Deconvolution of High Resolution Elastic Recoil Detection (ERD) Spectra with the Ion Beam Analysis (IBA) Data Furnace

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1. Introduction

The ERD setup at the Munich accelerator laboratory in combination with the Q3D-magnet spectrograph gives the possibility to achieve monolayer depth resolution in Elastic Recoil Detection (ERD) experiments. However, this resolution deteriorates rapidly with increasing depth due to different energy broadening effects.

Depth resolution can be increased by deconvolution of the spectra, if the resolution function is known. Therefore, the program NDF [1] (Nunos Data Furnace) was adapted to ERD analysis and applied. NDF uses a fitting algorithm based on simulated annealing [2].

The energy spectra obtained from ERD analysis were deconvoluted by NDF with an external resolution function. This function was calculated with the program DEPTH [3] by Edit Szilágyi. DEPTH considers both detector resolution and experiment inherent energy broadening effects.

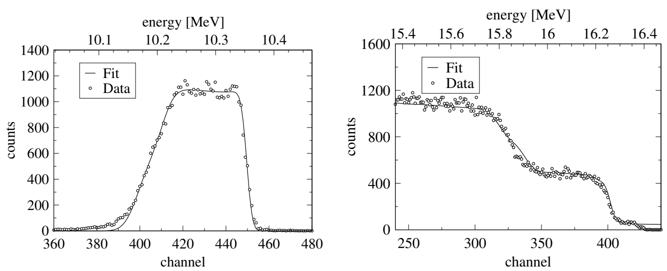

Fig. 1: Fits for the spectra for O and Si of a nominal 6 nm SiO_2 layer on Si substrate as calculated by NDF.

2. NDF

NDF is a fitting program, which calculates depth profiles from spectra given the experimental data. The result is achieved by simulating a depth profile for an arbitrary target structure and comparing the simulated and experimental results. With the simulated annealing algorithm it is possible for the program to obtain the global minimum of the solution to this multidimensional boundary value problem within acceptable time (Fig. 1).

The main task was to adapt the program to the ERD analysis and test it. NDF has never been applied to spectra from heavy ion ERD before, especially not to data from high resolution experiments. Similary DEPTH had to be adjusted to the Munich ERD experiment and the usage with NDF.

First deconvolutions were performed on measurement results from thin silicon oxide layers grown on silicon substrate. This material system provides a good test case because of its sharp interface.

NDF in combination with the DEPTH resolution function was able to deconvolute the spectra. The resolution of the interface SiO_2/Si interface at a depth of 6 nm could be improved from 1.7 nm to 0.9 nm.

Also NDF was used to calculate error margins for the target structure. The error margins were obtained with bayes inference (BI) (Fig. 2).

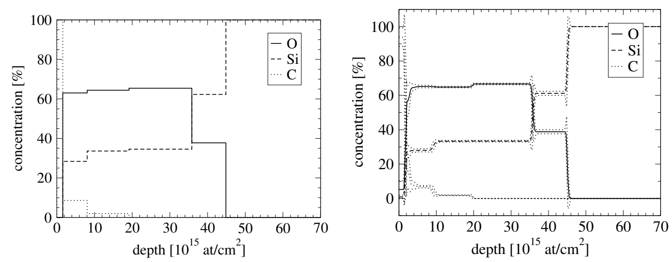

Fig. 2: Calculated depth profile of a 6 nm SiO_2 layer on Si substrate and error margins obtained with BI.

3. Conclusion

The ERD at the Munich Q3D magnet spectrograph is quite unique with its extrem high depth resolution. Thus, it is understandable when common programs like DEPTH and NDF reach their limits of accuracy and possiblities.

Especially the ERD model used for the simulations is often too crude when heavy ion ERD with grazing angle incidence and the high resolution measurements at the Q3D should be analyzed. In this case some approximations are no longer suitable and lead to errors obstructing the improvement of depth resolution. This also holds for DEPTH as it calculates the depth dependent energy resolution used in NDF.

Unclear as well is the reliability of the error margin calculation with bayes inference. Their results seem arguable.

Conclusively, NDF offers an interesting way for the analysis of high resolution heavy ion ERD measurements, but – applied to the Munich high resolution setup – still has flaws concerning the calculation of the target composition and error margins, and the consideration of typical ERD effects such as roughness and double scattering.

References

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