High-resolution ERD Utilizing Bayesian Data Analysis

P. Neumaier, G. Dollinger, A. Bergmaier, R. Fischer [a], and H. J. Körner
[a] Centre for Interdisciplinary Plasma Science, MPI für Plasmaphysik, Garching

The depth resolution in high–resolution ERD is at least limited due to energy–loss straggling and small–angle scattering effects of the incident and analysed ions [1]. In order to improve depth resolution in larger depths and to calculate the accuracy of deduced elemental profiles, the measured spectra have to be deconvoluted with respect to an apparatus function which contains all effects of ion–beam and detector induced energy spreads as well as energy–loss straggling and small–angle scattering effects.

In order to supress insignificant oszillations within the reconstructed spectra we deconvoluted the measured high resolution ERD profiles utilizing a recently developed extension of Bayesian data analysis, the adaptive kernel method, which is described in detail in Ref. [2]. For investigating carbon samples an apparatus function is generated via measuring a $^{13}C/^{12}C$ multilayer sample as well as via calculating the energy spreads using the DEPTH code of Szilágy *et al.* [3]. We demonstrated, that the experimental way can be used to determine a reasonable upper limit for the width of the apparatus function A [4]. Treating the theoretical approach the energy spreads were calculated only with respect to the energy broadening induced by energy–loss straggling, multiple scattering and an intrinsic detector resolution $\Delta E/E = 2{\times}10^{-4}$. Therefore, the calculated values are considered as a lower limit for the variance of the apparatus function A (Fig. 1).

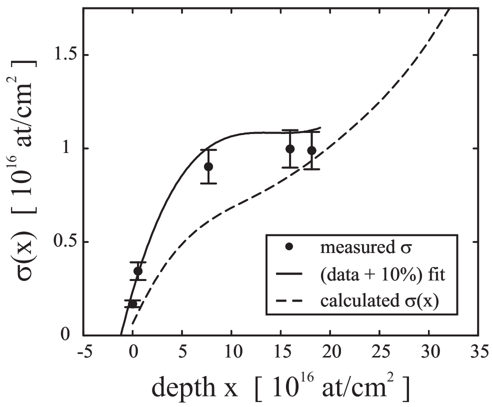

Fig. 1: Comparison of the standard deviations of the measured apparatus function with the corresponding calculated (DEPTH) values for $^{13}C^{4+}$ ions recoiled off a carbon sample utilizing a 40 MeV ^{197}Au beam, an incident angle of 4° and a scattering angle of 15°.

The measured spectra are deconvoluted with regard to the measured apparatus function A_{exp} and the calculated apparatus function A_{DEPTH}, respectively. As the deconvolution formalism using Bayes theorem inherently considers statistical errors, confidence intervals for each reconstructed spectra can be evaluated. Fig. 2 shows the most probable solutions $\widehat{f}_{exp}$ (with respect to A_{exp}) and $\widehat{f}_{DEPTH}$ (with respect to A_{DEPTH}) for the ^{13}C profiles of ta–C samples, that were grown with deposition energy $E = 40$ eV, respectively, and that contain either directly on the surface or about 7 nm beneath the surface about 5×10^{14} at/cm^2 ^{13}C. The solutions for the interfacial profile are much wider than the respective reconstructions for the surface profile. This marks a mixing of the carbon during subplantation. With respect to the apparatus functions A_{exp} and A_{DEPTH}, the mean ion range and the standard deviation of the mixing structure as well as the corresponding errors are calculated via Markov–Chain Monte Carlo (MCMC) integration. Taking into account the respective results for both apparatus functions A_{exp} and A_{DEPTH} reveals a mean ion range of $(4.5 \pm 1.8) \times 10^{15}$ at/cm^2 for carbon ions deposited with kinetic energy $E = 40$ eV and a standard deviation of $(12.0 \pm 1.5) \times 10^{15}$ at/cm^2 for the respective mixing profile. Notice that the dominating part of the derived error for the ion range is due to the uncertainty of zero thickness, that was quantified with an accuracy of $\pm\, 1.4 \times 10^{15}$ at/cm^2 due to MCMC integration [4].

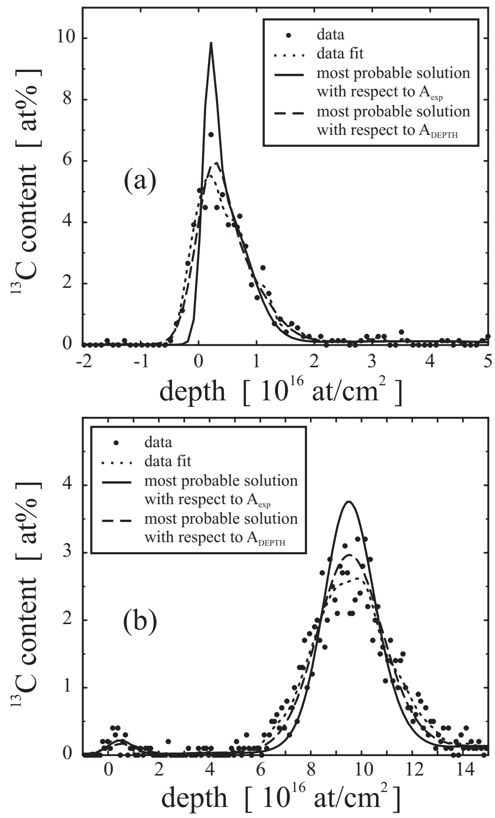

Fig. 2: Most probable reconstructions of (a) the surface profile and (b) the mixing profile for the deposition energy $E = 40$ eV.

Utilizing Bayesian data analysis allows to determine the uncertainty of the deconvoluted spectra and, for this reason, to quantify e. g. mixing widths and ion ranges of low–energy ions with respect to ta–C growth. Therefore, a wide field for quantitative investigations of light–elements depth distributions in ultra–thin films, at surfaces and at interfaces, is offered using the described technique.

References

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