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Combined evaluation of grazing incidence X-ray fluorescence and X-ray reflectivity data for improved profiling of ultra-shallow depth distributions☆

D. Ingerle [a,]*, F. Meirer [b], G. Pepponi [c], E. Demenev [c], D. Giubertoni [c], P. Wobrauschek [a], C. Streli [a]

[a] *Atominstitut, Vienna University of Technology, Stadionallee 2, A-1020 Vienna, Austria*
[b] *Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Universiteitsweg 99, 3584 CG Utrecht, Netherlands*
[c] *MiNALab, CMM-irst, Fondazione Bruno Kessler, Via Sommarive 18, I-38050 Povo, Italy*

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ABSTRACT

The continuous downscaling of the process size for semiconductor devices pushes the junction depths and consequentially the implantation depths to the top few nanometers of the Si substrate. This motivates the need for sensitive methods capable of analyzing dopant distribution, total dose and possible impurities. X-ray techniques utilizing the external reflection of X-rays are very surface sensitive, hence providing a non-destructive tool for process analysis and control.

X-ray reflectometry (XRR) is an established technique for the characterization of single- and multi-layered thin film structures with layer thicknesses in the nanometer range. XRR spectra are acquired by varying the incident angle in the grazing incidence regime while measuring the specular reflected X-ray beam. The shape of the resulting angle-dependent curve is correlated to changes of the electron density in the sample, but does not provide direct information on the presence or distribution of chemical elements in the sample.

Grazing Incidence XRF (GIXRF) measures the X-ray fluorescence induced by an X-ray beam incident under grazing angles. The resulting angle dependent intensity curves are correlated to the depth distribution and mass density of the elements in the sample. GIXRF provides information on contaminations, total implanted dose and to some extent on the depth of the dopant distribution, but is ambiguous with regard to the exact distribution function.

Both techniques use similar measurement procedures and data evaluation strategies, i.e. optimization of a sample model by fitting measured and calculated angle curves. Moreover, the applied sample models can be derived from the same physical properties, like atomic scattering/form factors and elemental concentrations; a simultaneous analysis is therefore a straightforward approach. This combined analysis in turn reduces the uncertainties of the individual techniques, allowing a determination of dose and depth profile of the implanted elements with drastically increased confidence level.

Silicon wafers implanted with Arsenic at different implantation energies were measured by XRR and GIXRF using a combined, simultaneous measurement and data evaluation procedure. The data were processed using a self-developed software package (JGIXA), designed for simultaneous fitting of GIXRF and XRR data. The results were compared with depth profiles obtained by Secondary Ion Mass Spectrometry (SIMS).

1. Introduction

1.1. Historical

Grazing incidence x-ray fluorescence (GIXRF) is a surface sensitive technique for the characterization of dopant profiles and thin layers in the nanometer regime on flat and smooth surfaces. The grazing incidence angular dependence of the X-ray fluorescence signal provides information on the depth distribution and total concentration per unit area of the elements in the near surface region. At glancing incidence the predominant part of the incident radiation is reflected and forms – within the limits of coherence – standing waves above the surface while the other part of the field intensity penetrates into the refracting medium as an evanescent wave. In 1954 Parratt [1] first showed in his seminal paper how the modulation of the electromagnetic field can be calculated as a function of the angle of incidence based on reflection, refraction and interference in the vicinity of a flat, sufficiently smooth

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* Corresponding author. Tel.: +43 1 58801 141338; fax: +43 1 58801 14199.
E-mail address: dingerle@ati.ac.at (D. Ingerle).

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surface. He also proposed a recursive method for the calculation in the presence of stratified media. Parratt implemented the complete field calculation for the prediction of the reflected part of the beam not only paving the way for X-ray reflectivity (XRR) analysis but also providing the basis for GIXRF analysis. In fact, once the field is known, the number of photoelectric absorption events and hence fluorescence photons can be predicted. This was first demonstrated in 1983 by Becker et al. for a homogeneous sample [2] where an exponentially decaying field excites the atoms in the material. In 1986 Iida et al. [3] used this approach for the study of an Arsenic implanted layer in silicon at a synchrotron radiation facility. In 1991 de Boer [4] published a thorough derivation of the fluorescence emitted from layered samples based on the calculation of the derivative of the Poynting vector through the calculation of the reflection and transmission coefficients at each layer and making use of Parratt's recursive calculation of the electromagnetic field. He showed for the first time the combined measurement and analysis of GIXRF and XRR signals for layered media. Based on deBoer's work, most developments in the theory of GIXRF were achieved during the 1990s, predicting an analytical potential being ahead of the technological capabilities and requirements at that time to produce thin, near surface layers with overall thicknesses in the nanometer region. In 1993 a combination of X-ray techniques for the analysis of thin layered materials was suggested by van den Hoogenhof and de Boer in [5] as Glancing-incidence X-ray analysis (GIXA), they even presented a spectrometer for combined analysis [6]. However, GIXRF being much less sensitive for sample thicknesses of more then a few tens of nanometers it is today, 20 years later, when technologically highly relevant materials with thicknesses of few nanometers are manufactured, that GIXRF attracts new attention. In 2010 Tiwari et al. [7] published the application of combined XRR and GIXRF measurements for the investigation of thin films and multilayered materials. For the calculation of fluorescence intensities in depth profile analysis the authors suggest a numerical integration using the field intensity of an unaltered substrate or layer. This approach is only valid in the dilute regime, i.e. if the change in refractive index due to the dopant is insignificant.

A more general procedure is presented in detail in this work, respecting the physical relevant parameters and avoiding possibly time-consuming numerical integration.

1.2. Technical

Measuring the angle dependent fluorescence signal in grazing incidence on an optical flat results in distinct shapes of the recorded angle curve depending on whether an element is present in the bulk material, a thin layer or implant near the surface or a residue on the surface [8,9]. For implants the curve shape below and near the critical angle is mainly depending on the average implantation depth, whereas the curve at larger angles corresponds to the implanted dose. The measured fluorescence intensity below the critical angle is given by the integration of the product of the implantation profile and the intensity of the exponentially decaying evanescent wave. Unfortunately, an unambiguous de-convolution of the angle dependent fluorescence signal in order to determine the concentration profile is not possible. To overcome this problem, a simultaneous measurement of the intensity of the specular reflected beam was performed. This XRR measurement is done in a classical θ–2θ geometry with one detector rotating on 2θ collecting the reflected photons while simultaneously recording the emitted X-ray fluorescence with a fluorescence detector. The intensity of the reflected beam depends on the electron density, thus on the atomic scattering factors and

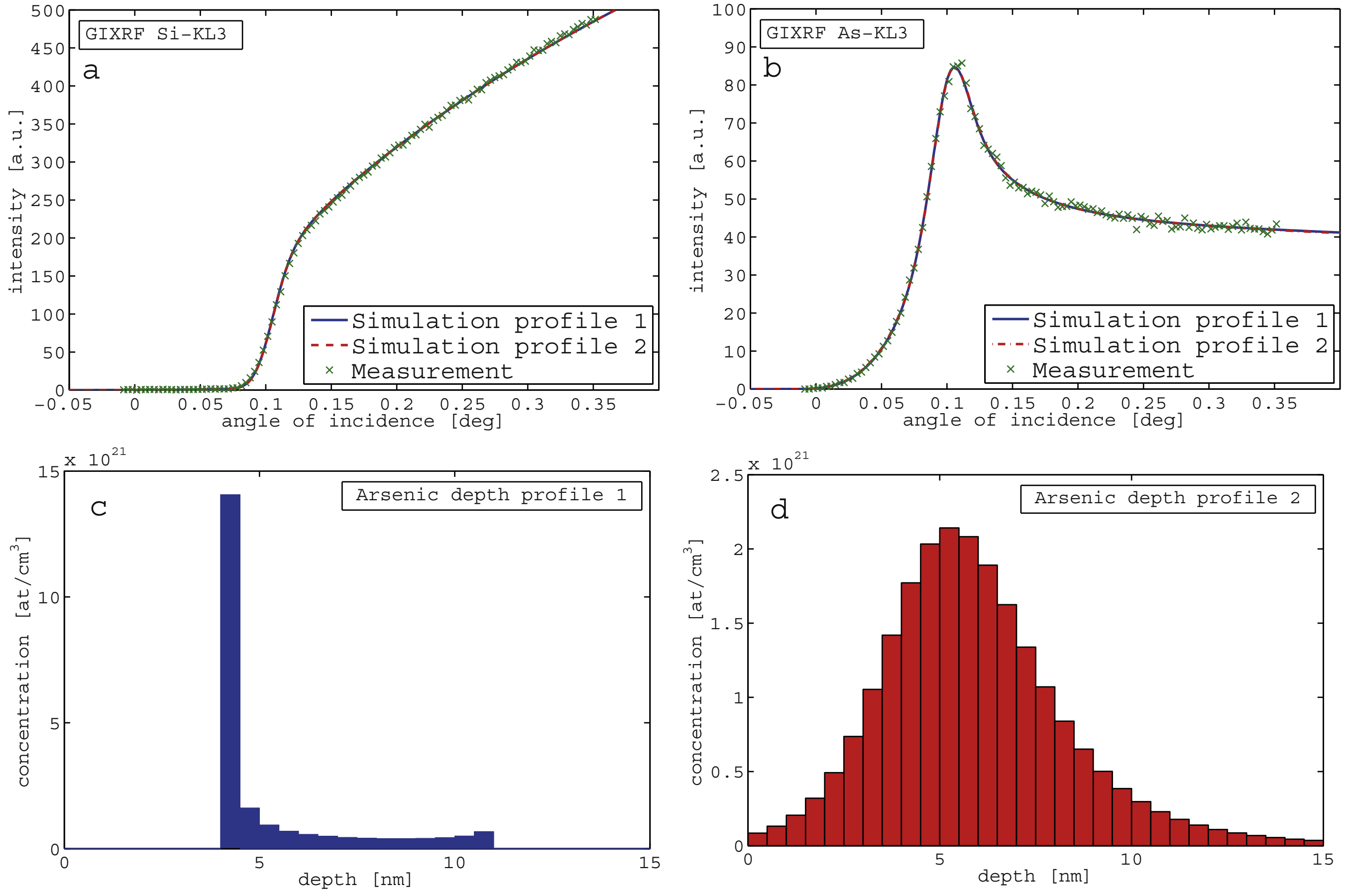

Fig. 1. (a) GIXRF Silicon bulk signal (fitted and experimental), (b) GIXRF Arsenic implant signal (fitted and experimental), and (c and d) assumed Arsenic depth profiles for the GIXRF simulation in (a) and (b).