JGIXA – a software package for the calculation and fitting of grazing incidence X-ray fluorescence and X-ray reflectivity data for the characterization of nanometer-layers and ultra-shallow-implants

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Grazing Incidence XRF (GIXRF) is a TXRF related technique, which is making use of the phenomenon of total external reflection of X-rays on smooth polished surfaces. As the penetration depth of the incident X-ray beam in the total-reflection regime is very small, i.e. in the order of only a few nanometers, the XRF spectra represent the elemental concentrations of this near surface region. Furthermore, varying the angle of incidence in the grazing incident regime and collecting XRF spectra at several angle positions results in angle dependent intensity curves for each element, which contain information on depth distribution and mass density of the elements in the sample. By fitting calculated curves to these experimental data, density and thickness of layers or depth distributions of implanted atoms can be determined.

Since the downscaling of the process size for semiconductor devices has reduced junction depths as well as layer thicknesses to just a few nanometers, a length scale where GIXRF is highly sensitive, the method has experienced a revival as a complimentary technique (e.g. to Secondary Ion Mass Spectrometry) and also on its own as a powerful non-destructive tool for process analysis and control in the fabrication of semiconductor devices.

In order to overcome an ambiguity of GIXRF concerning the exact distribution function for implants and a correlation of thickness and density for layers, the method is combined with X-ray reflectometry (XRR) as both techniques use similar measurement procedures and data evaluation strategies. Moreover, the physical properties for the calculation can be derived directly from the same sample model, thus making the approach straightforward. This combined analysis reduces the uncertainties of the parameters of the individual techniques.

The software JGIXA, which was programmed in Java and MATLAB, was specifically developed for the simultaneous calculation and fitting of GIXRF and XRR data, but also allows separate evaluation. The quality of the fit is determined via a total chi-square value of all available measurement data and the refinement of sample parameters is done by using global optimization algorithms. The software is available on multiple platforms and equipped with a user-friendly graphical user interface (GUI). Several evaluation examples for implants as well as layers in/on Silicon, which were obtained using the software, will be presented.