by the collimator's slits, and it is about 0.25° at all angles. But in energy representation, this means that in higher orders the thickness of the lines clearly diminishes, as can also be seen in Figure 6. The second order's lines are less than half as wide as the first order's and clearly show the X-ray crossovers' structure better.

Having said that, however, the lines are clearly less intensive, so that lines that are on principle weak, such as the Ll and Lν lines, can only be seen in the first order.

Analysis

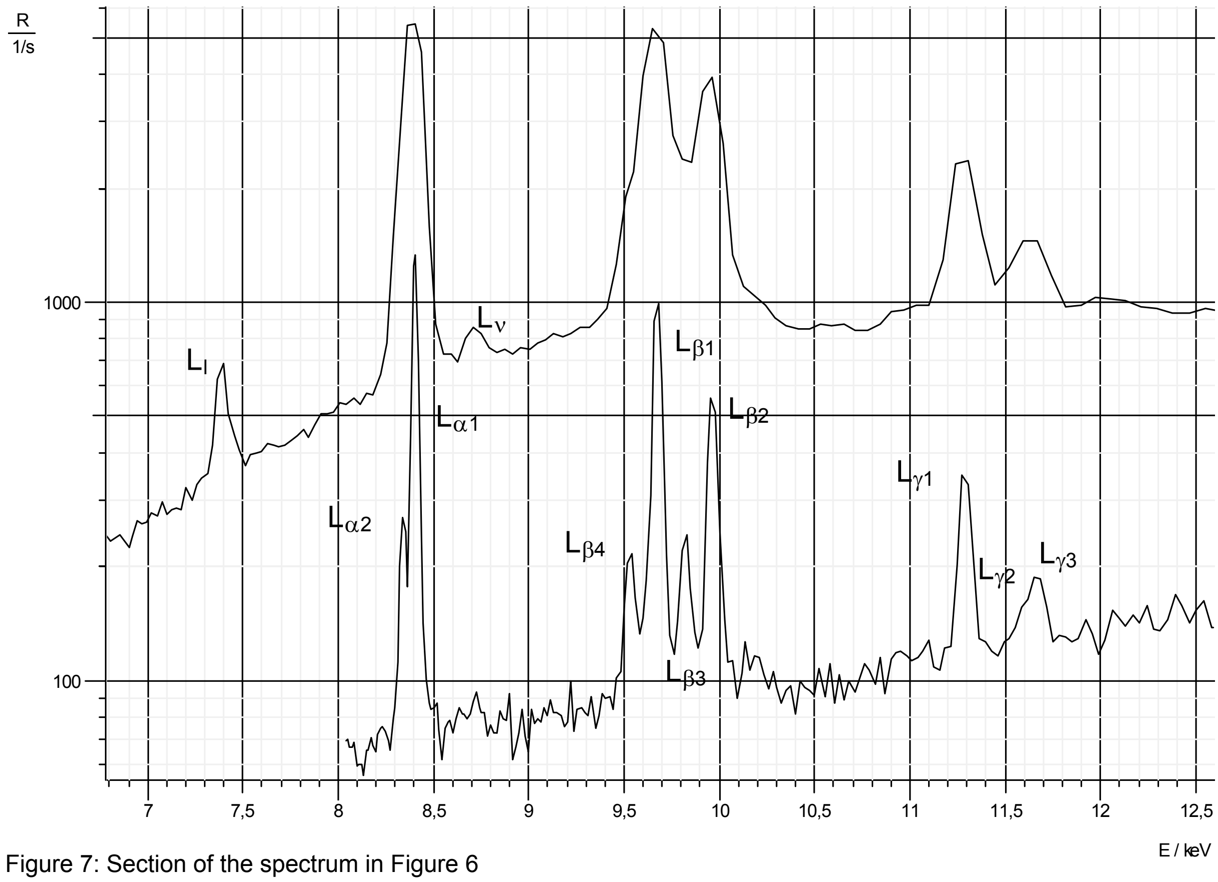

Figure 7: Section of the spectrum in Figure 6

Crossover	Measured data (keV)	Literature value (keV)
Lα1	8.40	8.3976
Lα2	8.34	8.3352
Lβ1	9.67	9.6724
Lβ2	9.96	9.948
Lβ3	9.82	9.8188
Lβ4	9.53	9.5249
Lγ1	11.29	11.2852
Lγ2	11.59	11.6082
Lγ3	11.67	11.6745
Ln	8.7	8.7244
Ll	7.4	7.3872

The individual levels' divisions can now be determined from the measured energy of the individual crossovers.

In the preceding leaflets, the fine structure division between the L3 and L2 levels for light elements is determined from the Kα1 - Kα2 difference. Since with tungsten the K shell cannot be stimulated with the experimentally available 35 kV, the K lines in this experiment cannot be observed. But as can be seen in Figure 2 and Table 1, there are two crossovers from level M4 and to L2 as well as L3. So the division of L2 and L3 can also be determined by the difference of lines Lα2 and Lβ1 and accounts for 1.33 keV.

The same interval should also be found between the Ll and Lν lines, since these proceed from the M1 level toward L2 and L3 respectively. The measurement produces a value of 1.3 keV, vaguely, since the weak lines were only visible in the first order.

The same is repeated for Lβ2 and Lγ1, likewise with an interval of 1.33 keV.