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A general artificial neural network for analysis of RBS data of any element with Z between 18 and 83 implanted into any lighter one- or two-element target

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Abstract

We report a generalisation of previous works where artificial neural networks (ANNs) were successfully applied for specific implantations such as Er in sapphire or Ge in Si. We have now developed a code that it is able to analyse data from implantations of any element with Z between 18 and 83 into any target composed of one or two lighter elements. Although this problem is considerably more complex than single-system ANNs, the ANN developed produced excellent results when applied to experimental data.

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1. Introduction

We have previously used artificial neural networks (ANNs) to analyse Rutherford backscattering (RBS) data in a fully automated and instantaneous way [1,2], and also to develop a method for automated control and of the experimental conditions such as the angle of incidence, angle of scattering, and beam energy and their optimisation for given samples [3].

The accuracy reached in the analysis is only slightly worse than what is achievable with state of the art methods [4]. The main disadvantage of ANNs is that they are better suited for single-systems, of similar data. When the data fall into different categories, it is often necessary to develop separate ANNs for each category in order to obtain reliable results [3]. This should mean that the goal of having an all-purpose ANN, able to analyse any RBS spectrum, is not attainable.

Generalisation of the ANNs for classes of systems or problems would nevertheless be an important goal. We started with an ANN able to deal with a given single element implanted in a given one-element substrate (Ge in Si [1]), then one-element in a two-element substrate (Er in

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Al_2O_3 [5]), then any element in a given lighter two-element substrate (anything in Al_2O_3 [6]). We now present an ANN able to analyse RBS data from any element with Z between 18 and 83 implanted into any lighter one- or two-element substrate.

2. Experimental data

RBS spectra of implanted sapphire [7] and Ge-implanted Si [1] previously presented were used to test the ANN. They include data from three experimental setups and five detectors. A wide range of implant dose and energy and of experimental conditions is covered.

3. Artificial neural networks

The theory of feedforward ANNs [8] and their application to RBS [3] is described elsewhere. The number of layers and nodes determines the ANN architecture, which can be represented by $(N, I_1, \ldots, I_n, M)$, where N is the number of inputs and M the number of outputs (in our case, the implanted dose and depth, and $M = 2$), and I_i the number of nodes in each intermediate layer. In supervised learning, the training is done by presenting a large set of known examples (the training set), and minimising the difference between the ANN outputs and the known results. The correctness of the training is verified by testing the ANN with another set of data, the test set. Root mean square errors are calculated for both sets.

We generated a training set consisting of theoretical spectra. The atomic number of the implanted element was chosen randomly between 18 and 83. The elements of the substrate were chosen randomly but imposing that they should be lighter than the implanted ion, and in 40% of the cases we chose a monoatomic substrate. The atomic fractions of the two substrate elements were also chosen randomly. The implant doses were between 10^{15} and 10^{17} at/cm^2, for depths between 100 and 3700 at/cm^2. Each implant was simulated as a perfect Gaussian. Only spectra where the signal of the implanted element was at least partially separated from the substrate signal were generated.

The spectra were calculated for different beam and detection parameters chosen at random, in order to simulate a very broad range of realistic experimental conditions. The beam was He, with energy between 1 and 2.1 MeV and resolution between 10 and 40 keV FWHM. The scattering angle was between 135° and 180°, and the detection angle was between −20° and 20° in the IBM geometry. The charge was between 1 and 200 μC for a solid angle of 1 msr. Pulse pileup and Poisson noise were added to the theoretical spectra [9].

The inputs consists of four experimental parameters to characterize the setup (beam energy, incidence angle, scattering angle and charge), and an extra set of six describing the atomic charge (Z) and mass (M) of the implanted element, and the atomic charge (Z_1, Z_2) of the substrate elements and their atomic fraction (f_1, f_2). Note that a monoelemental substrate was given simply by $Z_1 = Z_2$, with the fractions taking random values.

Instead of increasing the complexity of the ANN to match the problem, we reduced the complexity of the problem by using appropriate pre-processing. We used a peak identification routine to extract automatically the centroid and area of each implant, which were made part of the input instead of the 512 channel yields. These two features are enough to calculate a good first approximation of the implanted depth and dose. The routine uses Poisson statistics to find statistically significant peaks and edges, and then, from the peaks found at higher channels than the edges, chooses the one with the highest yield. This peak is then fitted with a joined half Gaussian function, used to calculate its position and area accurately.

The peak identification routine is not perfect and fails in about 10% of the cases. This is generally due to a small peak, a large pileup background, or partial superposition to the substrate signal, and sometimes to the fact that the peak recognition routine itself fails. These "wrong data" would lead to a high ANN error. We used the worst case elimination strategy [1], whereby the spectra for which the error is substantially above the average are eliminated.

We tested several network architectures as shown in Table 1. They show very similar results, and we choose the (12:30:10:2) topology as it is the

Table 1
Train and test errors for different networks after automatic worst case elimination

Network topology	Train error (%)	Test error (%)	# Eliminated cases (%)
(12:30:10:2)	3.15	3.37	19.7
(12:30:20:2)	3.12	3.70	20.7
(12:40:10:2)	3.20	3.25	19.8
(12:40:20:2)	2.98	3.22	20.5

simplest one and has the smallest number of eliminated cases, for a comparable error. Although this architecture is much simpler, and the number of eliminated cases has not increased substantially compared to ANNs dedicated to single-systems [4], the performance of the network is similar.

4. Results and discussion

We show the results obtained for experimental data in Table 2 for cases with all parameters well within the training range, in Table 3 for cases with at least one parameter outside the training range, and in Table 4 for border cases. The numbering of samples 1–43 follows that of [6]; samples 44–53 are samples 1–10 of [1].

For samples with parameters outside the training range, the ANN performs very poorly. This is a known feature of ANNs, which are able to do non-linear mappings and interpolations, but are in general unable of extrapolation [8]. That is, they can only analyse data that lies within the training universe.

Table 2
Results for samples with all parameters well within the training range

N	Nominal dose (at/cm^2)	Implant energy (keV)	Beam energy (MeV)	Setup/ scattering angle	Angle of incidence (°)	Solid angle-charge (μC msr)	Dose (10^{15} at/cm^2)		Depth (10^{15} at/cm^2)	
							ANN	NDF	ANN	NDF
TiAl_2O_3										
29	1×10^{16}	100	1.6	II/160°	5	9.86	10.8	9.8	701	848
33	1×10^{16}	100	1.6	II/180°	5	54.0	11.4	9.3	907	795.8
30	5×10^{16}	100	1.6	II/160°	4	9.82	55.4	58.9	593	769
34	5×10^{16}	100	1.6	II/180°	4	55.3	52.7	53.0	722	565
FeAl_2O_3										
36	1×10^{16}	160	1.6	II/160°	4	17.55	16.2	10.6	1223	1222
40	1×10^{16}	160	1.6	II/180°	4	99.0	9.8	10.3	880	904
37	4×10^{16}	160	1.6	II/160°	5	9.02	46.0	41.7	999	1180
41	4×10^{16}	160	1.6	II/180°	5	50.2	42.7	38.2	860	912
CoAl_2O_3										
22	5×10^{16}	150	2	I/180°	3	94.8	58.5	48.4	814	730
ErAl_2O_3										
11	4×10^{15}	200	1.6	II/160°	0	6.87	3.5	3.75	698	726
15	4×10^{15}	200	1.6	II/180°	0	20.48	4.0	3.83	615	736
AuAl_2O_3										
26	6×10^{16}	160	2	II/180°	2	52.0	60.1	59.3	668	395
GeSi										
44	15×10^{15}	100	1.5	III/165°	7	7.72	13.1	16.7	361	333
45	15×10^{15}	100	1.5	III/165°	7	5.41	9.7	14.4	367	302
46	15×10^{15}	100	1.5	III/165°	7	6.91	10.5	13.6	364	318
48	15×10^{15}	100	1.5	III/165°	7	8.68	11.7	15.7	353	378
49	10×10^{15}	100	1.5	III/165°	7	140.73	7.3	9.3	309	251
50	25×10^{15}	100	1.5	III/165°	7	104.98	24.7	26.8	322	246
51	10×10^{15}	100	1.5	III/165°	7	63.93	7.8	9.8	347	349
52	10×10^{15}	100	1.5	III/165°	7	113.49	8.1	9.6	348	357
53	10×10^{15}	100	1.5	III/165°	7	96.54	7.9	9.7	331	316

Table 3
Results for samples with at least one parameter outside the training range

N	Nominal dose (at/cm^2)	Implant energy (keV)	Beam energy (MeV)	Setup/scattering angle	Angle of incidence (°)	Solid angle-charge (μC msr)	Dose (10^{15} at/cm^2)		Depth (10^{15} at/cm^2)	
							ANN	NDF	ANN	NDF
$TiAl_2O_3$										
31	1×10^{17}	100	1.6	II/160°	5	9.89	70.6	106	618	769
$FeAl_2O_3$										
38	1×10^{17}	160	1.6	II/160°	4	9.63	73.7	105	1029	1163
39	5×10^{17}	160	1.6	II/160°	4	10.68	120.8	417	520	603
43	5×10^{17}	160	1.6	II/180°	4	55.7	133.6	407	495.1	488
$CoAl_2O_3$										
21	1×10^{15}	150	2	I/180°	7	99.2	1.7	0.96	851	681
23	2×10^{17}	150	2	I/180°	2	124.1	131	187	821	734
24	5×10^{17}	150	2	I/180°	2	64.3	156	448	555	623
$ErAl_2O_3$										
8	8×10^{13}	200	1.6	II/160°	0	5.83	2.4	0.07	1120	770
12	8×10^{13}	200	1.6	II/180°	0	94.59	1.6	0.07	928	805
6	3×10^{14}	800	1.6	I/180°	0	92.1	1.4	0.33	1401	1658
9	6×10^{14}	200	1.6	II/160°	0	6.94	1.9	0.67	885	701
13	6×10^{14}	200	1.6	II/180°	0	31.14	1.8	0.70	677	715
10	1×10^{15}	200	1.6	II/160°	0	3.31	1.9	0.99	842	744
1	3×10^{14}	800	1.6	I/140°	0	19.96	1.5	0.31	1437	1595

Table 4
Results for samples with at least one parameter near the limits of the training range

N	Nominal dose (at/cm^2)	Implant energy (keV)	Beam energy (MeV)	Setup/scattering angle	Angle of incidence (°)	Solid angle-charge (μC msr)	Dose (10^{15} at/cm^2)		Depth (10^{15} at/cm^2)	
							ANN	NDF	ANN	NDF
$TiAl_2O_3$										
28	1×10^{15}	100	1.6	II/160°	6	18.0	2.3	1.34	599	742
32	1×10^{15}	100	1.6	II/180°	6	104.4	1.6	1.08	647	706
35	1×10^{17}	100	1.6	II/180°	5	57.6	76.3	92.4	644	633
$FeAl_2O_3$										
42	1×10^{17}	160	1.6	II/180°	4	52.9	82.9	98.5	791	869
$ErAl_2O_3$										
14	1×10^{15}	200	1.6	II/180°	0	20.97	2.1	1.05	695	636
GeSi										
47	15×10^{15}	100	1.5	III/165°	7	4.12	8.5	14.7	379	335
7	1.3×10^{15}	800	1.6	I/180°	0	92.0	2.1	1.64	1012	1649
3	1.3×10^{15}	800	1.6	I/140°	0	18.98	2.1	1.60	1192	1577
4	5×10^{15}	800	1.6	I/140°	0	20.03	4.9	5.17	1432	1590
5	2×10^{16}	800	1.6	I/140°	0	19.63	9.0	25.21	1340	1756

For the samples within the training range, the general ANN developed here performs in most cases as well or better than the specialized ANNs developed previously. This is, by all means, a great success. We calculated the ANN results as compared to NDF, averaged for all the samples, for the ANN developed here and for previously developed single-system ANNs [1,5,6]. The results

Table 5
Average results for different ANNs

ANN	$Dose_{ANN}/Dose_{NDF}$	$\lvert Depth_{ANN} - Depth_{NDF} \rvert$ (10^{15} at/cm^2)
Ge in Si	1.11	53
Er in Al_2O_3	1.17	106
All in Al_2O_3	1.02	235
All in all	**0.96**	**83**

The "all in all" row refers to the present work for samples with all parameters well within the training range.

are shown in Table 5. Using as input only the peak position and area instead of the entire spectrum, which leads for instance to ignoring the dip in the substrate signal, might lead to reduced accuracy. This is, however, more than compensated by the increased efficiency and accuracy of a much smaller and simpler ANN architecture.

Finally, border cases are relatively well analysed, but with a large error. In particular, samples with small implanted doses are difficult to analyse no matter what the method of analysis, and the ANN error is consequently large.

5. Summary and outlook

We developed a ANN able to analyse RBS data of any element with Z between 18 and 83 implanted into any lighter one- or two-element substrate. Pre-processing, consisting in reducing each spectrum to two parameters, namely the peak position and area, led to a substantial reduction of the complexity of the problem, and thus to a general ANN that, within its range of applicability, performs as well or better than single-system ANNs previously developed.

We had previously developed an algorithm for the automated optimisation of the experimental parameters in RBS analysis of a well-defined system, namely Ge-implanted Si. The prospects of extending that to any implanted system are now excellent.

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