FUNDAMENTAL PARAMETER PROGRAMS:
ALGORITHMS FOR THE DESCRIPTION OF K, L AND M SPECTRA
OF X-RAY TUBES

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ABSTRACT
Electron excited continuous and characteristic x radiations of pure elements were
investigated employing an electron probe micro analyzer with an energy dispersive detection
system. The measurements were performed on 23 elements and acceleration voltages from
5kV to 30kV. Continuous spectra are described by a modified Kramers cross section. For
absorption correction of continuous and characteristic spectra in the target Love and Scott’s
concept of a constant depth distribution function of x-ray generation is employed. Thus, it is
possible to describe the x radiations of an x-ray tube with arbitrarily chosen target by a set of
three fundamental parameters. These parameters are \textit{const} and \(x\) for continuous radiation and
\(\text{Const}_{kl}\) for characteristic radiations. Numerical values of \(\text{const}\), \(x\) and \(\text{Const}_{kl}\) were obtained
by least squares fits of theoretical responses to measured data. When compared to the results
of earlier investigations a considerably improved description of characteristic spectra is
possible.

EXPERIMENTAL
For the investigations of x-ray spectra an electron probe microanalyzer Philips XL30 ESEM
TMP was employed equipped with an EDAX New XL30, 135-10 Si-Li detector. Continuous
spectra of elements Mg, Al, Si, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ge, Mo, Rh, Ag, Sn,
Gd, Er, W, Au and Bi, characteristic K spectra of elements from Mg to Ag, characteristic L
spectra of elements from Mo to Bi and characteristic M spectra of elements from W to Bi
were measured and evaluated. The beam geometry of the instrument was defined by an angle
\(\varphi = 90^\circ\) between incident electrons and specimen surface, an angle \(\epsilon = 35^\circ\) between take-off
of x radiation and the specimen surface and a solid angle \(\Omega = 0.00367\) sr of x-ray detection.
The channel width of the multichannel analyzer is \(dE = 0.01\) keV. After a careful
investigation of Cu K radiation depending on experimental conditions such as deadtime of
photon detection, setting of shaping time of pulses, line width of the K lines, statistical error
and stability of the system the time \(t\) of data accumulation was chosen between 300 s and
1000 s and typical values of the beam current \(i\) were a few hundred pA at highvoltages from 5
to 30kV.

CONTINUOUS SPECTRUM
Equ.1 gives the spectral response \(^{1,2)} dN(E)\) with Love and Scott’s \(^{3-6})\) absorption correction
\(f_{\text{abs,cont}}\).

Equation 1
\[
dN(E) = \text{const} \cdot \Omega \cdot i \cdot t \cdot Z \cdot \left(\frac{E}{E_0} - 1\right)^x \cdot f_{\text{abs,cont}} \cdot dE
\]
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where

\[ f_{\text{abs,cont}} = \frac{1 - \exp \left( -\tau_{E,j} \cdot 2 \cdot \overline{\rho_2} \cdot \sin \phi / \sin \epsilon \right)}{\tau_{E,j} \cdot 2 \cdot \overline{\rho_2} \cdot \sin \phi / \sin \epsilon} \]

\[ \overline{\rho_2} = \rho_{\text{m}} \cdot \frac{0.49269 - 1.0987 \cdot \eta + 0.78557 \cdot \eta^2}{0.70256 - 1.09865 \cdot \eta + 1.0046 \cdot \eta^2 + \ln U_0} \cdot \ln U_0 \]

\[ \rho_{\text{m}} = \frac{A}{Z} \cdot \left( 0.787 \cdot 10^{-5} \cdot \sqrt[3]{J} \cdot E_0^{3/2} + 0.735 \cdot 10^{-6} \cdot E_0^2 \right) \]

\[ \eta = E_0^{m} \cdot \left( 0.1904 - 0.2236 \cdot \ln Z + 0.1292 \cdot (\ln Z)^2 - 0.0149 \cdot (\ln Z)^3 \right) \]

\[ U_0 = \frac{E_0}{E} \]

\[ J = 0.0135 \cdot Z \]

\[ m = 0.1382 - \frac{0.9211}{\sqrt{Z}} \]

with

const
fit parameter between theoretical and measured continuum \(^1\)

\( \Omega \)
solid angle of x-ray detection (sr)

\( i \)
current (beam current) (mA)

\( t \)
time of data accumulation (s)

\( Z \)
atomic number

\( E_0 \)
maximum energy of continuous spectrum (keV)

\( E \)
photon energy (keV)

\( U_0 \)
overvoltage ratio

\( x \)
fit parameter between theoretical and measured response \(^1,2\)

\( \tau_{E,j} \)
photoelectric absorption coefficient \(^7,8\) of radiation \( E \) in element \( j \) (cm\(^2\)/g)

\( \phi \)
incidence angle of electrons with regard to the specimen surface

\( \epsilon \)
take-off angle of photons with regard to the specimen surface

\( dE \)
energy interval (keV)

\( A \)
atomic weight

The evaluation of measured continuous spectra for const and \( x \) was performed in four steps

1. Reduction of the measured response considering the detector efficiency.
2. Entering the numerical values of experimental parameters \( t, \Omega, E_0, \phi, \epsilon, dE \) into Equ.1.
3. Definition of spectral ranges for the evaluation procedure.
4. The two unknowns const and \( x \) are obtained by an iterative minimization of absolute differences (errors) between “measured” and “theoretical” responses.

The following numerical values are mean values from evaluations of 200 measured responses.

\[ \text{const} = 1.35 \cdot 10^9 \text{ (sr}^{-1}\text{mA}^{-1}\text{s}^{-1}\text{keV}^{-1}) \quad \text{standard deviation 15%} \]

\[ x = 1.109 - 0.00435Z + 0.00175E_0 \text{standard deviation 5%} \]

Fig.1 gives an example of the evaluation of continuous radiation. The fitting procedure is valid for photon energies \( E > 1 \text{keV} \). The computed response of the continuum can also be used for background subtraction in quantitative microprobe analysis. Thus, a precise description of the background of characteristic spectra became possible.
Fig. 1 Measured and computed response of continuous spectrum. Measurements were performed on Cu with an electron energy of 30 keV. At photon energies of less than 1 keV the characteristic Cu L lines and at 8 keV to 9 keV the characteristic Cu K lines can be observed.

CHARACTERISTIC SPECTRA

Characteristic signals \( N_{jkl} \) are given by Eqn. 2.

Equation 2

\[
N_{jkl} = \text{Const}_{jkl} \cdot \Omega \cdot i \cdot t \cdot R \cdot \frac{1}{S_{jk}} \cdot \overline{\rho}_{jk} \cdot p_{jkl} \cdot f_{\text{abs},jkl}
\]

where

\[
R = 1 - 0.0081517 \cdot Z + 3.613 \cdot 10^{-5} \cdot Z^2 + 0.009583 \cdot Z \cdot e^{-U_0} + 0.001141 \cdot E_0
\]

\[
\frac{1}{S_{jk}} = \frac{z_j b_{j0}}{Z} \left( U_0 \ln U_0 + 1 - U_0 \right) \left[ 1 + 16.05 \sqrt{\frac{J}{E_{jk}}} \cdot \sqrt{U_0 \ln U_0 + 2 \left( 1 - \sqrt{U_0} \right)} \right]
\]

\[
f_{\text{abs},jkl} = \frac{1 - \exp \left( - \tau_{E_{jk},ij} \cdot 2 \cdot \overline{\rho}_z \cdot \sin \varphi / \sin \epsilon \right)}{\tau_{E_{jk},ij} \cdot 2 \cdot \overline{\rho}_z \cdot \sin \varphi / \sin \epsilon}
\]

\[
\overline{\rho}_z = \rho_z = \frac{0.49269 - 1.0987 \cdot \eta + 0.78557 \cdot \eta^2}{0.70256 - 1.09865 \cdot \eta + 1.0046 \cdot \eta^2 + \ln U_0} \cdot \ln U_0
\]

\[
\rho_z = \frac{A}{Z} \left( 0.787 \cdot 10^{-5} \cdot \sqrt{J} \cdot E_0^{3/2} + 0.735 \cdot 10^{-6} \cdot E_0^2 \right)
\]

\[
\eta = E_0^{m} \left( 0.1904 - 0.2236 \cdot \ln Z + 0.1292 \cdot (\ln Z)^2 - 0.0149 \cdot (\ln Z)^3 \right)
\]
\[ U_0 = \frac{E_0}{E_{jk}} \]
\[ J = 0.0135 \cdot Z \]
\[ m = 0.1382 - \frac{0.9211}{\sqrt{Z}} \]

with

- \( j \) index characterizing the element
- \( k \) index characterizing the ionised atomic level
- \( l \) index characterizing the atomic level from where the ionised level is filled under emission of characteristic radiation

- \( Const_{jkl} \) fit parameter between theoretical and measured characteristic signals \(^{1,9}\)
- \( \overline{\omega}_{jk} \) averaged fluorescence yield \(^{10}\)
- \( p_{jkl} \) transition probability \(^7\)
- \( R \) backscattering factor \(^{11}\)
- \( U_0 \) the overvoltage ratio is defined with regard to \( E_{jk} \)
- \( E_{jk} \) absorption edge energy \(^{7,8}\) (keV)
- \( \tau_{E_{jkl},j} \) photoelectric absorption coefficient \(^{7,8}\) of characteristic radiation with photon energy \( E_{jkl} \) in element \( j \) (cm\(^2\)/g)
- \( E_{jkl} \) photon energy of characteristic jkl radiation (keV) \(^7\)
- \( z_k, b_k \) constants depending on shell index \( k \) \(^{12}\),

\[
\begin{align*}
  k &= K & z_k &= 2 & b_k &= 0.35 \\
  k &= L & z_k &= 8 & b_k &= 0.25 \\
  k &= M & z_k &= 1.2 & b_k &= 0.7
\end{align*}
\]

**K SPECTRA**

![Graph showing the relationship between Const\(j_{K\alpha}\) and overvoltage ratio from the evaluation of K\(\alpha\) and K\(\beta\) lines of 17 elements.](image)

**Fig.2** Const\(_{jK\alpha}\) versus overvoltage ratio from the evaluation of K\(\alpha\) and K\(\beta\) lines of 17 elements.
The result of evaluations of $\text{Const}_{ji}$ depending on the overvoltage ratio is given in Fig.2. Earlier investigations \(^1\) proposed $\text{Const}_{ji} = 6 \cdot 10^{13}$ (sr\(^{-1}\)mA\(^{-1}\)s\(^{-1}\)). The result of the present investigation can be described by

$$
\text{Const}_{ji} = \frac{4.697 + 0.134 \cdot U_0 - 0.00268 \cdot U_0^2}{1 - e^{-\gamma(U_0)}} \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1})
$$

At overvoltage ratios above 1.5 a standard deviation of 10% can be assumed.

L SPECTRA

The evaluation of L-spectra \(^9\) gave the following results:

L1-based radiations (L1M3, L1M2, L1N2, L1N3 and L1N23)

$$
\text{Const}_{jL1} = f_{\text{corr}} \cdot 0.71 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 20%}
$$

L2-based radiations (L2M4, L2N4, L2M1)

$$
\text{Const}_{jL2} = f_{\text{corr}} \cdot 2.70 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 5%}
$$

L3-based radiations (L3M5, L3M4, L3N5, L3N4, L3N45, L3O45, L3N1, L3M1)

$$
\text{Const}_{jL3} = 4.94 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 2%}
$$

where

$$
f_{\text{corr}} = -0.4814 + 0.03781 \cdot Z - 2.413 \cdot 10^{-4} \cdot Z^2 \quad \text{(for } Z > 80 f_{\text{corr}} = 1) \]

M SPECTRA

M3-based line (M3N5)

$$
\text{Const}_{jM3} = 2.32 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 10%}
$$

M4-based lines (M4N2, M4N6)

$$
\text{Const}_{jM4} = 15.8 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 30%}
$$

M5-based lines (M5N3, M5N6, M5N7)

$$
\text{Const}_{jM5} = 20.5 \cdot 10^{13} \text{(sr}^{-1}\text{mA}^{-1}\text{s}^{-1}) \quad \text{standard deviation 10%}
$$

It has to be pointed out that the tables of Johnson and White \(^{13}\) contain Mζ1 and Mζ2 lines with relative intensities of 0.01. In Elam’s tables \(^7\) the Mζ line is attributed to the transition M45N67 with transition probability 0.00293. In accordance with the IUPAC recommendation Mζ is defined by M45N23. Besides, it has to be emphasized that the measured signal strengths of Mζ lines are much stronger than the given numerical values of relative intensities or transition probabilities. As an example the M spectrum of W is given in Fig.3. From the measured signal strength a relative intensity or transition probability of 5% to 10% with regard to Mα (M5N6, M5N7) seems to be more realistic. This strong Mζ line can be found in all investigated M spectra from Gd to Bi. Additionally, the origin of this line - M4N2 or M5N3 or a superposition of both transitions – leads to the question, is it an M4 or an M5 based line or is it both? Therefore, two assumptions were made: Mζ is an M5 based line (M5N3) and the best agreement with measured signal strengths can be found with a transition probability of 0.088. Consequently, the transition probability of Mα decreases from 1 to 0.088. The agreement between the measured and the computed response of Fig.3 supports these assumptions. Labar \(^{14}\) came to similar conclusions and proposed for M5N3 transitions probabilities three orders of magnitude larger than the tabulated values.
Reduced Response (Photons/pA/sr/s/keV)

Photon Energy (keV)

1.2 1.4 1.6 1.8 2 2.2 2.4

Conclusions

1. The agreement between experiment and theory has been improved by the description of the K spectra under consideration of the overvoltage ratio.
2. A further progress has been realized by the careful analysis of the M spectra of the elements from Gd to Bi.
3. The experiments were performed under an incidence angle of the electrons $\phi=90^\circ$ and a take-off angle of the x rays $\epsilon=35^\circ$. Therefore, it could be assumed that the numerical values of the present investigation are only valid for the given angles. But, earlier investigations of electron excited x-ray spectra in dependence on the angle of electron incidence demonstrated the possibility to extend the angular range of the validity of the algorithms by the ratio $\sin\phi \sin\epsilon$ in the absorption terms $f_{\text{abs,cont}}$ and $f_{\text{abs,jkl}}$. Thus, the results of the present investigation can be applied to the angular ranges of $\phi$ from $30^\circ$ to $90^\circ$ and of $\epsilon$ from $15^\circ$ to $65^\circ$.

References


Fig.3 Measured and computed M spectrum of W with M$\zeta$ (1.38keV), M$\alpha$ (1.78keV), M$\beta$ (1.84keV) and M$\gamma$ (2.04keV). The slightly higher measured values at photon energies around 1.6keV are from incomplete charge collection in the SiLi detector.