

Application of Neural-Network Technique to Analysis of PIXE Spectra

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Introduction

Recently, artificial neural network techniques have been developed and successfully applied in the spectrum analysis in various fields. We have also proposed a analysis method based on the linear associative neural network (LANN) technique for the high speed analysis of the gamma-ray spectrum^{1,2)}. The principle of the LANN is very simple and calculation is very fast. In this paper, the LANN technique is introduced as a new method for the PIXE spectrum analysis; the method has high potential for the analysis in the on-line real-time and/or automatic modes.

LANN Method

The principle of the LANN technique has been described elsewhere,^{1,2} but brief explanation is given here. The LANN can realize the direct mapping of the observed pulse height spectrum to elemental content of samples. Namely, the function of the network is the linear transformation of an input vector $\mathbf{x}=[x_1, \dots, x_n]^T$, where T denotes the transposition and x_i is counts of channel i of the objective pulse height spectrum, to another space vector $\mathbf{y}=[y_1, \dots, y_m]^T$, where y_j is the concentration of element j in the sample, as shown schematically in Figure 1. The mapping is carried out just by multiplying the $m \times n$ weight coefficients matrix \mathbf{W} , whose elements are gained by the learning phase of the network before the analysis, to \mathbf{x} as $\mathbf{y}=\mathbf{W}\mathbf{x}$. The values of the matrix elements of \mathbf{W} are determined to satisfy the condition: $\|\mathbf{Y}-\mathbf{W}\mathbf{X}\|^2=\min$.^{3,4)} where the $n \times m$ matrix \mathbf{X} consists of \mathbf{x}_j 's, the reference spectra of the each element j 's, and the $m \times m$ matrix \mathbf{Y} consists of output \mathbf{y}_j 's corresponding to \mathbf{x}_j 's; for $j=1, m$, \mathbf{y}_j is usually taken as a unit vector $\mathbf{y}_j=[y_{1j}=0, \dots, y_{jj}=1, \dots, y_{mj}=0]^T$. Thus, \mathbf{Y} is a unit matrix, and the matrix \mathbf{W} turns out to be \mathbf{X}^+ : the Moore-Penrose pseudo-inverse matrix of \mathbf{X} . The matrix elements of \mathbf{W} are usually obtained by a supervised learning method of the network called Widrow-Hoff⁴⁾, or by a pure mathematical algorithm.

Experimental

We conducted performance test of this method for two types of samples: the first ones were mixed metal samples consisting of iron and nickel of various compositions, and the other one was a thin SUS 316 sample. Here we show only the results for the SUS 316 sample. A sample of SUS316 and pure metal samples of chromium, manganese, iron and nickel, the principal elements of the SUS316 (a trace element copper not included) were prepared by the evaporation method on Mylar films in vacuum. The experiment was carried out in the PIXE course at Cyclotron and Radioisotope Center, Tohoku University using a proton beam of 3 MeV. We employed a graphite collimator of 3-mm diameter to limit the size of the proton beam on the samples. The beam after passing through the samples stopped in a Faraday cup at 3 m behind the sample position. A 100- μm Mylar absorber was inserted between the sample and X-ray detector to suppress the strong Bremsstrahlung continuum and elastically scattered protons. X-rays emitted from the samples were observed by a conventional type Si(Li) detector in the direction of 90 deg. with respect to the incident beam. The pulse signals were analyzed by a 1024-ch PHA, and the data were stored in a bulk memory of a micro-computer. We have measured a set of spectra for all alloys as well as the single elemental samples, and a sample of backing film alone.

Spectrum Analysis

First, we constructed an LANN having 1024 input units and 5 output units corresponding to the four principal elements of SUS316: Cr, Mn, Fe, and Ni, and Mylar backing. The reference spectra for the network learning were made by subtracting the Mylar data from each metal sample data after normalization by Coulomb numbers of the proton beam bombarded. Here, we adopted a conventional single-spectrum learning method². The analysis of the objective spectra from the Fe-Ni alloys and SUS316 were made just by feeding those to the network.

The output of the LANN is compared to those of the peak fitting analysis using a sophisticated code SAPIX⁵) as shown in Figure 2. Error bars for both results in the figures are due to the statistical uncertainties. The uncertainties for the network output dy_j 's were evaluated by the following formula as variance matrix,

$$\langle dy dy^T \rangle = W \langle dx dx^T \rangle W^T,$$

where $\langle . \rangle$ denotes the ensemble average, $dy = W dx$, and $dy^T = dx^T W^T$. We adopted the assumption of independence between counts in each channel as follows,

$$\langle dx_i dx_k \rangle = (x_i x_k)^{1/2} \delta_{ik} \quad (\delta_{ik} = 1, \text{ if } i=k; =0, \text{ otherwise}).$$

Both results are almost consistent for the Fe and Ni alloys. As for the SUS316, the agreement is good except the manganese case ((1) of Figure 2 for SAPIX). In the manganese case, the SAPIX result is not correct because the resulting K_{β}/K_{α} value for manganese is far from the data base value given in (Ref.6). In the network analysis, the K_{β}/K_{α} is in principle assured because the both K_{α} and K_{β} peaks were included in the experimental observed reference spectrum used for the network learning. Figure 3 presents the comparison of the constructed spectra using the output of the network and the reference spectra data with the objective SUS spectrum. Excellent agreement is shown except the small discrepancy both in the lower and higher tails of the Ni- K_{β} peak that correspond to the K_{α} and K_{β} peaks of copper, respectively, not included in the reference spectra as mentioned above. The simple use of the SAPIX code could not correctly resolve the overlapping of Cr- K_{β} and Mn- K_{α} peaks. These two peaks were too close with each other, and the separation problem was quite ill-posed. Conversely using the data of K_{β}/K_{α} for these elements, another result for Mn could be obtained as SAPIX(2) (Figure 2), and is consistent with the network result. Such additional information was necessary to resolve the ill-posedness. The present network analysis is almost free of this kind of problem because the each reference spectrum includes all X-ray peaks of a single element, not only peaks of K-X lines but also of L- and M-lines, if observed; whereby the independence among the spectra for the different elements is very high.

More detailed description on the present method and tests is given elsewhere⁷⁾.

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References

- 1) Iwasaki S., Fukuda H., and Kitamura M., *Intelligent Engineering Systems Through Artificial Neural Networks*, 3 (1993) 199 (ASME Press, New York).
- 2) Iwasaki S., Fukuda H., and Kitamura M., *Internat. J. PIXE*, 3, No.3 (1993) 267.
- 3) Kohonen T., *Self-Organization and Associative Memory*, (Springer-Verlag, Berlin, 1984).
- 4) Hecht-Nielsen R., *Neurocomputing*, (Addison-Wesley Pub. Co., New York, 1990).
- 5) Sera K., et al., *Internat. J. PIXE*, 2, No.3 (1992) 325.
- 6) Johansson S. A. E. and Campbell J. L., *PIXE: A Novel Technique for Elemental Analysis*, (John Wiley & Sons, Ltd., Chichester, 1988).
- 7) Iwasaki S., et al., *Internat. J. PIXE*, to be published in Vol. 4, Nos. 2&3.

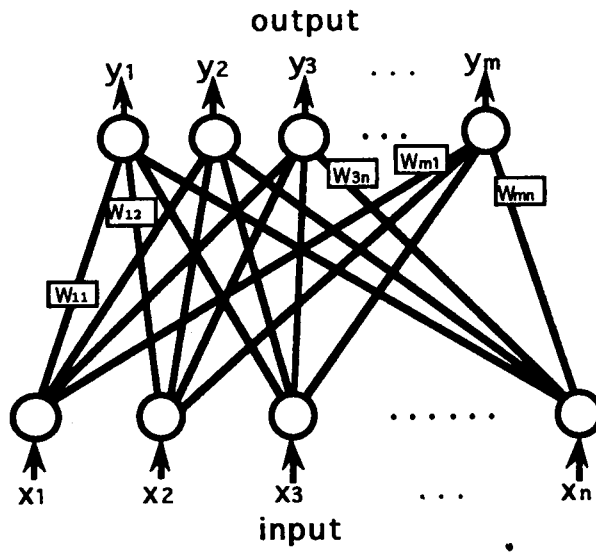


Fig. 1 Structure of linear associative neural network for the spectral analysis. The symbol (O) represents a unit of the network, and w_{ij} is weight coefficient of unit j for i input value.

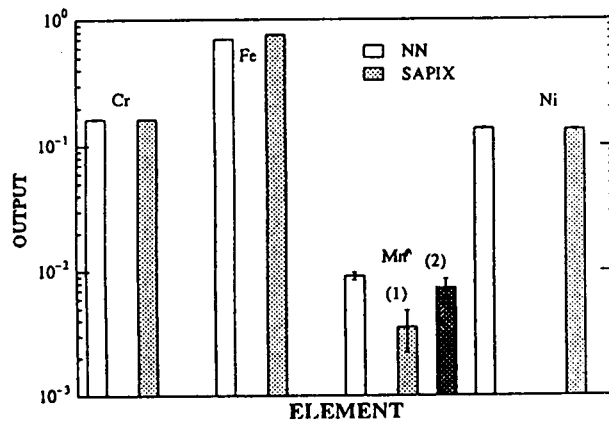


Fig. 2 Comparison of the results for SUS 316 with those of the SAPIX code. See text for the two results (1) and (2) of manganese.

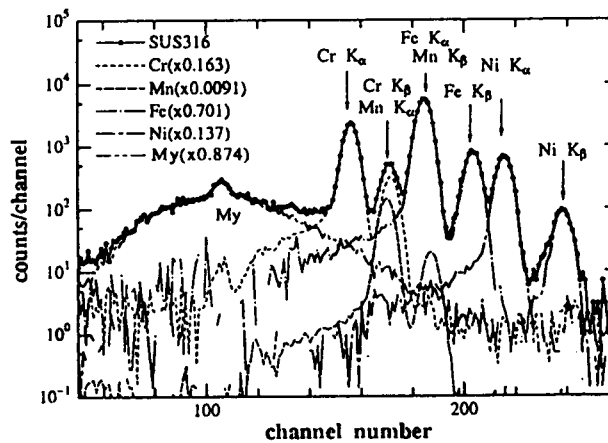


Fig. 3 Comparison of the spectrum for the SUS 316 (see. Fig. 2) with the reconstructed ones.