Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

doc. Ing. Tomáš Trojek, Ph.D.

Cesta k 3D rentgenové fluorescenční analýze

The way to 3D X-ray fluorescence analysis

Summary

This work summarizes some results of the author's twenty-year work on the improvement of the X-ray fluorescence analysis (XRF) at the Department of Dosimetry and Applications of Ionizing Radiation, FNSPE CTU in Prague. It is devoted to the development of techniques that have enabled non-destructive measurements of the elemental composition of objects with a heterogeneous structure. The aim was to design such instrumentation and to propose techniques of measurements and data evaluation that differences in surface or depth distributions of elements were possible to identify and quantify.

In the second half of the twentieth century, XRF was used as an analytical method for determining the elemental composition of samples which were taken, homogenized, and prepare in a suitable form before an XRF analysis. However, this approach began to change gradually. Especially in the last two decades, the effort is to apply XRF as an instrumental analytical method enabling to perform the analysis directly on a studied subject. Such analysis is non-destructive, and it can also determine how the individual elements are distributed in an investigated object.

The knowledge of 3D distributions of elements is more beneficial than the information on the averaged concentrations of elements obtained within the measurements of homogenized samples. For this purpose, XRF techniques were studied for a microanalysis, a 2D scanning of a surface, and a confocal XRF, which make us possible to determine elemental composition at a selected depth under a surface.

Souhrn

Tato práce shrnuje některé výsledky dvacetileté práce autora na zdokonalování metody rentgenové fluorescenční analýzy (RFA) na katedře dozimetrie a aplikace ionizujícího záření, FJFI ČVUT v Praze. Je věnována vývoji technik, které umožnily nedestruktivní měření prvkového složení předmětů s heterogenní strukturou. Ať už se jednalo o rozdíly v plošné distribuci prvků nebo byly studovány předměty obsahující vrstvy o různém složení, bylo snahou vyvinout takové přístrojové vybavení a postupy měření a vyhodnocování naměřených dat, aby byly tyto rozdíly v prvkovém složení identifikovány a kvantitativně popsány.

Rentgenová fluorescenční analýza sloužila v druhé polovině dvacátého století jako analytická metoda ke stanovení prvkového složení vzorků, které byly před analýzou odebrány, homogenizovány a převedeny do podoby vhodné k analýze. Tento přístup se však začal postupně měnit. Především v posledních dvou desetiletích je snahou využívat RFA jako instrumentální analytickou metodu, která nevyžaduje odběr vzorku a analýza může být provedena přímo na studovaném předmětu. Nejen že je taková analýza nedestruktivní, ale může také stanovit, jak jsou jednotlivé prvky v předmětu rozloženy, což je mnohem přínosnější než informace o průměrné koncentraci prvků získaná z měření homogenizovaných vzorků. Za tímto účelem byly studovány RFA techniky pro mikroanalýzu, 2D skenování plošného rozložení prvků a konfokální RFA, která umožňuje stanovit složení materiálu ve zvolené hloubce pod povrchem.

Klíčová slova

záření X, rentgenová fluorescenční analýza, měření in situ, kvantitativní analýza, zobrazování

Keywords

X-rays, X-ray fluorescence analysis, in situ measurement, quantitative analysis, imaging

Contents

1. Introduction …………………………………………………….. 6

2. Macro-X-ray fluorescence scanning ………………………… 7

3. Micro-X-ray fluorescence scanning ………………...…….. 8

4. Quantitative evaluation ……………………………………… 10

5. Depth analysis based on Kα/Kβ intensity ratio……………… 12

6. Application of Monte Carlo method in XRF………………… 13

7. Confocal X-ray fluorescence analysis……………………….. 17

8. Conclusions …………………………………………………. 20

References ……………………………………………………….. 21

Curriculum Vitae – doc. Ing. Tomáš Trojek, Ph.D. ……….…..... 23

1. Introduction

X-ray fluorescence analysis (XRF) is an analytical method based on excitation and detection of so-called characteristic X-ray radiation. In the case of handheld or small laboratory devices for energy dispersive XRF, typical instrumentation includes a miniature X-ray tube (source of X-rays for excitation and ionization of atoms in an investigated material) and a silicon detector providing X-ray spectrometry in energy range at least 2-30 keV with the energy resolution better than 190 eV for X-rays with energy of 5.9 keV. Such XRF systems provide information on chemical elements present close to a surface of a sample. The analyzed area depends to the diameter of an excitation beam (usually several millimeters) and the present chemical elements are detected up to the depth of tens or hundreds of micrometers depending on the material composition and the energy of characteristic X-rays. XRF method is used as a method of a qualitative analysis, as well as a quantitative analysis. The qualitative analysis consists in identification of individual elements in X-ray fluorescence spectra using the Moseley's law [1]. In quantitative analysis, elemental concentrations or a thickness of a thin layer is derived from the X-ray intensity (net peak area) of a particular X-ray line in an X-ray spectrum.

Main advantages of XRF:

- non-invasive analysis – XRF analysis can be performed without taking samples and an investigated object is not damaged.
- in-situ analysis – there are handheld or small portable XRF systems which make us possible to perform the measurements out of a laboratory.
- short acquisition time – analysis is very quick and first results are available within few seconds of a measurement.
- multi-elemental analysis – lot of elements can be identified within one analysis.

Main disadvantages and limitations of XRF:

- elemental analysis – XRF does not provide information on chemical compounds.
- identification of only heavier elements – light elements (with Z lower than about 13) cannot be detected due to low energy of their X-rays.
- surface analysis – only a surface area of an investigated object is analyzed due to high attenuation coefficient of characteristic X-rays in most of materials.
- quantitative analysis – quantitative XRF analysis is possible but it is difficult especially in the case of in-situ analysis.

2. Macro-X-ray fluorescence scanning

Standard X-ray fluorescence techniques enable only a point analysis which provides information on an averaged elemental composition in a volume given by the excitation beam diameter and the attenuation of the X-rays in a material. In some cases, it may be beneficial to visualize more accurately the element distribution on a selected area or even whole surface of an object under investigation. For this purpose, scanning techniques are used [2]. A measuring probe with a source and a detector slowly moves over a flat surface of an object and detects differences in composition in this preselected area. A narrow beam of X-rays strike upon the surface of an examined object and so-called characteristic X-rays are emitted. The results of this scanning are maps showing the areas with the highest and the smallest quantity of all measurable elements.

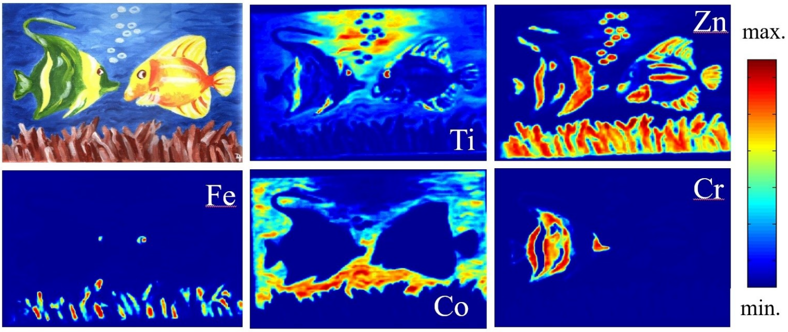

Fig. 1. Photograph of the painting “Two Fish” and the distributions of five elements obtained with macro-XRF scanning. Scanned area: 305 x 262.5 mm^2

The whole “Two Fish” painting was scanned with the XRF system with a Mini-X X-ray generator operated at a voltage of 35 kV. The net peak areas of the Kα lines of titanium (Ti), zinc (Zn), iron (Fe), cobalt (Co), and chromium (Cr) were automatically evaluated in a total of 12 810 X-ray spectra acquired with a step of 2.5 mm. The maps were drawn for each element. The results are shown in Figure 1 [3]. The highest net peak areas are indicated with a red color, and they display the regions where most of a given element (corresponding pigment) was applied. Lower net peak areas are related to a thinner layer of certain paint or indicate that this layer is overlapped with another layer. The distribution of a selected element is associated with a presence of a corresponding pigment or a group of pigments. Typically, titanium is present in titanium white (TiO_2), for instance.

Analytical capabilities of X-ray fluorescence for 2-dimensional elemental analysis were also tested on low-grade uranium-bearing sediments with unique sandstone-hosted U–Zr mineralization (Bohemian Cretaceous Basin, Czech Republic). The applied approach was aimed at the detection of uranium and zirconium, visualization of their distribution across mineralized lithological units and description of their relationships with associated elements. Maps of uranium, zirconium, and other identified elements demonstrated their patchy distribution and a frequent association of the elements with mineral fillings, see Figure 2 [4].

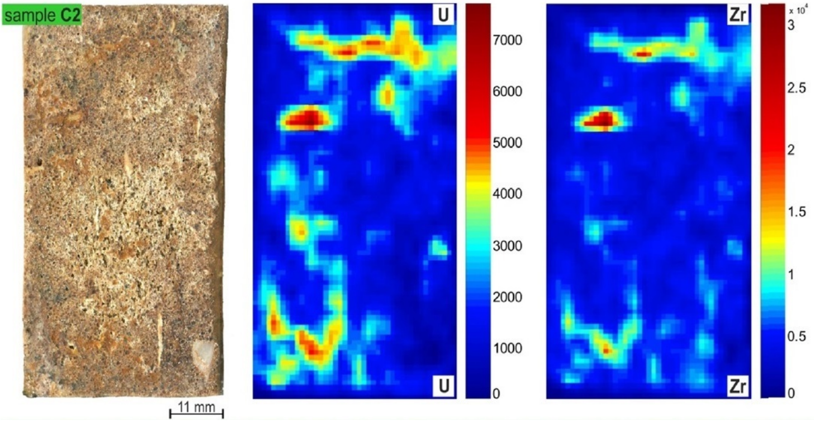

Fig. 2. Photograph from optical microscope (left) and surface distributions of uranium and zirconium obtained with macro-XRF scanning.

3. Micro-X-ray fluorescence scanning

Portable XRF systems for the point analysis and laboratory devices for the macro-scanning use X-ray sources with X-ray beams collimated to a diameter of a few millimeters. However, if better spatial resolution is required, further narrowing of the beam width with a collimator is undesirable because of a significant reduction of the beam intensity.

Fortunately, there are already ways how to narrow the X-ray beam diameter down to tens of micrometers. In micro-XRF, so-called polycapillary X-ray optics is used. This focusing is based on total reflection of X-rays in narrow curved glass capillaries. A microfocus X-ray tube with focusing polycapillary optics produces a narrowing beam reaching its minimum diameter at a certain distance from the optics. Thus, a diameter of analyzed area can be chosen from about 20 up to 500 μm by means of setting the distance of an object from this source. X-ray sources with a narrow micro-X-ray beam can be also used in scanning XRF systems and make us possible to draw elemental distribution in a microscopic scale.

Typical application of micro-XRF scanning is an investigation of archaeological artefacts, see Figure 3. A fragment of a silver enameled box, which was found at Hradisko near Mušov, was the subject of interest of this study [5]. The aim of micro-XRF scanning was to get information on elemental composition, and thus to contribute to correct dating of this archaeological find.

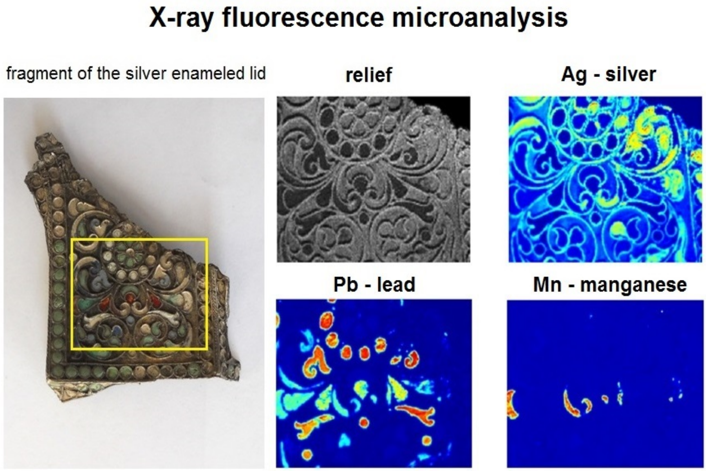

Fig. 3. Micro-XRF scanning of the lid, area: 25 x 32 mm^2, lateral resolution: 200 μm

The dating of this fragment into the Roman period was excluded by the discovery of traces of purple enamel colored with manganese and zinc, which does not occur in the ancient times.

X-ray florescence method can be even applied to organic samples and it was used to study of a survival response of Larix sibirica to the Tunguska explosion. The Tunguska explosion (June 30, 1908) resulted in catastrophic environmental changes in which only few trees near the epicenter survived.

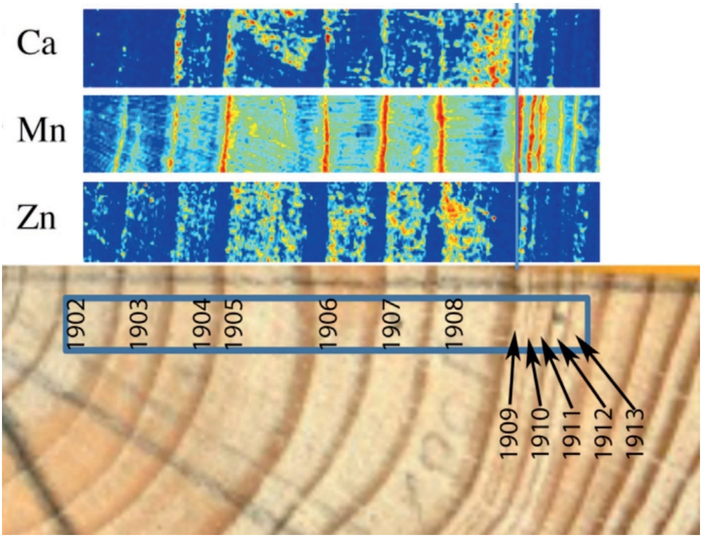

Fig. 4. micro-XRF profile across the wood section. Blue vertical line marks the 1908/1909 ring boundary

Figure 4 shows anomalies as a result of the Tunguska explosion. It indicates that Zn accumulated in the earlywood part of the xylem. At the time of Tunguska explosion, this part of the tree served as a main transport system for nutrients. The biochemical data revealed maxima of Ca, Mn in the bark/phloem tissue, consistent with the transport of compounds providing energy and structural building blocks [6].

4. Quantitative evaluation

The quantitative evaluation includes all processes leading to the determination of the quantity of individual chemical elements in a sample of unknown composition. While qualitative analysis consists in identifying a peak with a given energy in a spectrum, the quantitative analysis is based on the net peak areas of the individual elements in the spectrum. Usually only the most intensive X-ray line of an element is used for its quantification ($K\alpha$ or $L\alpha$ line).

Various quantitative methods have been already developed to determine the concentrations of elements in an analyzed sample. These methods differ in the number of reference materials required, demands on sample preparation, and the procedures of calculation of concentrations. A method called “Fundamental parameter method” seems to be the most appropriate in the case of analyzes performed directly on objects without sampling. It is based on known physical constants describing interaction of ionization radiation with matter and production of characteristic X-rays. In general, the relationship between the concentration and the net peak area of a given element may not be linear and is affected by the presence of other elements in a matrix. From a mathematical point of view, the net peak area of the given element is a function of the concentrations of all elements present in an analyzed volume. This is evident from the basic equation named after Jacob Sherman [7], which describes measured count rate of the K line (Kα or Kβ) of an element *i* with energy E_i:

$$\dot{N}_i(E_i) = \int_{\Omega_1}\int_{\Omega_2} \frac{\eta(E_i)}{4\pi\sin(\varphi_1)} \int_{E_{\min}}^{E_{\max}} C_i \tau_i(E_0)\varpi_{i,K} \frac{r_K - 1}{r_K} f\; S\; I(E_0)\, dE_0\, d\Omega_2\, d\Omega_1 \qquad (1)$$

where

$$S = \frac{1 - \exp\left\{-\rho\, T\left[\mu'(E_0) + \mu''(E_i)\right]\right\}}{\mu'(E_0) + \mu''(E_i)} \qquad (2)$$

$$\mu'(E_0) = \frac{\sum_j C_j \mu_j(E_0)}{\sin(\varphi_1)} \qquad \mu''(E_i) = \frac{\sum_j C_j \mu_j(E_i)}{\sin(\varphi_2)}$$

$\eta(E_i)$	detection efficiency of a detector for photon energy *E*
Ω_1	solid angle of incident photons
Ω_2	solid angle of detected photons
C_i	concentration of an element *i* (mass fraction)
$\tau_i(E_0)$	mass attenuation coefficient of photoelectric effect for element *i* and photon energy E_0
$\omega_{i,K}$	fluorescent yield for an element *i* and *K* series
r_K	ratio of mass attenuation coefficients of photoelectric effect for an element *i* for energy above and below K absorption edge
f	probability of Kα or Kβ transition
φ_1	incidence angle
φ_2	take-off angle
ρ	density of material
μ_j	mass attenuation coefficients for an element *i*
T	thickness of a sample
$I(E_0)$	intensity of the excitation beam

This equation includes only production of characteristic X-rays by the incident X-ray beam, and it does not consider emission of secondary (tertiary, etc.) characteristic X-rays produced by interaction of primary characteristic X-rays in an analyzed object [8]. The effects of other interactions are neglected too. The equation (1) also neglects the phenomena that occur in in-situ analyzes (variable distances, tilting of an object, surface effects, or heterogeneity of on object). Nevertheless, this equation allows to explain the basic principles of quantitative X-ray fluorescence analysis.

5. Depth analysis based on Kα/Kβ intensity ratio

In X-ray fluorescence analysis, various X-ray lines are produced with different intensities. Quantitative methods usually use the spectral net peak areas of Kα (or Lα) lines for calculating the element concentrations. The Kα/Kβ (or L lines) ratio then describes the depth distribution of an element [9].

The principle of the proposed Kα/Kβ technique lies in the different attenuation coefficients for the Kα and Kβ lines. If an element is deposited on the surface, the emitted X-rays are only slightly affected by absorption in an analyzed material. On the other hand, if an element is present at some depth in the specimen, its characteristic radiation must penetrate through a thick layer of the matrix, and the characteristic X-ray fluxes are significantly changed. The Kα/Kβ ratio is reduced because the attenuation coefficient for a Kα line is higher than for the line Kβ. An increase is possible only if a specimen contains an element with an absorption edge between these two lines. Then the Kβ line can be absorbed to a greater extent than the Kα line [10].

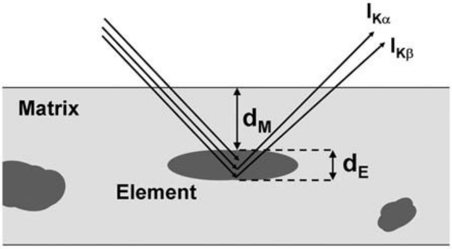

Fig. 5 Emission of characteristic X-rays from a heterogeneous specimen

This effect is evident from the equation (2) where higher attenuation coefficient for characteristic X-ray line of the energy E_i reduces the value of the parameter S. Although the energy difference of Kα and Kβ lines is not very high, the difference in the values of the attenuation coefficients causes a measurable variation in the Kα/Kβ ratio.

The Kα/Kβ ratio can be used to verify the sample homogeneity. For instance, it can identify that a given element is not distributed homogeneously but it is located at a certain depth d_M below the surface, see Figure 5 [11]. After a specimen has been analyzed, the element concentrations are calculated ‘‘conventionally’’ under the assumption that the sample is homogeneous. Based on the established composition, the Kα/Kβ ratios for all present elements are then calculated and compared with the ratios derived from the X-ray spectrum. If the depth distribution of the elements is inhomogeneous, the corresponding measured and computed Kα/Kβ ratios differ due to the different absorptions of the characteristic radiation. This measurement and calculation can provide primary information on the distribution of different elements and can confirm the correctness of the quantitative analysis.

6. Application of Monte Carlo method in XRF

It has been described that any heterogeneity in elemental depth distribution could significantly affect the shape of acquired X-ray spectra. The typical example is a presence of coating on a surface of a metallic object, see Figure 6. When brass reference material is covered with an iron foil of a thickness of 5 μm, the intensities of copper and zinc lines are reduced, and high peaks of iron appear in a spectrum. When a standard method of quantitative analysis (assuming homogeneity) is applied to such experimental data, it provides high concentrations of major elements (iron, copper, and zinc) and low concentration of lead. But this is a misleading result because iron is present dominantly only in the surface layer.

The quantitative analysis of heterogeneous samples can be based on modified equations (1) and (2). However, such approach becomes difficult if the experimental conditions and properties of a sample are more complicated. Another option is to use the Monte Carlo (MC) numerical method based on random number generator. This method is generally more time consuming but the results of XRF analyses can be predicted for almost arbitrary conditions of the measurements.

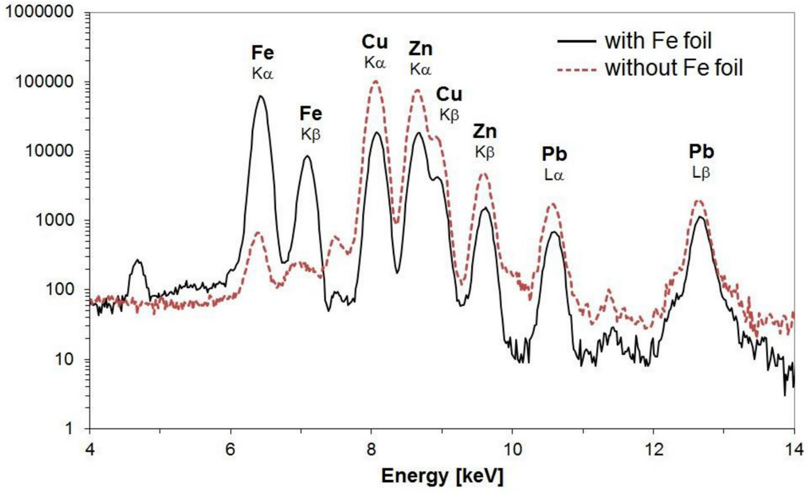

Fig. 6. X-ray spectrum of NIST SRM 1103 (brass) with and without 5 μm iron foil on its surface.

There are some MC codes and their various applications in the field of XRF. Application of MC method for radionuclide excitation XRF was described in [12]. The MCSHAPE code is a well-known code nowadays [13], and a Monte Carlo simulation code for confocal 3D micro-beam X-ray fluorescence analysis of stratified materials has been already developed [14].

The MCNP code was applied to the simulation of radiation transport in matter at the CTU in Prague. It is a Monte Carlo transport code for photons, neutrons, and electrons. A package for atomic relaxation processes is implemented, the emission of characteristic radiation is taken into account, and therefore the emission and interactions of X-rays in the material can be studied. If only X-ray counts or count rates of certain elements are to be determined, the computing time could be much shorter than for simulating of the whole detector spectrum. The calculation procedure for chosen characteristic X-ray lines is described in the article [15]. The MCNP code is a user-friendly Monte Carlo transport code suitable for photons with energy higher than 1 keV. Tally F5 implemented in this code enables to calculate X-ray fluence in a desired point which could be associated with a position of an X-ray detector. The X-ray fluences calculated at the point in front of the position of a real detector can be converted into X-ray count rates, if following requirements are fulfilled for an XRF setup, reference materials, and an investigated sample.

These requirements are:

a) geometric setup and X-ray source spectrum are known

b) a reference material of known composition is measured under the same conditions as an investigated sample

c) the reference material includes the same element which should be determined in the sample

Then the count rate of a certain X-ray line in a spectrum X-ray can be obtained with a simple formula (3),

$$N_s = N_R \frac{F_s}{F_R} \tag{3}$$

where is

N_S	predicted count rate for a sample *S*
N_R	measured count rate for a reference material *R*
F_S	computed fluence for a sample *S*
F_R	computed fluence for a reference material *R*

Monte Carlo method predicts the measurement results when experimental conditions, including the properties of a sample, are known and implemented in the computing code. Thus, the composition of the sample cannot be determined with only one simulation, but elemental concentrations or the coating thicknesses must be obtained with an iterative procedure, see Figure 7. The results are then shown in Figure 8 [16].

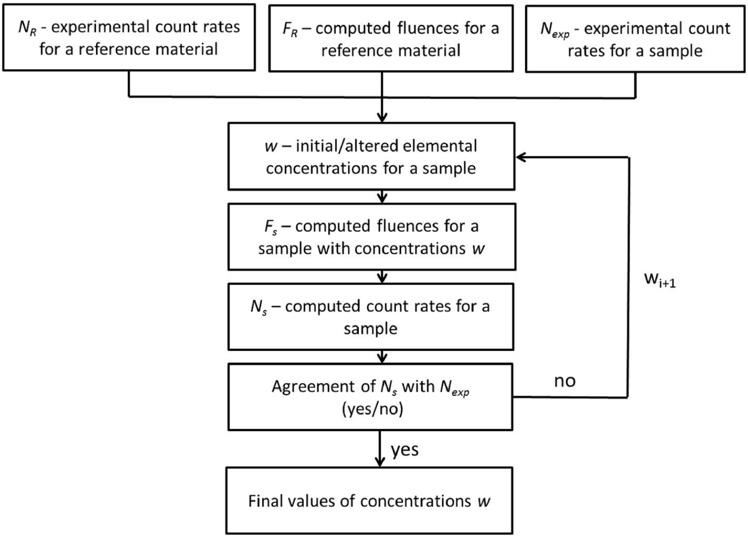

Fig. 7. Flowchart diagram of the Monte Carlo iterative procedure.

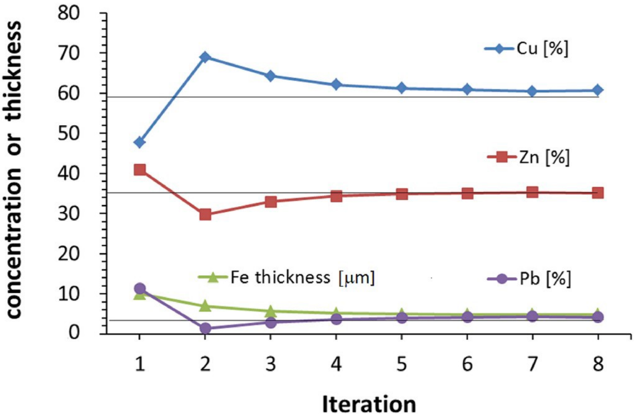

Fig. 8. Iterative Monte Carlo procedure for quantitative analysis of SRM 1103 considering Fe foil on its surface.

7. Confocal X-ray fluorescence analysis

Confocal X-ray fluorescence analysis is a promising analytical technique intended for non-destructive investigation of objects with a layered structure. Its principle consists in detection of characteristic X-rays from a small confocal volume that is defined by the overlap of the foci of the focusing and the collimating optics located at the source and the detector side of a confocal XRF setup, see Figure 9. Experimental setups for the confocal micro-XRF analysis differ in X-ray sources. It is possible to use a synchrotron beam [17, 18], or confocal XRF analysis has also been realized under laboratory conditions using X-ray tubes as an X-ray source [19, 20].

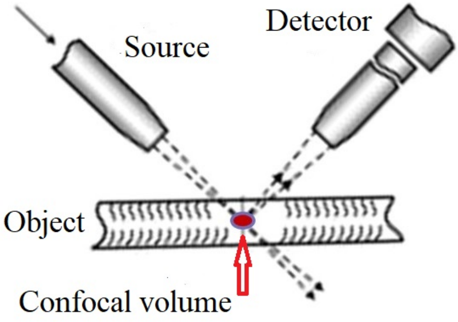

Fig. 9. Principle of confocal XRF – confocal volume is created by means of the intersection of the axes of the X-ray micro-beam and the collimation optics located in front of the detector.

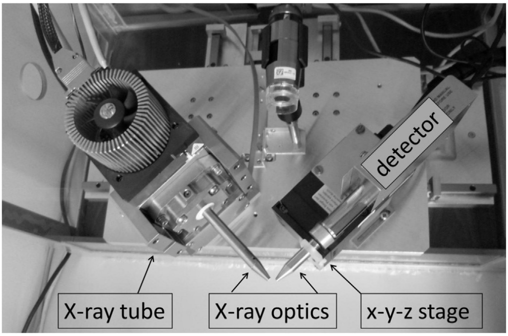

Fig. 10. Detailed view of the board with the main components of the confocal XRF device

The basis of the confocal XRF spectrometer developed at the CTU is a robust metallic board on which the XRF components are mounted, see Figure 10. The main XRF components include an X-ray source, a spectrometric detector, and two X-ray lenses. The board is movable along a horizontal plane thanks to two durable screw-bolts with stepping motors. While the shifting in one direction (perpendicular to the surface of the object) is necessary for depth profiling, the second one can be used for a surface line scan, for instance.

The properties of this new confocal XRF setup were tested with samples of paint layers - sample plate divided into 20 segments with various combinations of two single pigment layers. The result of confocal XRF analysis of one segment is shown in Figure 11. The signal of mercury was acquired close to the surface, while a lead containing layer is located approximately 20 µm deeper. Mercury is present in a red pigment – vermilion HgS. Lead is a part of typical medieval white pigment – lead white $2PbCO_3 \cdot Pb(OH)_2$. This result is consistent with the stratigraphy of this segment shown in the Figure 12. It consists of a ground covered with a layer of lead white and a layer of vermilion is present on the surface [21].

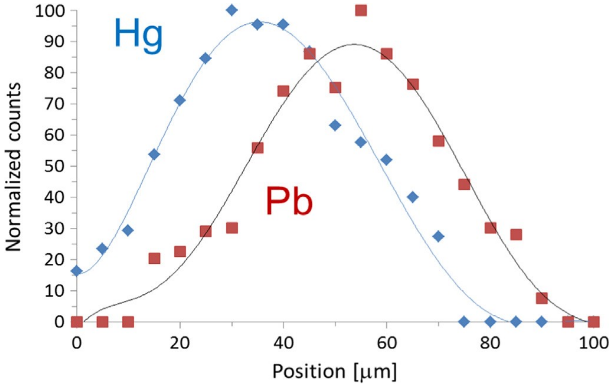

Fig. 11 The normalized count rates of the Lα lines of mercury and lead obtained with confocal XRF depth profiling.

It has been demonstrated that the depth profiling with this confocal XRF system enabled us to recognize paint layers with various historical pigments in the prepared sample plate. Of course, the analysis suffers from the expectable limitation arising generally from the interaction of X-rays with matter. It was possible to measure the characteristic X-rays with a sufficient count rate for all heavier elements present in the pigments. If an upper layer was too thick, we were not able to detect those elements from a bottom layer whose characteristic radiation had a high attenuation coefficient in the material of an upper layer.

Besides the relatively low weight of the new confocal device, enabling its transport, the setup has other advantages thanks to the movable collimating optics connected to the x–y–z stage. Firstly, the searching for the confocal configuration is quite quick and comfortable. Secondly, the collimating optics can be ejected and the confocal-XRF is then changed into a micro-XRF setup. Finally, the proper shifting of the collimation optics can switch the preference for high-count rate to better depth resolution.

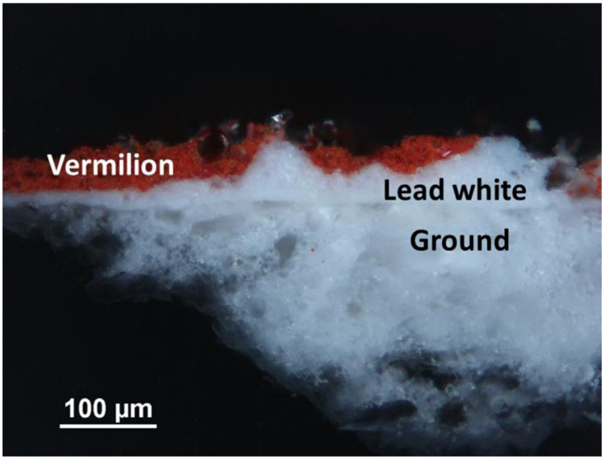

Fig. 12. Cross-section of a micro-sample with two paint layers

The quantitative evaluation of data in confocal XRF is a difficult task and its theory and application are described in the certified methodology [22]. It seems that the precise determination of concentrations of individual elements versus a depth in a general object of unknown composition is not yet possible. Therefore, the attention is paid to recognition of individual layers, determination of their thicknesses, and assignment of identified elements to those layers in an object.

8. Conclusions

This brochure deals with the author's work on a long way from classical XRF instruments used for point analyses of samples to non-invasive and non-contact 3D analyses of valuable objects that must not be damaged within their investigation. All presented results were achieved in the X-ray fluorescence laboratory at the Department of Dosimetry and Application of Ionizing Radiation, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague.

As can be seen, such development is based on three linked pillars. The first pillar includes the construction of own devices from available components for various XRF techniques. It allowed to analyze small details on the surface of investigated objects, to scan selected surface areas of objects in micro- and macro-scale, and finally to determine the depth distribution of elements. The reason for the construction of such devices was a lack of suitable commercial products. Even today after many years of using 2D scanning XRF techniques at the CTU, it is still not a standard and commonly available technique. There are no commercially available devices for confocal XRF even today, and this technique is only being developed in research institutions. Using our own instruments was advantageous due to the flexibility, as the instrument's properties can be easily changed with respect to measurement requirements. This is also beneficial from a pedagogical point of view because students can easily familiarize with the advantages and disadvantages of a particular configuration.

The second pillar of this work is the development of new measurement and data evaluation procedures. These include methods for the recognition of a layered structure, elimination of surface effects, or the quantitative analysis using the Monte Carlo method.

The last pillar is represented by XRF applications in various fields. With respect to the advantages and disadvantages of XRF, this method is used to investigating of art and historical objects, industrial materials, as well as geological and some biological samples. Especially in the case of heritage science, XRF is one of the key methods because it is non-destructive and can provide at least basic information on elemental composition very quickly. Thus, XRF is often used to examine non-standard objects and samples, which requires an individual approach. Thanks to the feedback from the end-users, XRF instruments and measurement techniques can be further improved in such a way that they would be best adapted to real requirements.

References

[1] MOSELEY, H. G. J. The High-Frequency Spectra of the Elements. Part II". *Philosophical Magazine and Journal of Science*. 1914, 6, 27, 703-713

[2] ALFELD, M., et al. A mobile instrument for in situ scanning macro-XRF investigation of historical paintings. *Journal of Analytical Atomic Spectrometry*. 2013, 28(5), 760-767

[3] TROJEK, T. and D. TROJKOVÁ. Several approaches to the investigation of paintings with the use of portable X-ray fluorescence analysis. *Radiation Physics and Chemistry*. 2015, 116, 321-325

[4] MIKYSEK, P., et al. X-ray fluorescence mapping as a first-hand tool in disseminated ore assessment: sandstone-hosted U–Zr mineralization. *Minerals Engineering*. 2019, 141, 1-13

[5] HLOŽEK, M., et al. Recent or Roman enamel? Resolution of dating of the unique find from Mušov - Burgstall using techniques of X-ray fluorescence analysis. *Radiation Physics and Chemistry*. 2020, 167, 108254

[6] KLETETSCHKA, G., et al. Survival Response of Larix Sibirica to the Tunguska Explosion. *Tree-Ring Research*. 2017, 73(2), 75-90

[7] SHERMAN, J. The theoretical derivation of fluorescent X-ray intensities from mixtures. *Spectrochimica Acta*. 1955, 7, 283-306

[8] ROUSSEAU, R. M. Corrections for matrix effects in X-ray fluorescence analysis-A tutorial. *Spectrochimica Acta Part B: Atomic Spectroscopy*. 2006, 61, 7, 759-777

[9] NEELMEIJER, C., et al. Paintings— a challenge for XRF and PIXE analysis, *X-ray Spectrometry*. 2000, 29, 101-110

[10] TROJEK, T., T. ČECHÁK, L. MUSÍLEK. Techniques for depth heterogeneity identification in X-ray fluorescence. *Nuclear Instruments and Methods in Physics Research B*. 2007, 263, 76-78

[11] TROJEK, T., T. ČECHÁK, L. MUSÍLEK. Kα/Kβ Ratios of Fluorescence X-rays as an Information Source on the Depth Distribution of Iron in a Low Z Matrix. Analytical Sciences, 2008, 24, 851-854

[12] YAP, C. T., and P. P. SALIGAN, 1986. A Monte Carlo approach to X-ray analysis at low energies using an annular 55Fe source. *Nuclear Instruments and Methods in Physics Research A*. 1986, 251 (1), 140-143

[13] SCOT, V., et al. 3D extension of the Monte Carlo code MCSHAPE for photon-matter interactions in heterogeneous media. *Nuclear Instruments and Methods in Physics Research B*. 2007, 263, 204-208

[14] CZYZYCKI, M., et al. Monte Carlo simulation code for confocal 3D micro-beam X-ray fluorescence analysis of stratified materials. *X-ray Spectrometry*. 2011, 40, 88-95

[15] TROJEK, T., and T. ČECHÁK. Use of MCNP code in energy dispersive X-ray fluorescence. *Nuclear Instruments and Methods in Physics Research B*. 2007, 263, 72-75

[16] TROJEK, T. Iterative Monte Carlo procedure for quantitative X-ray fluorescence analysis of copper alloys with a covering layer. *Radiation Physics and Chemistry*. 2020, 167, 108294

[17] JANSSENS, K., K. PROOST and G. FALKENBERG. Confocal microscopic X-ray fluorescence at the HASYLAB microfocus beamline: characteristics and possibilities. *Spectrochimica Acta Part B: Atomic Spectroscopy*. 2004, 59(10-11), 1637-1645.

[18] WOLL, A.R., et al. Development of confocal X-ray fluorescence (XRF) microscopy at the Cornell high energy synchrotron source. *Applied Physics A*. 2006, 83(2), 235-238

[19] KANNGIESSER, B., et al. Three-dimensional micro-XRF investigations of paint layers with a tabletop setup. *Spectrochimica Acta Part B: Atomic Spectroscopy*. 2005, 60(1), 41-47.

[20] LIN, X., et al. Characterization and applications of a new tabletop confocal micro X-ray fluorescence setup. *Nuclear Instruments and Methods in Physics Research Section B*. 2008, 266(11), 2638-2642

[21] TROJEK, T., et al. Confocal X-ray fluorescence spectrometer for in-situ analyses of paintings. *Radiation Physics and Chemistry*. 2017, 137, 238-242.

[22] PROKEŠ, R. and T. TROJEK. Konfokální rentgenová fluorescenční analýza, certified methodology, 2018, FJFI, ČVUT v Praze

Curriculum Vitae

doc. Ing. Tomáš Trojek, Ph.D.

Born: February 6, 1978 in Ostrava

E-mail: tomas.trojek@fjfi.cvut.cz

	Education and diplomas
2013	doc., Applied Physics, FNSPE, CTU in Prague
2001 - 2006	Ph.D., Nuclear Engineering, FNSPE, CTU in Prague
1996 - 2001	Ing., Dosimetry and Application of Ionizing Radiation, FNSPE, CTU in Prague

	Professional Experience
2001 – now	Department of Dosimetry and Application of Ionizing Radiation, FNSPE, CTU in Prague, Czech Republic 2001 – 2006 Assistant 2006 – 2011 Secretary of department 2011 – 2014 Deputy head of department 2012 – 2014 Chairman of Academic Senate of FNSPE 2014 – now Head of department
2001 - 2010	Experiment DIRAC, CERN, Switzerland (1 month yearly as the CTU employee)
2009 - now	Czech Accreditation Institute, ISO 17025 professional evaluator
2015 - now	International Radiation Physics Society, executive councillor

	Internship
2005, 2006	International Atomic Energy Agency, Seibersdorf, Austria, 2 x 1 month
2004	Joint Institute for Nuclear Research, Dubna, Russia, 1 month
2003	Universidad Politécnica de Valencia, Velencia, Spain, 5 weeks
2002	Institut Supérieur Industriel de Bruxelles, Brussels, Belgium, 3 months

Research interests

X-ray fluorescence analysis, spectrometry of ionizing radiation, application of Monte Carlo method, dosimetry of ionizing radiation

Pedagogical and scientific activities	
Papers in impacted journals	62
Citations in Scopus with/without self-citations	631/405
H-index with/without self-citations	15/10
Defended doctoral theses	5
Defended master's theses	8
Defended bachelor's theses	3
International scientific projects	2
National scientific projects	12

Selected projects

CAAS - Centre of Advanced Applied Sciences, OPVVV, EF16_019/0000778, 2018-2023

AD-BANG - Advanced Detectors for Better Awareness of Neutrons and Gamma rays in environment, Norway grants, 7F14358, 2014-2017

RadoNORM - Towards effective radiation protection based on improved scientific evidence and social considerations, Horizon 2020, 900009, 2020-2025

Historical technologies and modern methods of research. The interpretative possibilities of the specialized methods of the research of the medieval artworks using the innovative technologies, NAKI, DF13P01OVV010, 2013-2017

Selected publications

TROJEK, T. Iterative Monte Carlo procedure for quantitative X-ray fluorescence analysis of copper alloys with a covering layer. *Radiation Physics and Chemistry*. 2020, **167**. DOI: 10.1016/j.radphyschem.2019.04.044. ISSN 0969806X.

TROJEK, T. a H. BÁRTOVÁ. Calibration of handheld X-ray fluorescence spectrometer for identification and semi-quantitative analysis of objects with stratified structure. *Radiation Physics and Chemistry*. 2019, **155**, 310-314. DOI: 10.1016/j.radphyschem.2018.08.004. ISSN 0969806X.

TROJEK, T. a L. MUSÍLEK. X-ray fluorescence – a non-destructive tool in investigation of Czech fine and applied art objects. *Radiation Physics and Chemistry*. 2017, **137**, 230-233. DOI: 10.1016/j.radphyschem.2017.01.007. ISSN 0969806X.

TROJEK, T. a D. TROJKOVÁ. Several approaches to the investigation of paintings with the use of portable X-ray fluorescence analysis. *Radiation Physics and Chemistry*. 2015, **116**, 321-325. DOI: 10.1016/j.radphyschem.2015.01.002. ISSN 0969806X.

TROJEK, T. Reconstruction of the relief of an investigated object with scanning X-ray fluorescence microanalysis and Monte Carlo simulations of surface effects. *Applied Radiation and Isotopes*. 2012, **70**(7), 1206-1209. DOI: 10.1016/j.apradiso.2011.11.012. ISSN 09698043.

TROJEK, T. a M. HLOŽEK. X-ray fluorescence analysis of archaeological finds and art objects: Recognizing gold and gilding. *Applied Radiation and Isotopes*. 2012, **70**(7), 1420-1423. DOI: 10.1016/j.apradiso.2012.03.033. ISSN 09698043.

TROJEK, T. Reduction of surface effects and relief reconstruction in X-ray fluorescence microanalysis of metallic objects. *Journal of Analytical Atomic Spectrometry*. 2011, **26**(6). DOI: 10.1039/c0ja00187b. ISSN 0267-9477.

TROJEK, T. a D. WEGRZYNEK. X-ray fluorescence Kα/Kβ ratios for a layered specimen: Comparison of measurements and Monte Carlo calculations with the MCNPX code. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*. 2010, **619**(1-3), 311-315. DOI: 10.1016/j.nima.2009.10.157. ISSN 01689002.

TROJEK, T., M. HLOŽEK, T. ČECHÁK a L. MUSÍLEK. X-ray fluorescence analyzers for investigating postmediaeval pottery from Southern Moravia. *Applied Radiation and Isotopes*. 2010, **68**(4-5), 879-883. DOI: 10.1016/j.apradiso.2009.10.038. ISSN 09698043.