A Versatile Fundamental Parameter Software for Quantification in XRF Considering Various Spectral Modification Modes Including X-ray optics

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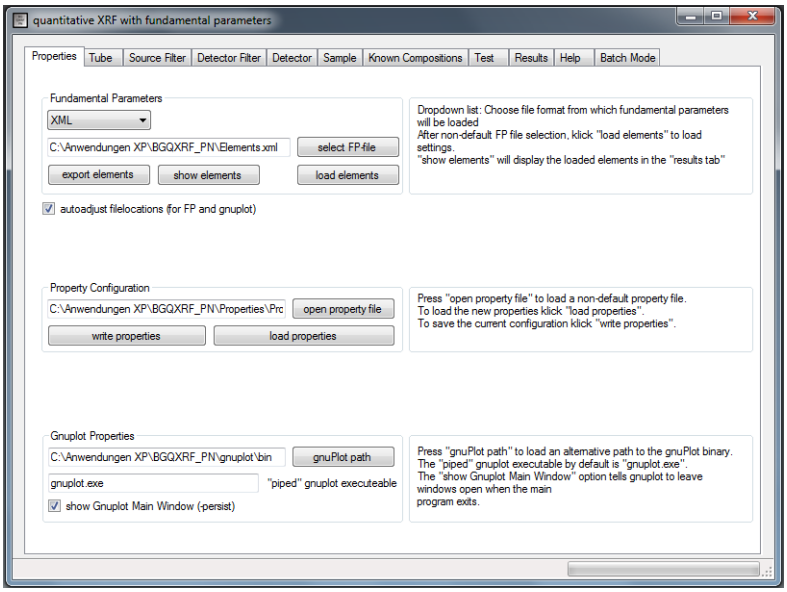
In this presentation all steps to perform a quantitative XRF analysis are demonstrated. Data obtained from fitting of a measured spectrum through background subtraction and peak deconvolution - i.e. net counts of the elements in a sample, serves as basic input information for the quantitative results. A versatile software package ATI-QUANT developed at Atominstitut, TU Wien in scope of several Master's theses is applied to obtain quantitative information. The software is taking into account all experimental data of source, sample and detector. In particular, following tube parameters are considered: anode material, details of the tube design, e.g. electron incident/photon emission angle, window material and thickness, solid angle for the emission/detection, finally data of high voltage and current - thus allowing the calculation of the source photon flux on the sample. Further, the originally calculated tube spectra can be corrected according to the usage of spectral modification devices. This typically includes filter materials or high energy cut-off reflectors, multilayers or crystals, resulting in a quasi- or monoenergetic beam. Moreover, changes in the spectral distribution by using polycapillaries can be simulated by applying mathematical functions. The detector parameters are requested to calculate the efficiency, and even a filter in front of the detector can be added. User can choose between thin films, intermediate and thick sample for further fundamental parameters calculations. ATI-QUANT is not only correcting for absorption, but also respects inter-element effects. The software factors in various experimental conditions, e.g. analysis in total reflection geometry with internal standard; thick/thin samples, or presence of oxides. Results from standard reference materials measured under different conditions are presented to show the applicability of various excitation conditions.



References:

1. B.Großmayer, master thesis TU Wien, 2008
2. Philip Necker, master thesis TU Wien 2017