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Thin film depth profiling using simultaneous particle backscattering and nuclear resonance profiling

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ABSTRACT

We report an important extension to the DataFurnace code for Ion Beam Analysis which allows users to simultaneously and self-consistently analyse Rutherford (RBS) or non-Rutherford (EBS) elastic backscattering together with particle-induced gamma-ray (PIGE) spectra. We show that the code works correctly with a well-known sample. Previously it has not been feasible to self-consistently treat PIGE and RBS/EBS data to extract the depth profiles. The PIGE data can be supplied to the code in the usual way as counts versus beam energy, but the differential cross-sections for the PIGE reaction are required. We also compared the results obtained by the new routine with high resolution narrow resonance profiling (NRP) simulations obtained with the stochastic model of energy loss.

1. Introduction

The IBA DataFurnace (NDF) is a general purpose program for analysis of IBA data [1]. It currently includes Rutherford backscattering (RBS), elastic (non-Rutherford) backscattering (EBS), elastic recoil detection analysis (ERDA), non-resonant nuclear reaction analysis (NRA), and particle-induced X-ray emission (PIXE). Any number of spectra taken from the same sample with any of these techniques can be analysed and fitted simultaneously.

In nuclear resonance profiling (NRP, often called resonant nuclear reaction analysis or RNRA), the yield of the nuclear reaction product is measured as a function of beam energy in the vicinity of a narrow resonance, preferably isolated, in a nuclear reaction cross section. Useful resonances exist for many light elements, and often NRP is the technique of choice for profiling of light elements in heavy substrates with high sensitivity. Thus NRP is highly complementary to techniques such as RBS or PIXE.

Several NRP codes have been previously presented, with various approaches [2–7]. However, they are all dedicated codes, i.e. they can only analyse NRP data. We have developed an open source routine for analysis of excitation curves obtained in NRP, based on our previous code ERYA developed for particle-induced gamma-ray emission (PIGE) [8,9]. We integrated this new routine in NDF. The existing features of DataFurnace, such as automated fitting of complex layered samples, calculation of confidence limits on the results obtained can therefore also be used in a seamless way. This even includes the inverse operation of automatically extracting cross-sections from the data, by treating the cross section as a free parameter in a fit procedure where multiple spectra obtained form a well-known sample at different energies are analysed. The procedure is the same for NRP or RBS [10].

We show examples for bulk and multilayered samples, for NRP data alone, and in combination with other techniques.

2. Calculation model

We follow the model given in [8,9], with the following improvements: first, the energy spread of the incoming beam is used to calculate the correct cross section at each depth [11]. Second, the shape of the energy loss function can be either Gaussian, which is appropriate in many cases, or it can follow the gamma function, which we have previously showed to lead to results comparable to those obtained using a stochastic model for the energy loss in high resolution near-surface region medium energy ion scattering experiments [12].

The width of the beam energy spread due to transport within the sample can be calculated with the Bohr or Chu models, or with the code DEPTH [13], which also includes the effect of multiple scattering and geometrical straggling. Different sets of stopping powers such as SRIM2008 (previous versions of SRIM are also available) [14], MSTAR [15], or user-input values can also be used.

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3. Results

We show in Fig. 1 the results obtained with both NDF and ERYA for a measurement of bulk PbF_2 with the 197 keV emission of the $^{19}F(p,p'\gamma)^{19}F$ reaction. The experimental details and the cross section measurement are given in [8]. For both codes, the discrepancy with the experimental data is always smaller than 4%, and could be due to inaccuracies in the cross section. We also note that the errors shown are from counting statistics only, and other sources of error are not taken in consideration. The ERYA and NDF calculations are slightly different, with NDF systematically obtaining yield values smaller by ≈0.5%. This could be due to the different stopping power used (ERYA uses SRIM2000 stopping), or even to numerical differences in the implementation (similar differences were observed for RBS, ERDA and NRA simulations made with different codes [16]), but it is more likely to be due to the different handling of the cross section and energy straggling in the two codes. In any case, both codes describe very well the experimental results.

A second example is shown in Fig. 2. The 1014 keV emission of the $^{27}Al(p,p'\gamma)^{27}Al$ reaction was used to measure bulk $AlTiO_5$. The experimental conditions are given in [17]. Again, both the ERYA and NDF results are consistent with the experimental data, and amongst themselves. Again, NDF leads to slightly smaller calculated yield values, as can be seen in Fig. 2a), where the ratio between calculation and yield is shown. The shape of the calculated excitation curves, however, is almost undistinguishable, as can be seen in Fig. 2b).

We used NRP in conjunction with RBS and PIXE to analyse a Si/SiO_2 1000 nm/CoFeBSi 450 nm sample, where all three techniques are essential for its complete characterisation. For NRP, the 4.43 MeV emission of the $^{11}B(p,\gamma)^{12}C$ reaction was detected, using the 163 keV resonance which has a width of 7 keV. A 2 MeV ^4He RBS spectrum was collected, and a 2.2 MeV proton beam was used for the PIXE measurement. From the PIXE, a Co:Fe ratio of 71:29 is determined; from the RBS spectrum, shown in Fig. 3a), the total CoFe content is determined, as well as the Si content of the film. For all three elements a uniform depth profile is derived. Finally, from the NRP data, shown in Fig. 3b), the B profile is determined, being also consistent with a homogeneous film. We derive a $(Fe_{29}Co_{71})_{47.9}B_{24.4}Si_{27.7}$ composition and an areal density of 4.1×10^{18} at./cm^2, which would correspond to a 460 nm thickness assuming a weighted average of the elemental densities. We note that all data were fitted simultaneously, with the same depth profile, ensuring full consistency between all data.

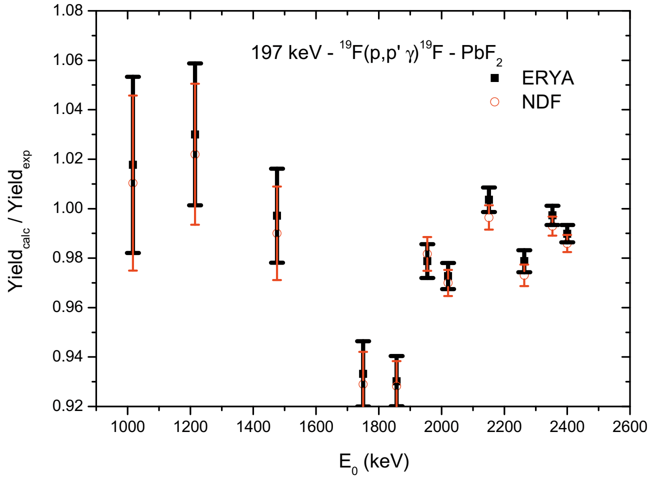

Fig. 1. NRP results obtained with both NDF and ERYA for a measurement of a bulk PbF_2 sample with the 197 keV emission of the $^{19}F(p,p'\gamma)^{19}F$ reaction.

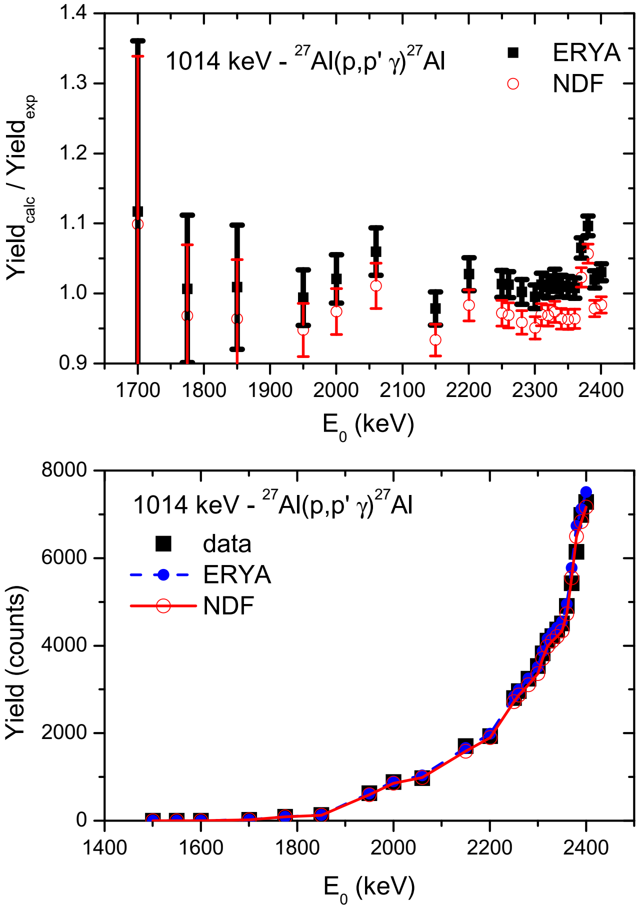

Fig. 2. NRP results obtained with both NDF and ERYA for a measurement of a bulk $AlTiO_5$ sample with the 1014 keV emission of the $^{27}Al(p,p'\gamma)^{27}Al$ reaction.

As a more stringent test we used the code SPACES [2,3] to calculate the excitation curve of protons in 15 μg/cm^2 Si film, considering a Lorentzian shaped resonance centered at 151 keV with 100 eV FWHM, and a Gaussian shaped 100 eV FWHM combined beam energy spread and Doppler effect. SPACES implements the stochastic theory for charged-particle energy loss [18], which provides a rigorous calculation of yield excitation curves even for very narrow resonances of width comparable to the energy loss in a single proton–electron scattering event. In this case the discrete nature of the energy loss process gives rise to an observable overshoot on the leading edge of the excitation curve – the Lewis effect [19,20]. Accurate calculation of the magnitude and shape of the Lewis effect is a stringent test orf the underlying energy straggling functions. Firstly, we show in Fig. 4a) the energy loss functions calculated by SPACES for some penetration depths. At the very surface, before any collision of the proton ions with electrons, the energy loss is a delta function. After a small depth (e.g. 0.5 μg/cm^2), some ions still did not interact with any electrons, some met one single electron, and some already underwent a number of collisions. The resulting energy loss function is highly discontinuous. As the depth increases, all ions undergo many collisions with electrons and the energy loss function becomes smoother and ultimately tends towards a Gaussian shape.

We also show in Fig. 4a) the energy loss functions calculated by NDF using the gamma function. Already for a depth of 1 μg/cm^2 they approach well the stochastic theory functions. Below that depth, the fine discontinuous structure that comes from the discrete nature of the energy loss process is missed. However, the actual energy distribution of the nuclear reaction process is not only