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Bayesian reconstruction of surface roughness and depth profiles

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Abstract

Bayesian data analysis provides a consistent probabilistic theory for the extraction of sample parameters from spectra measured with MeV ion beam analysis methods. The application of Bayesian data analysis is demonstrated on three different examples, namely the deconvolution of the apparatus function for improving the energy resolution of solid state detectors, the reconstruction of depth profiles of individual elements with confidence intervals from Rutherford backscattering measurements, and the reconstruction of surface-roughness distributions using Rutherford backscattering.

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1. Introduction

Ion beam analysis (IBA) methods using MeV ions are powerful tools for the determination of the near-surface layer composition of solids and depth profiling of individual elements [1,2]. IBA methods include Rutherford backscattering (RBS), elastic recoil detection analysis (ERDA), and nuclear reaction analysis (NRA). These analysis methods are quantitative without need for reference samples, non-destructive, have a good to very good depth resolution from the order of several nm to atomic resolution [3], and a very good sensitivity for heavy elements of the order of parts-per-million (ppm). In many applications cheap, small and easy-to-use semiconductor detectors like silicon-surface barrier detectors or

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particle-implanted and passivated silicon (PIPS) detectors can be used for the detection and energy analysis of backscattered or recoiled particles.

Major disadvantages of IBA methods, however, are the limited energy resolution of semiconductor detectors (typically 10–15 keV full width at half maximum (FWHM) for typical incident proton or ^{4}He energies in the range 1–3 MeV), and the complicated data analysis: Except for special cases like very thin layers, the determination of the sample composition from a measured spectrum is not possible analytically and requires the use of computer codes. This is especially the case for RBS, where the sub-spectra of individual elements may overlap and light elements like hydrogen are not visible in the spectrum.

Several computer codes for the analysis of RBS, ERDA and NRA measurements were developed during the last two decades [4–10]. State-of-the-art software includes a large number of different physical effects in simulation calculations, such as electronic and nuclear stopping for incident and outgoing ions, non-Rutherford scattering and reaction cross-sections, the broadening of measured spectra due to finite detector resolution, electronic and nuclear energy loss straggling of incident and outgoing particles, multiple small angle scattering [6], plural large angle scattering [11,9,12], and surface roughness effects [13–16]. These programs always perform a *forward* calculation, i.e. they calculate a simulated spectrum for a given target composition. The quantities seeked by the experimentalists, like sample composition, depth profiles of elements, thicknesses of deposited layers, layer roughnesses etc., are then obtained by fitting, i.e. by varying the sample parameters until best fit to the measured spectrum is obtained. The best fit is typically defined by minimum quadratic deviation χ^2 between the simulated and measured spectrum, taking the counting statistics of experimental data into account. The fit can be done either manually or in an automatic manner [5,10], and may consider additional constraints (like known ratios of elements or known total amounts of some elements), or additional information (like simultaneous measurements at different angles or measurements at different energies).

Although this approach to IBA data analysis by fitting has proven to be very successful, and the results are often sufficient from a practical point of view, it does *not* provide a full solution of the *inverse* problem, i.e. the determination of a depth or surface-roughness profile from a measured spectrum, and it does *not* exploit the full information present in the experimental data: A good fit is a necessary, but not a sufficient condition. The solution of the inverse problem is difficult due to the presence of noise in the experimental data, insufficient information, and above all by the ill-posed nature of the underlying inversion problem [17,18]. It has been shown during the last decade, that Bayesian data analysis together with the maximum-entropy concept is particularly suited for this type of data analysis problems. It provides a consistent probabilistic theory to obtain unbiased results. Additional prior knowledge can be incorporated effectively into the computations, leading to more stringent confidence intervals. In this paper, we will demonstrate the use of Bayesian data analysis for RBS measurements on three different problems: The deconvolution of the apparatus function for improving the energy resolution of solid state detectors, the reconstruction of depth profiles, and the reconstruction of surface-roughness profiles.

2. Bayesian data analysis

The goal of Bayesian data analysis is the determination of the *posterior probability density* $p(\vec{\theta} \mid \vec{d}, I)$, where $\vec{d}$ are (experimental) data and $\vec{\theta}$ are (model-) parameters. I summarizes all other available information, and $\mid$ separates variables from conditions. That is, we want to obtain the probability distribution of the parameters $\vec{\theta}$ (in RBS data analysis these might be layer thicknesses, concentrations of elements in a given depth, etc.), given the experimental data $\vec{d}$ and additional knowledge I. The yet unknown posterior density $p(\vec{\theta} \mid \vec{d}, I)$ is linked with already known quantities through Bayes' theorem, which is given by

$$p(\vec{\theta} \mid \vec{d}, I) = \frac{p(\vec{\theta} \mid I) \cdot p(\vec{d} \mid \vec{\theta}, I)}{p(\vec{d} \mid I)}. \quad (1)$$