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BadgerFilm: a versatile thin film analysis program for EPMA and more

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Electron probe microanalysis (EPMA) is a technique widely used to identify and quantify materials. The most recent EPMA quantification methods use models that accurately describe the ionization depth distribution, the so-called phi-rho-z distribution. While these models were first developed to quantify bulk samples, extensive research efforts have been made in the 1990's to extend their applicability to the analysis of layered specimens. Several phi-rho-z models for thin film quantifications have been published, such as PAP, XPP [1] or XPHI [2]. However, their implementation into actual computer programs that can be used by EPMA labs is scarce and their availability is limited, either because of compatibility problems with modern computers or because of the cost of the license to acquire the program. In an intent to give more access to thin film analysis tools to EPMA labs, we have developed BadgerFilm, a free and open-source thin film analysis software [3,4]. The main purpose of BadgerFilm is to determine the compositions and thicknesses of thin film specimens by EPMA. The program uses the multi-voltage method in which experimental k-ratios are measured at several accelerating voltages. The algorithm iterates on the composition and thickness of the films (or substrate) until the calculated k-ratios match the experimental k-ratios. Complex multilayered specimen can easily be analyzed using this method. For example, it is possible to determine composition and thicknesses of a bilayer of Ni-Cr/Fe-Gd-Pt on top of a Si substrate [5]. As shown on Figure 1, BadgerFilm produces results in good agreement with experimental measurements. The results were also shown to agree well with results obtained with other thin film analysis programs and other thin film characterization techniques (e.g., the Rutherford Backscattering technique) [4]. However, the capabilities of the program go beyond the characterization of multilayers specimens. BadgerFilm can be used to accurately quantify bulk samples [3]. During the analysis of geological materials, oxygen is sometimes difficult to quantify – because of interferences (especially with EDS detectors), because of the difficulty of having an accurate, stable, O standard, or to reduce the analysis time – and is determined by stoichiometry relative to the other elements. BadgerFilm implements the possibility of quantifying materials using O defined by stoichiometry as well as another element defined by stoichiometry relative to O. For example, a dolomite sample, of stoichiometric formula CaMg(CO3)2, can be quantified by only measuring Ca and Mg (and trace elements such as Fe and Sr) and by calculating O and C by stoichiometry. Multi-voltage measurements traditionally used for thin film analysis can also be utilized in BadgerFilm to determine mass absorption coefficients (MACs). By knowing the composition and geometry (film thickness) of the sample, the MAC of a given element and characteristic X-ray line absorbed by another element or itself (self-absorption) can be determined. The MAC is set as a free parameter and the fitting algorithm will iterate on its value until the calculated k-ratios match the experimental k-ratios. As an example, the MAC of Si Kα by Hf can be measured by recording the Si Kα X-ray intensity on a HfSiO4 samples at several accelerating voltages. The fitting algorithm will then find the MAC value that gives the best agreement between measured and calculated X-ray intensities (Figure 2). BadgerFilm is a versatile, free, thin film analysis program, able to quantify multilayered specimens as well as bulk materials. By comparison with most software that are "black boxes" – which sometime makes it difficult to understand the internal mechanisms and interpret the data – BadgerFilm is open-source and was designed to be easily modifiable. Its flexibility allows the program to easily be adapted to solve other types of problems. BadgerFilm can be downloaded at this address:

https://github.com/Aurelien354/BadgerFilm

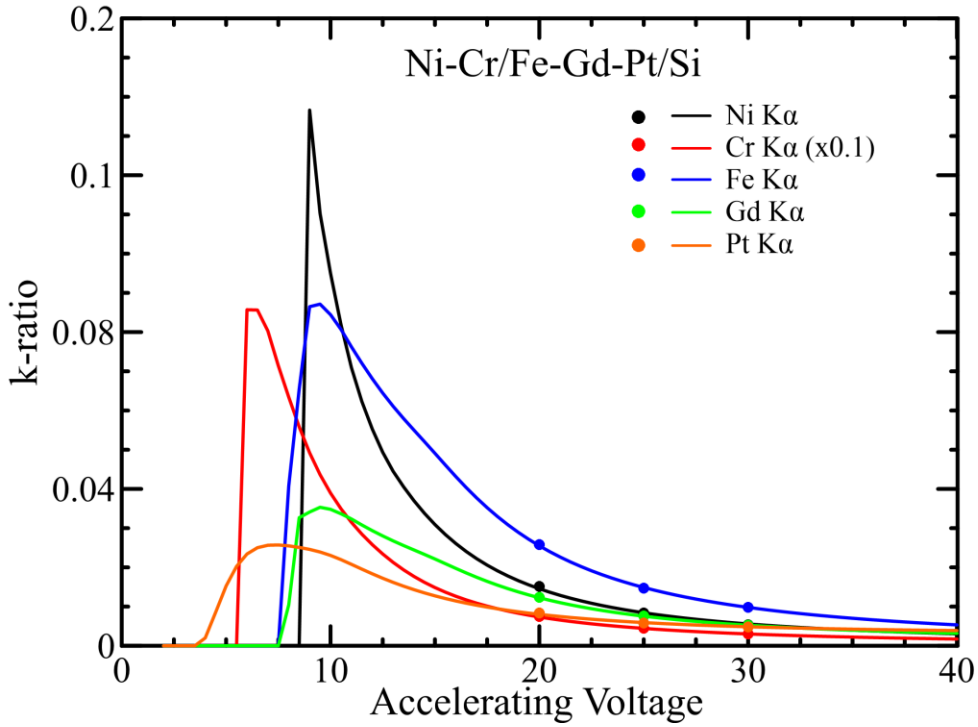

Figure 1. Experimental (dots) [5] and calculated (lines) k-ratios for a Ni-Cr/Fe-d-Pt/Si multilayer. Compositions and thicknesses were set as unknown and iterated on until the calculated data match the experimental data.

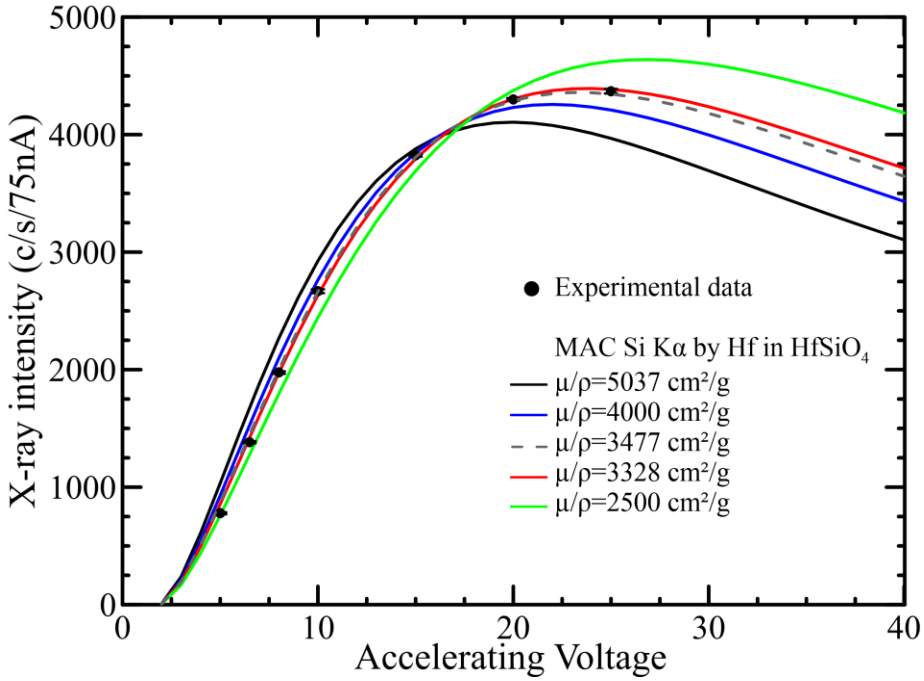

Figure 2. Si Kα X-ray intensities measured at several accelerating voltages (dots). Calculated X-ray intensities are fitted to the experimental data by varying the Si Kα by Hf MAC from 5037 cm²/g (original MAC value from Heinrich's MAC30 MACs algorithm [6]) to 2500 cm²/g. The best fit was obtained for a MAC value of 3328 cm²/g. This number is very close to the value of 3477 cm²/g experimentally found by J. Donovan in 2011, available in Probe for EPMA and CalcZAF [7].

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