

**QUANTITATIVE CHARACTERIZATION OF STRATIFIED MATERIALS BY CONFOCAL 3D
MICRO-BEAM X-RAY FLUORESCENCE SPECTROSCOPY.
MONTE CARLO SIMULATION VS. FUNDAMENTAL PARAMETERS MODEL**

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Nowadays, heterogeneous, stratified structures are utilized in many areas of surface and materials technology. Multi-layered components are commonly used in many branches of modern industry: e.g. electronics (dielectric coating for superconductor devices), energy production and storage (new rechargeable lithium batteries), optics (optical fibre), environmental solutions (functional membranes for gas separation), automotive industry (lacquer systems) and in biomedical applications (biosensors, biocatalysts and biopharmaceuticals). Examination of chemical composition of individual layers and determination of their thickness helps to get information on their properties and function. A confocal 3D micro X-ray fluorescence (3D μ XRF) spectroscopy is an analytical method giving the possibility to investigate 3D distribution of chemical elements within a sample with spatial resolution in micrometer regime in non-destructive way.

This paper demonstrates the practical application of the recently developed Monte Carlo (MC) simulation of the 3D μ XRF experiment on stratified materials. The MC code simulates interaction between X-ray photons and matter. The fate of each impact photon from polarized or unpolarized beam is being tracked from the point where it leaves a focusing optics, through sample penetration until detection in the X-ray detector. Primary and secondary fluorescence and multiple photon scattering effects are considered in this code. Results of the MC simulation were compared against predictions of a fundamental parameter model proposed to 3D μ XRF of multi-layered samples.

The stratified materials with thickness up to 200 μ m based on polymer matrix doped with small quantities of Fe_2O_3 and Cu_2O oxides were examined with synchrotron radiation as test samples. The investigated samples were scanned in depth to obtain profiles of X-ray fluorescence peak intensity of elements. Correlation coefficients between experimental vs. simulated and experimental vs. analytical model X-ray profiles were calculated. The homogeneity of areal dispersion of elements and depth-resolved distribution of elements within the samples were evaluated with statistical methods.

In order to perform a quantitative analysis, i.e. to determine chemical composition and thickness on individual layers, the experimental profiles were deconvoluted with the iterative MC simulation and with the fundamental parameter model.

The performed investigation allowed to test capabilities and limitations of the MC simulation and the fundamental parameter model to quantitative characterization of the stratified materials.