Artificial neural network techniques for analysis of ion backscattering spectra

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Abstract-*Ion backscattering spectrometry is an analysis technology that is dedicated to the compositional analysis of samples with the thickness of μm level. The problem of spectral data analysis, which is to determine the sample structure from the measured spectra, is generally ill-posed. In this study, artificial neural network (ANN) techniques have been developed for spectral data analysis. A multilayer feedforward neural network was constructed and applied to the specific case of SiGe thin films on a silicon substrate. The network was trained by the resilient backpropagation algorithm with hundreds of simulated spectra of samples for which the structures are known. Then the trained network was applied to analyse spectra with unknown structure of samples. The ANN prediction results are excellent. The constructed neural network can handle properly redundancies, which were caused by the constraint of output variables.*

Keywords: neural networks, resilient backpropagation, spectral analysis, intelligence techniques

1. Introduction

Over past two decades, artificial neural networks (ANN) have been successfully applied to solve a wide scope of hard problems owing to its ability to approximate nonlinear behavior without a prior knowledge of relations between the problem representation and its solution. Now ANN has gradually become a generic mathematical method and tool for solving some of hard problems. In recent years, some attempts have been made to use ANN techniques for analysis of complex scientific data. Complex scientific data may come from experimental measurements in various areas such as in astronomy, geophysics, environmental science, chemical drug design, and spectrometry [1-3] etc. Analysis of spectral data is a typical category of scientific data handling. Problems of spectral analysis are seemingly simple but there often exist high computational complexities and uncertainties. Traditionally, numerical and statistical approaches are employed for data analysis and interpretation. However, standard numerical methods sometimes may be incapable of solving some of complex problems, in which an inference process or optimization strategy may be required to extract relevant information from a large amount of measured spectral data. On the other hand, the neural network technique could be a suited-well approach, because a constructed network is good at learning from known instances and making inference for unknown cases. The extraordinary ability of approximating, learning and generalization of ANNs motivates us considering its application for data analysis of ion backscattering spectra.

Backscattering spectra of energetic ion beams come from experimental measurements based on the Rutherford backscattering spectrometry (RBS) principle [4]. Mathematically, for given experimental conditions, ion backscattering spectra are function curves of normalized yield $Y(E)$ versus energy E. Information related to sample structure are implicitly contained in the spectra. Conventionally, data analysis of backscattering spectra requires the analyst to have high skills and

much experience-based knowledge of what the spectra of known samples look like. In the present study, we demonstrate how artificial neural networks are used to analyze RBS spectral data to obtain the structural parameters of a sample. The spectra are as input data into a network with an appropriate architecture and the sample structural parameters are the output variables. Representative pairs of input and output are chosen for training the network. After adequate training, the constructed network is used to predict the sample structural parameters.

2. ANN approach for ion backscattering spectral analysis

2.1 Problem Definition

Using the technology of ion backscattering spectrometry, the sample to be analyzed is bombarded by an energetic ion beam (usually He+ ion with MeV incident energy), the number and energy of backscattered ions are recorded by a spectrometer. The energy spectrum of the detected ions is a plot of the yield *Y(E)*, which contains implicitly information about the sample depth profile and composition. The sample structure can be described with a few parameters. For general problems, the elemental concentrations with depth distributions are concerned in the analysis. For relative simple cases, only elemental concentrations and sample thicknesses are required. We focus on the latter cases in this investigation.

From the mathematical transformation point of view, the problem of spectral data analysis can be abstracted as a pair of forward and inverse transformation between the input vector – the spectra data and the output vector – the structural parameters of a sample. A spectrum representing a physical process performs a smooth conversion of an input vector$\{c_1, c_2,\ldots c_n\}$, where $c_1, c_2,\ldots c_n$ are structural parameters of a sample including concentrations and thicknesses, into an output vector $\{y(E_1), y(E_2) , \ldots y(E_m)\}$, where $y(E)$ is a continuous function of energy E with the parameter set $\{c_1, c_2,\ldots c_n\}$. This input-output dependence can be written as a forward transformation equation $y(E)=f(E, c_1, c_2,\ldots c_n)$ and an inverse transformation $\boldsymbol{c}=F(\boldsymbol{y})$. The inverse problem, which is to determine the sample structure from the spectra, can be solved by the neural network method.

2.2 ANN approach

We have built a few multilayer feedforward perceptron networks (MLP) to tackle our analysis problem, where the structural information of a sample will be predicted from the corresponding spectra available. Initially a number of different network structures were explored. After some trials, three layer networks were found to be appropriate. The network consists of three layers of nodes: one input layer, one output layer and a hidden layer. All the nodes in one layer are connected the next layer (feedforward), as shown in figure 1. The spectral data are input from the nodes at the input layer. The sample structural parameters are as output variables at the nodes of output layer. The numbers of nodes in the input and output layers were determined according to the imposed task of a specific problem. The number of nodes at the hidden layer is adjustable so that an optimal network architecture can be achieved.

After determination of the architecture of the network, a series of input data (i.e., spectra) with their corresponding expected output values (i.e. sample structural parameters) will be presented to the network for the purpose of training. There are a number of algorithms available for training a MLP network, such as Resilient Backpropagation, Conjugate gradient, Levenberg-Marquard, and Quasi-Newton etc. We adopted the Resilient Backpropagation algorithm for training our network.

The main advantage of the Resilient Backpropagation algorithm is to eliminate the harmful effects of the Gradients methods, due to partial derivative problem of the sigmoid functions that are used as transfer functions in the hidden layer[5-7]. This algorithm directly adjusts the weights of the network based on the sign of the partial derivative of the error function with respect to each weight. This could accelerate learning process in the flat regions of the error function.

2.3 Construction of the training set

The training examples must contain the necessary information to generalize the problem. They normally consist of realistic data from experimental measurements. However, when a reliable and accurate computational model is available, the training data could be generated with simulated experimental data. We utilized the simulation program SIMNRA5.0 [8] to generate representative examples for training and testing. Since the SIMNRA 5.0 was based on an accurate computational model, the simulated spectra have been proven to be very close to experimental ones. We consider a specific example for the demonstration of the neural network technique applied to spectral analysis. In this example, we assume the sample consisting of a thin film SiGe on the Si substrate. The thicknesses of the sample are set between 1000 and 2500 ($\times 10^{15}$at/cm^2). The concentrations for Ge and Si both are between 0.2 – 0.8. There is a constraint, namely $C_{Ge}+C_{Si}=1.0$. Fig.2 shows a typical training spectrum with corresponding structural parameters. The training set and testing set consist of 412 and 60 simulated spectra and corresponding sample structures respectively. Each spectrum was generated by SIMNRA 5.0 for sample structural parameters chosen at random in specific ranges. The spectral data, made up of 54 data points, are as input for the network. There are 3 outputs representing the concentrations of c_1 (Ge), c_2 (Si) and the thickness (t).

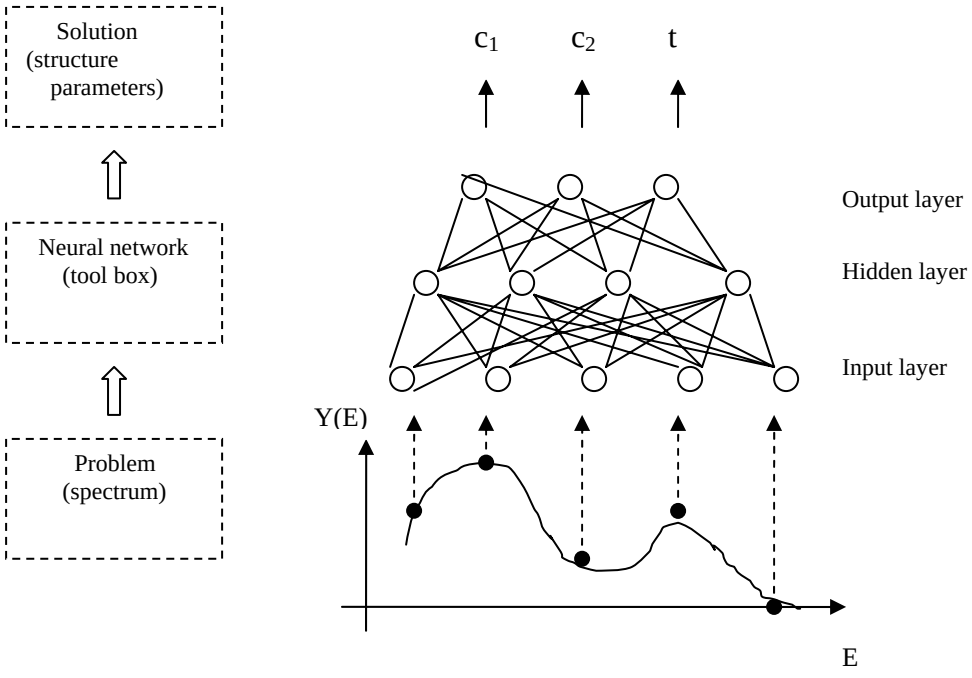

Fig.1. Schematic diagram of neural network for solving spectral analysis problem. Values of spectra at energy position E_1, E_2,… E_m are as input for the network. Structural parameters are the output.

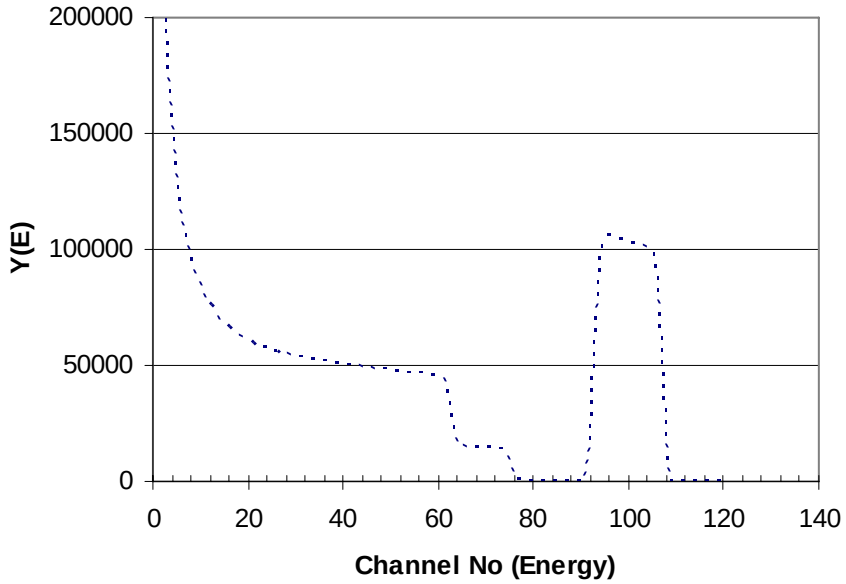

Fig.2. A typical training spectrum corresponding to the sample structure (t: $1700*10^{15}$at/cm^2, c_1: 0.59, c_2: 0.41).

3. Results and discussions

We have used the MATLAB® neural network toolbox to perform the computer experiments. A number of trials with different number of hidden neurons between 8 and 80 have been tested. It was found that 48 hidden units were sufficient to obtain a good performance on the training and testing data set. Typically 250 epochs were completed before the performance ceased improvement.

During training the mean squared errors (m.s.e) for the training set and the test set are plotted in Fig.3 as a function of epoch. This figure displays that a large initial value of errors is sharply decreased and followed by slow convergence to a minimum value. The final errors achieved on both the training and test set were 0.00038. In addition to the mean squared error curves, the performance of the network response can also be examined by analysis of predicted outputs versus the corresponding targets for some of test spectra or training data. We have performed some regression analysis for three output variables, using some of test spectra. As plotted in figures 4, all three outputs track the targets very well. Fig.4a shows that ANN can accurately predict the thicknesses of samples. Fig.4b and c also shows that AAN predictions for concentrations are also quite well.

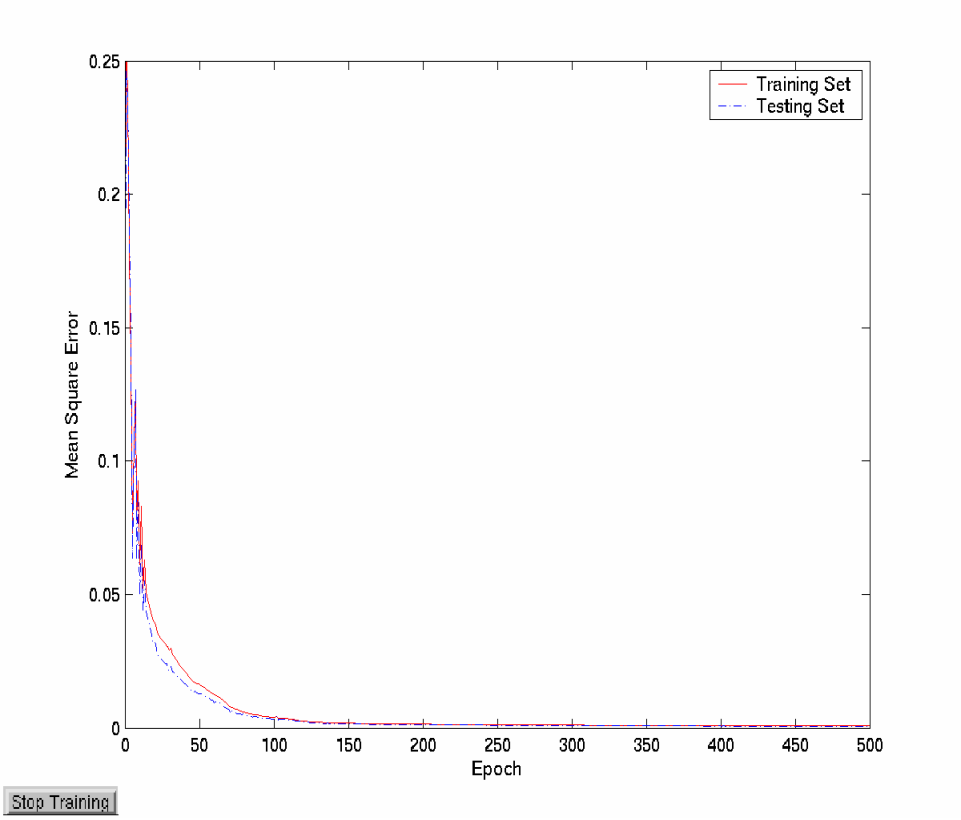

Fig.3. Mean squared errors for training and test data.

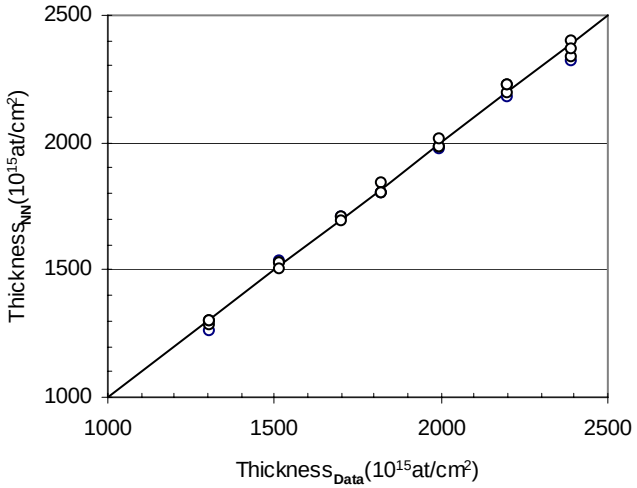

Fig.4a. Predicted output of thickness.The values obtained with ANN are labelled 'NN'. The original values with which the data were constructed are labelled 'Data'.

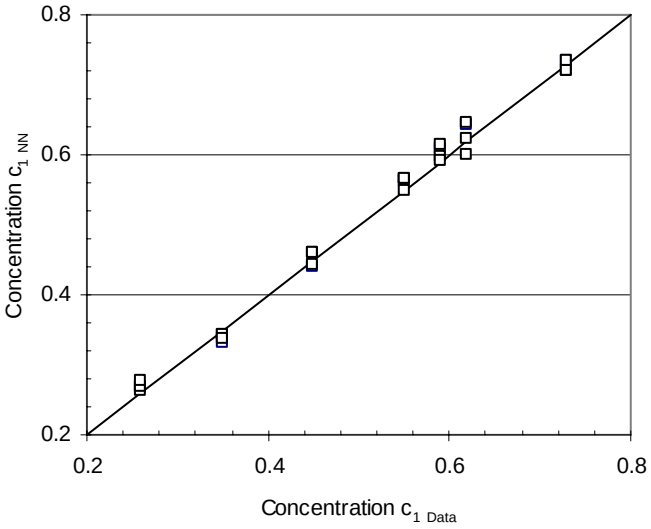

Fig4b. Predicted concentration c1. The values obtained with ANN are labelled 'NN'. The original values with which the data were constructed are labelled 'Data'.

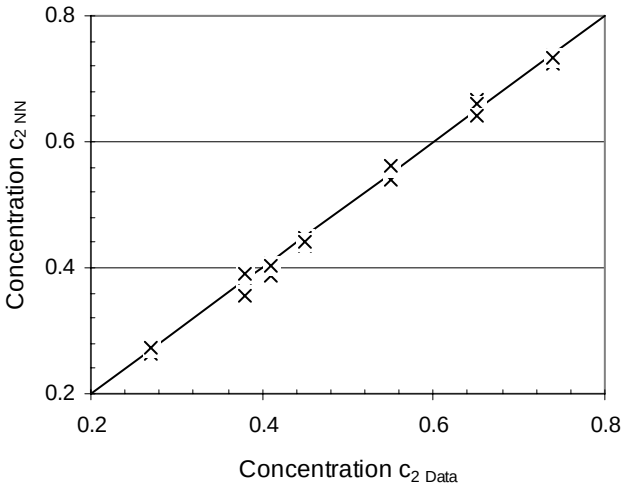

Fig.4c. Predicted output for concentration c2.The values obtained with ANN are labelled 'NN'. The origianl values with which the data were constructed are labelled 'Data'.

The trained network, with the fixed weights obtained during the training phase, was applied to generalization cases in which we analyzed 9 spectra. The predicted outputs are summarized in table 1. The neural network predictions were compared with the values determined using numerical simulation (namely, nominal). Overall, the agreement is excellent. The relative errors for thicknesses and concentrations are less than 3% and 9% respectively. The network correctly analyzed all cases within acceptable errors. Note there is a constraint for each pair of c_1 and c_2 and the summation of the network outputs of c_1 and c_2 meet the requirement of constraint (approximately equals to 1). This suggests that the constructed neural network can handle properly redundancies, which were caused by constraints of output variables.

Table 1. Comparison of the neural network predictions with simulated results

	Nominal (Numerical simulation)			NN prediction		
Sample No.	c_1	c_2	t ($\times 10^{15}$ at/cm^2)	c_1	c_2	t ($\times 10^{15}$ at/cm^2)
1	0.251	0.749	1173	0.264	0.729	1142
2	0.540	0.460	1173	0.545	0.453	1163
3	0.782	0.218	1173	0.755	0.240	1144
4	0.251	0.749	1768	0.261	0.737	1752
5	0.540	0.460	1768	0.540	0.452	1766
6	0.251	0.749	1914	0.262	0.738	1926
7	0.540	0.460	1914	0.549	0.461	1921
8	0.251	0.749	2211	0.254	0.742	2212
9	0.540	0.460	2211	0.539	0.457	2234

4. Conclusion

The results of this investigation show that properly configured MLP network is capable of performing spectral data analysis to extract structural parameters of the sample. The neural network method doesn't require any involvement of physics knowledge. The present study also shows that neutral network can be a new powerful tool for analysis of spectral data. In real data there is statistical error in the spectra – which is the input. It would be interesting to see what level of statistical uncertainty will hinder the accurate execution of the neural network algorithm.

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