Energy resolution of the X-ray energy detector

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/5f7b040f692dbb00031eed1c

General information

Application

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 required for this experiment is found in the Theory section.

Main principle

Various metal samples are subjected to polychromatic X-rays. The resulting fluorescence radiation is analysed with the aid of a semiconductor detector and a multi-channel analyser. The energy of the characteristic X-ray lines and their full widths at half maximum are determined. In addition, the dependence of the full widths at half maximum and the shift of the line centroid as a function of the counting rate are examined.

Other information (2/2)

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Learning objective

The goal of this experiment is to get to learn the handling of a multi-channel analyser system.

Tasks

- Calibrate the semiconductor detector with the aid of the characteristic radiation of the copper X-ray tube.
- Determine the energy levels and full widths at half maximum of the characteristic K_α-lines of the different metals and represent them graphically.
- Determination and graphical representation of the full widths at half maximum as a function of the counting rate, with the K_α-line of zircon used as an example.
- Determination and graphical representation of the shift of the line centroid as a function of the counting rate, with the K_α-line of zircon used as an example.

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Theory (1/3)

Because of Heisenberg's uncertainty principle, the energy levels of the terms of an atom are not certain. Instead, they have a finite, though small, width, so that the natural width of an X-ray line depends on the sum of the natural widths of the energy levels that are involved in the transition. The line widths, e.g. of characteristic X-ray lines, which are measured with the aid of an energy analyser, are wider than the natural line widths by several orders of magnitude. The energy resolution of a detector is particularly high if it can represent two closely adjacent lines in a clearly separate manner. If two closely adjacent lines A and B have the full widths at half maximum (FWHM = Full Width Half Maximum) ΔA and ΔB and if their line centroids have the distance W (see Fig. 3), the two lines can still be represented separately if W is approximately $\geq \Delta\mathrm{A} + \Delta\mathrm{B}$. If an X-ray line of the energy level E_0 is measured with the aid of an energy detector, the resolving power of the detector is called $\mathrm{E}_0/\Delta\mathrm{E}_{\mathrm{FWHM}}$. The reciprocal value of the quotient is called the resolution. The energy analysis of X-rays with the aid of a semiconductor detector is described briefly based on the example of a Si-pindetector (p-contact - intrinsic - n-contact). Incident X-ray quanta with a sufficient level of energy create free electrons in the Si-crystal due to the photoelectric effect. The kinetic energy of these electrons correlates with the energy of the X-ray quanta.

Theory (2/3)

Apart from the phonon excitation, the electrons also create electron-hole pairs on their way through the depletion layer of the semiconductor. The number of these electron-hole pairs is a measure of the energy of the incident quantum. Holes and electrons are withdrawn by voltage that is applied externally and, thereby, creates a charge pulse. The magnitude of the charge pulse, on the other hand, is a measure of the energy of the incident X-ray quantum. The resulting pulse height spectrum will then be analysed by a multi-channel analyser. The extension of the natural X-ray line through the detector has many causes (e.g. inelastic scattering of the incident particle/quantum in the solid body prior to the photoelectric effect). Other causes are deficiencies of the multi-channel analyser, such as noise, which affect the pulse height distribution. Therefore, the results of this experiment refer to the overall system, which comprises the detector and multi-channel analyser. If X-ray lines are analysed with a semiconductor detector, their full width at half maximum $\Delta\mathrm{E}_{\mathrm{FWHM}}$ depends on their energy level E_0.

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Theory (3/3)

The following applies (see appendix):

$$\frac{\Delta E_{FWHM}}{E_0} = 2.35\sqrt{\frac{E_1}{E_0}} \qquad (1)$$

(E_1 = energy for creating an electron-hole pair)

(1) leads to

$$\Delta E_{FWHM} \propto \sqrt{E_0} \Rightarrow (\Delta E_{FWHM})^2 \propto E_0$$

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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 material upgrade set	09165-88	1

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Setup and Procedure

Setup (1/2)

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- Screw the adapter ring onto the inlet tube of the energy detector and connect the signal and supply cables to the corresponding ports of the detector with the aid of the right-angle plugs.
- Connect the signal and supply cables to the corresponding ports in the experiment chamber of the X-ray unit. In Figure 1, the port for the signal cable is marked in red and the port for the supply cable is marked in green. Connect the external X RED ports of the x-ray unit (see Fig. 2) to the multi-channel analyser (MCA). Connect the signal cable to the “Input” port and the supply cable to the “X-Ray Energy Det.” port of the MCA.
- Secure the energy detector in the holder of the swivel arm of the goniometer. Lay the two cables with sufficient length so that the goniometer can be swivelled freely over the entire range. Connect the multi-channel analyser and computer with the aid of the USB cable.

Fig. 1: Connectors in the experiment chamber

Fig. 2: Connection of the multi-channel analyser

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Setup (2/2)

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- Connect the multi-channel analyser and computer with the aid of the USB cable.
- Insert the tube with the 2-mm-aperture.
- Bring the goniometer block and the detector to their respective end positions on the left. Bring the detector to the 90° position in the 2:1 coupling mode (Fig. 3).

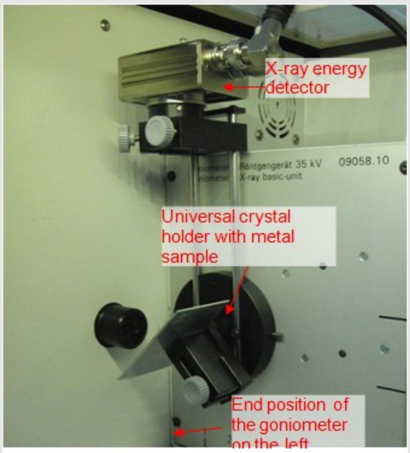

Fig. 3: Goniometer set-up

Procedure (1/6)

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- Bring the goniometer block and the detector to their respective end positions on the right.
- Insert the tube with the 1mm-aperture into the exit tube of the X-ray tube.
- With the X-ray unit switched on and the door locked, bring the detector to the 0° position. Then, shift the detector by some tenths degree out of the zero position in order to reduce the total rate.
- Operating data of the tungsten X-ray tube: Select an anode voltage U_A = 25 kV and an anode current I_A = 0.02 mA and confirm these values by pressing the “Enter” button.
- Switch on the X-radiation

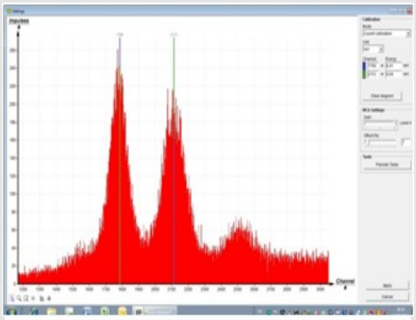

Fig. 4: calibration of the multi-channel analyser

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Procedure (2/6)

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- In the MEASURE program, select “Multi channel analyser” under “Gauge”. Then, select “Settings and calibration”. After the “Calibrate” button has been clicked, a spectrum can be measured. The counting rate should be < 300 c/s. Energy calibration settings: - 2-point calibration, - Unit = keV, Gain = 2 – Set the offset so that low-energy noise signals will be suppressed (usually a few per cent are sufficient), See Fig 4.
- Measuring time: 5 minutes. Use the timer of the X-ray unit.
- Make the two coloured calibration lines congruent with the line centres of the two characteristic X-ray lines. The corresponding energy values (see e.g. P2544705) $\mathrm{E(L_3M_5/L_3M_4)}$ = 8,41keV and $\mathrm{E(L_2N_4)}$ = 9,69 keV are entered into the corresponding fields, depending on the colour. (Note: Since a separation of the lines $\mathrm{L_3M_4}$ and $\mathrm{L_3M_5}$ Lines is not possible, the mean value of both lines is entered as the energy of the line).
- Name and save the calibration.

Procedure (3/6)

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Spectrum recording

- Bring the goniometer block and the detector to their respective end positions on the left. Bring the detector to the 90° position in the 1:2 coupling mode.
- Insert the metal sample with the universal crystal holder (sample at 45°).
- Operating data of the molybdenum X-ray tube: anode voltage $\mathrm{U_A}$ = 35 kV

1. Concerning task 1 and 2: Measurement of the full widths at half maximum as a function of energy.

Only the corresponding $\mathrm{K_\alpha}$-lines will be evaluated.

- Insert the tube with the 2-mm-aperture.
- Adjust the anode current so that the counting rate is approximately 100 c/s.

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Procedure (4/6)

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- Select the gain factor 4 (switch to gain factor 2 for the measurements of the silver and zinc samples).
- Measuring time: 5 minutes for each sample (use the timer of the X-ray unit).

2. Concerning task 4 and 5: Measurement of the full width at half maximum and determination of the shift of the line centroid as a function of the counting rate.

Only the zinc sample is used for this measurement and only its corresponding K_α-line will be evaluated.

- Insert the tube with the 5-mm-aperature.
- Select the gain factor 4.
- Adjust the required counting rate via the anode current.
- Measuring time: between 1 and 5 minutes, depending on the counting rate.

Procedure (5/6)

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- In order to determine the line position, switch from the bar display to the curve display. To do so, click “Display options” and then “Interpolation and straight lines”. Figure 7a shows the result concerning the spectrum of the zinc sample.
- Extend the relevant line section with the aid of the zoom function
- Then, select the various curve sections with

open the window “Function fitting"

Then, select “Scaled normal distribution“ (see Fig. 5b).

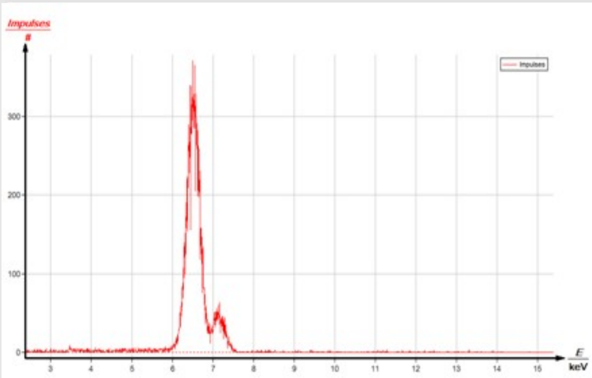

Fig. 5a: Fluorescence spectrum of iron

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Procedure (6/6)

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- Hide the original measurement curve and reselect the sections of the normal distributions. Find the line centroids of the normal distributions with “Peak analysis”

(see Fig. 5c) or determine them with the function “Survey”

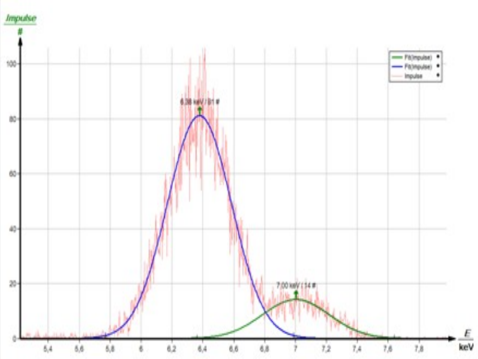
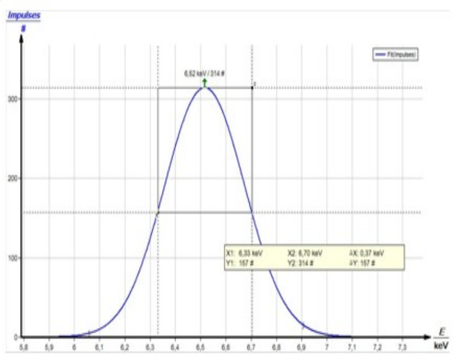


Fig. 5b: Fluorescence lines of iron with a fitted normal distribution

Fig. 5c: Normal distribution of the iron fluorescence lines for determining their channel position (original measurement curve not shown)



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Evaluation

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Task 2

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Determine the energy levels and full widths at half maximum of the characteristic K_α-lines of the different metals and represent them graphically.

Table 1 shows the line energies $\mathrm{E}(\mathrm{K}_\alpha)$ (column B) of the elements that were used, and the corresponding full widths at half maximum $\Delta\mathrm{E}_{\mathrm{FWHM}}$ (column C).

A	B	C
Element	$\mathrm{E}(\mathrm{K}_\alpha)$ [keV]	$\Delta\mathrm{E}_{\mathrm{FWHM}}$ [keV]
Fe	6,39	0,360
Ni	7,46	0,369
Cu	8,03	0,371
Zn	8,62	0,377
Zr	15,78	0,420
Mo	17,50	0,429
Ag	22,17	0,512

Table 1:Full width at half maximum $\Delta\mathrm{E}_{\mathrm{FWHM}}$ as a function of the line energy $\mathrm{E}(\mathrm{K}_\alpha)$

Task 2 (part 2)

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Figure 6 shows the corresponding course of the function. A square dependence of the full width at half maximum from the energy level, which could be expected in accordance with (2), cannot be clearly demonstrated, which is probably due to the narrow-band energy interval (approx. 6 keV – approx. 24 keV) that is available. The regression lines that were added show, however, that an approximate linear dependence can be assumed for small energy intervals.

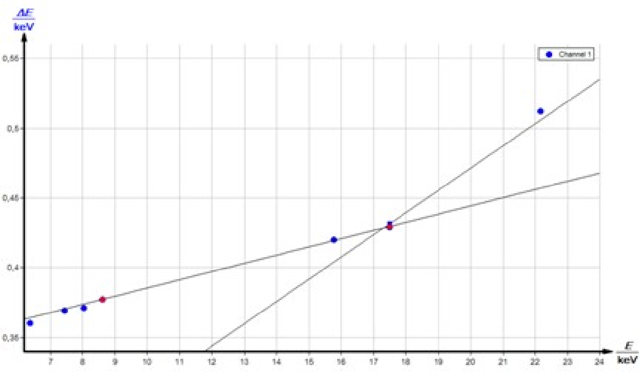

Fig. 6: Course of $\Delta\mathrm{E}_{\mathrm{FWHM}} = \mathrm{f}(\mathrm{E})$

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Task 3

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Determination and graphical representation of the full widths at half maximum as a function of the counting rate, with the K_{α}-line of zircon used as an example.

The dependence of the full width at half maximum and of the centroid of a fluorescence line on the counting rate can be determined particularly well with the aid of the K_{α}-line of zircon, since the two characteristic K_{α}- and K_{β}-lines are already well separated from each other (see Fig. 7a and 7b).
Figure 8 and 9 show the dependence of the full width at half maximum $\Delta\mathrm{E}_{\mathrm{FWHM}}$ of the zircon K_{α}-line as a function of the counting rate. It can be seen that the full width at half maximum of a line grows exponentially when the counting rate increases. Small and nearly constant full widths at half maximum can only be achieved in a small section with counting rates of approximately < 150 c/s.

Task 3 (part 2)

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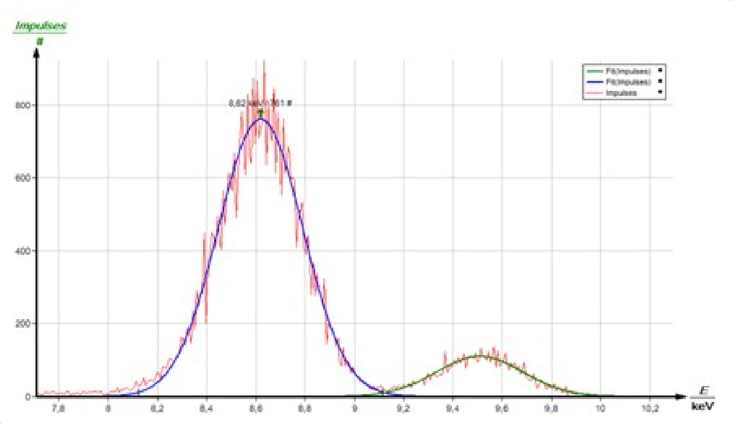

Fig. 7a: Fluorescence lines of zircon with a fitted normal distribution

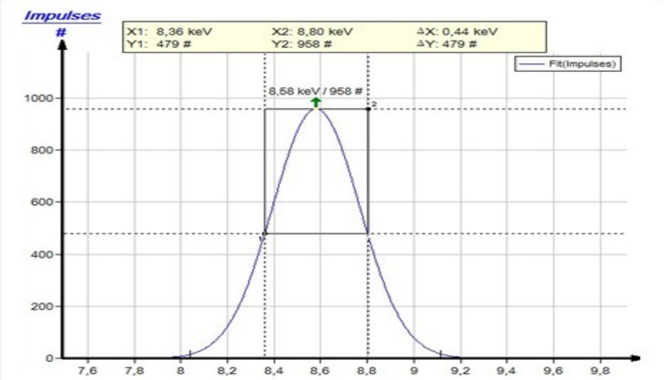

Fig. 7b: Normal distributions of the zircon K_{α}-line for determining the line energy and the full width at half maximum (the original measurement curve is hidden)

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Task 4

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Task 4: Determination and graphical representation of the shift of the line centroid as a function of the counting rate, with the K_{α}-line of zircon used as an example.

When the counting rate increases, the centroid of a line also moves towards lower energy values. This is only a slight shift, but it can be clearly measured (see Figure 8). The results of Figure 8 and 9 show that a good resolution of a line can only be achieved at low counting rates. The same is true for the sufficiently precise determination of their energy level.

Fig. 8: Full width at half maximum ΔEFWHM of the zircon Kα-line as a function of the counting rate

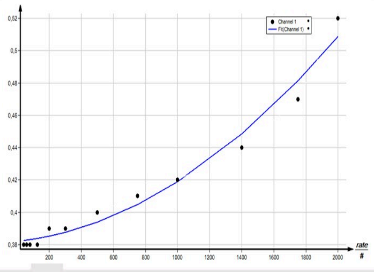
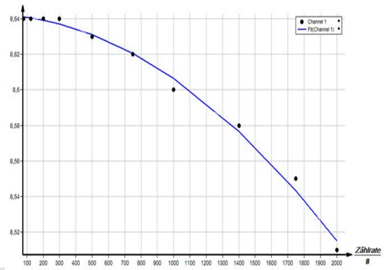


Fig. 9: Shift of the line centroid of the zircon Kα-line as a function of the counting rate



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Appendix

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Note

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The energy $\mathrm{E_0}$ of an incident X-ray quantum is used up in the semiconductor for the generation of electron-hole pairs and for the excitation of phonons.
The phonon excitation is neglected for the following analysis. This neglect is permissible, since the aim is not to determine an absolute value for the resolving power.
If $\mathrm{E_1}$ is the energy for producing an electron-hole pair, the average number of electron-hole pairs that are produced during the absorption is:

$$\bar{\mathrm{n}} = \frac{\mathrm{E_0}}{\mathrm{E_1}} \qquad (3)$$

In a simplified manner, one can assume that the statistical fluctuation σ of the average number of pairs can be represented by a normal distribution.

$$\sigma = \sqrt{\bar{\mathrm{n}}} = \sqrt{\frac{\mathrm{E_0}}{\mathrm{E_1}}} \qquad (4)$$

Note (part 2)

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(If one would also take the phonon excitation into consideration, the product $\mathrm{E_0 \cdot F}$ would stand in the numerator of the radicand (F = Fano factor = 0.13 for silicon).)
The following applies to the full width at half maximum of a normal distribution:

$$\Delta\bar{\mathrm{n}}_{1/2} = \sqrt{8\ln(2)} \cdot \sigma = 2.35 \cdot \sqrt{\frac{\mathrm{E_0}}{\mathrm{E_1}}} \qquad (5)$$

If one assumes that the spectral line with the energy level $\mathrm{E_0}$ also has a normal distribution, the following applies analogously:

$$\frac{\Delta\mathrm{E_{FWHM}}}{\mathrm{E_0}} = \frac{\Delta\bar{\mathrm{n}}_{1/2}}{\bar{\mathrm{n}}} = 2.35 \cdot \sqrt{\frac{\mathrm{E_0}}{\mathrm{E_1}}} \qquad (6)$$

For the full width at half maximum $\Delta\mathrm{E_{FWHM}}$ of the line, (4) results in:

$$\Delta\mathrm{E_{FWHM}} \propto \sqrt{\mathrm{E_0}} \Rightarrow (\Delta\mathrm{E_{FWHM}})^2 \propto \mathrm{E_0} \qquad (7)$$

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