Comparison of four data analysis software for combined X-ray reflectivity and grazing incidence X-ray fluorescence measurements

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X-ray specular reflectivity (XRR) is a non-destructive method for the characterization of multi-layered structures that provides highly accurate information on layers thickness, roughness and in-depth electronic density. Angle-dependent grazing incidence X-ray fluorescence (GIXRF) provides information on the elemental depth distribution and has been widely used to investigate thin films on substrate [1]. As these techniques are based on similar measurement procedures and data evaluation approaches, their combination reduces the uncertainties of the individual techniques and provides an accurate depth-resolving analysis of multilayers [2]. Several software have recently been developed to perform the combined modeling of XRR and GIXRF.

Our study focuses on the comparison of four combined XRR-GIXRF data analysis software (Maud [3], jGixa [4], Gimpy and MedePy). For each software, the representation of the layers, the atomic database used for X-ray calculations, the formalism implemented, the data reduction algorithms as well as the method to correct the effect of the geometrical factor on the measured angle-dependent fluorescence intensity are described and compared. Indeed, as the GIXRF signals depend on experimental setup parameters, a geometrical factor has to be evaluated when comparing theoretical calculations and experimental data [5].

Each XRR and GIXRF combined fitting methods have been compared with respect to their performance in diverse situations using simulated data (Figures 1 and 2), and using experimental data acquired on a Ni (50nm)/SiO$_2$/Si sample measured on a laboratory tool equipped with a Molybdenum tube.

![Fig. 1: XRR simulation software comparison](image1.png)

![Fig. 2: GIXRF simulation software comparison](image2.png)