Prototyping of chemical composition of complex crystals using method of neural networks

A V Blagin¹, V V Nefedov², N A Nefedova²

¹ Don State Technical University, 1, Gagarin Square, Rostov-on-Don, 344000, Russia
² Platov South - Russian State Polytechnic University (NPI), 132, Prosveshcheniya Street, Novocherkassk, 346428, Russia

E-mail: a-blagin@mail.ru

Abstract.
The traditional methods of study of multi-component crystal heterojunction structures by means of X-ray diffractometry and electroscopy are expensive and complex. The present paper discusses the information technology based on the use of artificial neural networks for identification of the chemical composition of complex semiconductor structures. The obtained results allow supposing the successful use of this method for many multi-component systems.

1. Introduction
The research of multi-component crystal heterojunction structures (hereinafter referred to as heterostructures) by means of traditional methods, such as X-ray diffractometry and electroscopy, is nowadays an expensive component of the technology of electronic devices. This serves as an impetus to find other methods and approaches in the field of computer statistic experiment. The present paper features a discussion of an approach applied to the new information technology based on use of artificial neural networks (hereinafter referred to as ANN) aimed at identification of chemical composition of complex semiconductor structures.

The ANN is built according to the following characteristics of live neural networks letting them effectively handle non-standard challenges [1]: 1) simple processing element – neuron; 2) huge quantity of neurons takes part in processing of information; 3) one neuron is connected to a vast number of other neurons (global connections); 4) connections between neurons alternate their strength; 5) massive parallelism in processing of information.

Biological neuron of human central nerve system serves as a prototype for construction of the neuron. Biological neuron has its body, complex of appendices – dendrites – allowing the neuron receive input signals, and one appendix – axon – transferring the neuron’s output signal to other cells. The point of connection between the dendrite and axon is synapse. A simplified function of the neuron can be pictured in the following way:

- Neuron receives a set (vector) of input signals from dendrite;
- Cumulative value of the input signals is evaluated in the neuron’s body;
- Neuron shapes an output signal with its intensity depending of the value of calculated dot product;
- Output signal is transferred to axon and transferred to dendrites of the other neurons.
The particular characteristic of such bio-physical system is that the inputs of the neuron are not equisignificant. Each input is characterized by certain weight coefficient defining the significance of the information that is received through it. Thus, the neuron does not only sum up values of input signals but calculates the dot product of input signals and vector of weight coefficients.

Neural network is a sum of a huge amount of relatively simple elements – neurons with the topology of their connections depending on network type. To build a neural network aimed on solution of a certain problem one should choose a type of connection between neurons and correspondently pick up the values of weight parameters on the connections. The set connections further define whether one element can affect the other. The power of affection is defined through the weight of a connection.

2. The essence of the method and task definition
Before discussing the issue of teaching of the ANN, the mathematic definition of function of a separate neuron should be mentioned. It is performed in two steps:

Summary weight input is found according to

\[ S_j = \sum_i Y_i \times W_{ij} \]

where \( Y_i \) – is the activity level of i-element in the preceding layer, \( W_{ij} \) is the connection strength between the i- and j-element, whereby the synaptic connections with positive strengths \( W_{ij} \) are designated as actuating and those with negative strengths – slowing; 2) the activity of \( Y_j \) is calculated by means of a certain function of the total weighed input. Regular solution implies the use of sigma-function: 

\[ Y_j = \frac{1}{1 + \exp(-S_j)} \]

The following procedure is used to teach the ANN solving a certain problem. Initially a series of training cases consisting of vector of activities of input elements with vector of desired activities of output elements was presented to the network with a further comparison of actual activity on output elements with the desired activity. Then a calculation of an error followed that is defined as a squared difference between the actual and the desired output. Further the strength of every connection has been changed to reduce the error. Starting from the output layer, these actions are executed consequently for all preceding layers. The process of “back propagation” (back propagation, [2,3]), as it is described here, has been replicated with many different training examples to teach the network to recognize them correctly.

**Back propagation algorithm consists of four steps:**

1. Calculate the velocity of change of an error in case of alteration of the output element. This derivative of the error (EA) is the difference between the actual and expected activity.

\[ EA_j = \frac{dE}{dY_j} = Y_j - D_j \]

2. Calculate the velocity of change of an error in the course of change of total input received by the output element. The amount (EI) is a result of Step 1 multiplied by the velocity of alternation of the output element with alteration of its total input.

\[ EI_j = \frac{dE}{dS_j} = \frac{dE}{dY_j} \times \frac{dY_j}{dS_j} = EA_j \times Y_j \times (1 - Y_j) \]

3. Calculate the velocity of alteration of the error in the course of alteration of the strength on the input connection of an output element. The resultant (EW) is the result of Step 2 multiplied by the activity level of the element, from which the connection starts.

\[ EW_{ij} = \frac{dE}{dW_{ij}} = \frac{dE}{dS_j} \times \frac{dS_j}{dW_{ij}} = EI_j \times Y_i \]

4. Calculate the velocity of alteration of the error in the course of alteration of the activity of an element from the preceding layer. This key step lets us to apply the back propagation to the multi-layer networks. When activity of the element from preceding layer changes, it affects the activities of all output elements that are connected to it. Therefore, to calculate the total summary affection
on the error all the affections on the output elements are summed up. These affections can be
calculated relatively easy. It is the result of Step 2 multiplied by the strength of the connection to
the correspondent output element.

\[ EA_i = \frac{dE}{dY_i} = \sum_j \left( \frac{dE}{dS_j} \times \frac{dX_j}{dY_i} \right) = \sum_j \{ E_{ij} \times W_{ij} \} \]

Using Step 2 and 4, the EA quantities of one layer of elements can be converted into EA of a
preceding layer. This procedure can be repeated with aim of calculation of the EA of all and every
preceding layer. Knowing the EA for an element, Step 2 and 3 can be used for calculating of the EW
on its output connections and correspondent adjusting the synaptic strengths.

3. Results of the author's studies
The described method can be used for identification of the qualitative composition of multicomponent
solid solutions (hereinafter referred to as MSS) in regard to their photoluminescence spectrum
(hereinafter referred to as PL spectrum). Assume there is a certain PL spectrum of a structure on the
basis of MSS that is described by the function \( S = S(\lambda) \).

It is proposed to use as identification parameter the amount of energy radiated in a sufficiently narrow
diapason of length of waves \([\lambda_i, \lambda_{i+1}]\), that can be evaluated as an integral \( S = S(\lambda) \) on that kind of
diapason.

The spectrum shall be divided into \( n \) sections with the length \( h \); assume that the spectrum is linear on
each of them. I.e.

\[
Q_i = \left\{ S(\lambda) = \frac{h}{2} \left[ S(\lambda_i + h \times i) + S(\lambda_{i+1} + h \times (i+1)) \right] \right\} \approx \frac{h}{2} \left[ S_i + S_{i+1} \right]
\]

The amounts of \( Q_i \) will depend on a large number of parameters; still their correlations for one and the
same MSS shall remain constant. Therefore, to reduce the affection of side factors, such as, for
example, the value of non-radiative recombination, \( P_i = \frac{Q_i}{A} \), where \( A = \max_{i=1}^n Q_i \) is chosen as
characteristics of \( i \)-segment.

By this means, \( n \) elements are compared to \( P_i \) values arriving to the input of neural network to the PL
spectrum of the MSS. There will be 9 signals corresponding to the components of the 3rd and 5th group
on the output of ANN. The experimentally received data for MSS’s specters on input as well as unit
values received on the outputs, corresponding to the defined MSS, will be used as references during
the teaching of the network. Other output values are set as zero values. Network status shall be
regarded as satisfying when all teaching examples produce response on the requested outputs not less
than 0.9; with not more than 0.1 on the others. The qualitative composition of an unknown example is
evaluated upon the amount of responses of neural network (with the largest values corresponding to
the most probable components of the presented sample).

Processing of benchmark data is performed in two steps and, correspondingly, assumes the use of
several ANN. The qualitative content of the MSS was evaluated initially. PL spectrums of MSS
GaAs_xBi_yP_{1-x-y}/GaP were presented to ANN as examples (see Ill. 1), whereby the amount x was
deemed to have values from 0.005 to 0.025, and \( y \) – from 0.0005 to 0.0020. 37 examples were used for
this. The output values for components were set according to the qualitative composition of the MSS:
1 corresponded to the component included into MSS, 0 – corresponded to all others. The use of the
back propagation method allows achieving the satisfying identification of 100% of teaching cases. The
second step featured the attempt to identify quantitative composition of the considered MSS.
This resulted in discovery of the following fact. The ANN turned out to be sensitive to the changes of
\( Y \), although the values set to this parameter were one order less than the values of X (Bismuth is
GaAs_xBi_yP_{1-x-y}/GaP light alloying additive in MSS). Experimental data [4] testifies that even subtle
changes in composition in regard to Bi lead to the significant modification of zonal energetic structure
of crystals. This fact explains the mentioned inequivalence – consistency of optical properties with respect to the changes of $X$ and inconsistency with respect to the alterations of $Y$.

![Figure 1. PL spectrums GaAP<sub>Bi</sub>/GaP(a) and GaAsP<sub>Bi</sub>/GaP(b). Content of Bi in solid phase $X_{Bi}$ mol. %, 1 – 0.03, 2 – 0.06, 3 – 0.1.](image)

This conclusion underwent experimental verification. PL characteristics of heterostructures GaAsP<sub>Bi</sub>/GaP are determined at 77 K and 300 K. Photoresponses with relative intensity of not less than 0.5 are obtained within diapason of 1.4 - 1.85 eV (GaAsP<sub>Bi</sub>), which is substantially broader than the luminescence domains of the correspondent solid solutions not alloyed by Bismuth. Luminescence specters have several maximums at 77 K. Half-width of the peaks is 10-30 MeV. Low-energy peaks arising of the formation of GaAs clusters have a relative intensity of not more than 0.25. Along with the growth of XSBi the intensity of low-energy peaks decrease and their diffusion is registered, which signifies the structuring role of Bismuth. The fact of additional shift of photoluminescence towards the short-wave region of spectrum is registered at the maximum values of XSBi. It can probably be conditioned by increase of Eg due to Burstein-Moss effect [5-8]. (The mentioned fact has significant operational applicability at the use of the GaAsP<sub>Bi</sub>/GaP structure in air pollution control devices ($CO_2$, $CO_2$, $SO_2$) and in other branches of electrooptics [9-12])

The obtained results allow supposing a possibility of successful use of this method also for the more complex four- and five-component systems as it is already shown at the beginning of 2000th [11], the neural networks method became widely used in the tasks of analysis of highly non-linear systems. At that, the amount of outputs of neural networks rises abruptly. This issue can be solved by use of data relating to the spheres of existence of solid solutions, and for components scarcely affecting the PL spectrum only one output can be used – indicating whether the component is present in the MSS. It is obvious that the described method can be effectively applied for solving of other problems in the technology of semiconductor materials – there where there is a possibility to apply methods of identification and forecasting by means of ANN.

4. Conclusion

The obtained results allow suggesting a possibility of successful application of the described method in other multi-component systems. However, it obviously leads to an increase of the amount of outputs of ANN. The problem can be solved using the data of the existence domains of MSS; and the issue with the components having little effect of the PL spectrum can be solved by the use of only one output – the test defining presence of this component in heterostructure. A shortcoming of the suggested method lays in the fact that the success ratio of attempts to define the composition is proportional to the volume of statistic data for spectrums of connections generating the MSS under examination. Still, in the cases when the volume is sufficiently huge, composition of the new samples can be evaluated in a timely manner and practically without any additional material costs, which undoubtedly can be regarded as a significant advantage for crystal physics and technology of multi-
component semiconductors. The described method can be of particular interest in different branches of modern physics dealing with the graphic representation of characteristics of matter and field.

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