The application of neural networks on analysis of optical glass properties

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Abstract - In the paper we present application of artificial neural network (ANN) on relation between glass composition versus optical transmittance of the chosen glass systems. The excellent prediction ability of ANN program shows a possibility to influence the glass composition to obtain required optical properties.

Keywords - antimonite glasses, artificial neural networks, optical properties.

I. Introduction

Artificial neural networks use the distributed parallel processing of information during the execution of calculations, which means that information recording, processing and transferring are carried out by means of the whole neural network, and then by means of particular memory places. The basis of mathematical model of the neural network is a formal neuron which describes by a simplified way a function of a biological neuron by means of mathematic relations (Fig. 1).

A neuron consists of a body, called a soma, which the input transmission channel in the form of dendrites leads to; the output is provided by axon [1]. The formal neuron has n of generally real inputs $x_1,\ldots,x_n$ corresponding to dendrites. All inputs are assessed by appropriate synaptic weights $w_1,\ldots,w_n$ which are generally also real. Weights determine the transmission rate of the input signal. The weighed sum of input values presents the inner potential of the neuron z [2, 3-6]:

$$\mathrm{z} = \sum_{i=1}^{n} w_i x_i - h \tag{1}$$

Output (state) of the neuron y modelling the electric impulse of the axon is generally given by a non-linear transfer function σ, the argument of which is the inner potential of z.

$$y = \sigma(z) \tag{2}$$

Learning is a basic and essential feature of neural networks. Knowledge is recorded especially through the strength of linkages between particular neurons. Linkages between neurons leading to a "correct answer" are strengthened and linkages leading to a "wrong answer" are weakened by means of the repeated exposure of examples describing the problem area. These examples create a so-called training set [3].

For all types of predictions neural networks are suitable to be used for their learning Back propagation algorithms. This algorithm is convenient for multilayer feed forward network learning which is created minimally by three layers of neurons: input, output and at least one inner (hidden) layer. Between the two adjoining layers there is always a so-called total connection of neurons, thus each neuron of the lower layer is connected to all neurons of the higher layer.

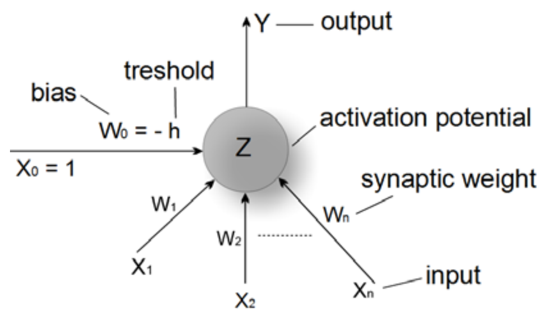

Fig. 1 Mathematical model of neuron

Learning in the neural network is realized by setting the values of synaptic weights between neurons, biases or inclines of activation functions of neurons. The adaptation at Back propagation types of networks is also called „supervised learning“, when the neural network learns by comparing the actual and the required output and by setting the values of the synaptic weights so that the difference between the actual and the required output decreases [3].

Artificial neural networks are suitable for approximation of relations among various process data, among data with a high degree of nonlinearity and inaccurate data. This type of data often occurs in industrial processes of metallurgy. Neural networks are able to simulate behaviour of systems with very complex internal structure and complicated external behaviour, where analytic description is considerably complex; eventually

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it does not exist at all. They can simulate dependences which are solved with difficulties by classic methods of statistic data evaluation (e.g. regression analysis) and they are able to express more complex relations than these methods. Regression analysis requires at least partial knowledge of the internal structure of the system (system is known as a grey or white box), i.e. it is necessary to assess the structure of the regression function beforehand, which is difficult especially for multiparametric systems. Neural networks do not need knowledge of the system internal structure (system can be given as a black box); they are able to derive the dependency among variables just from the nature of the data by means of learning.

II. Experimental Procedure

Investigated glasses were prepared from materials of high purity (> 98 %) at the Université de Rennes in France. Production of glasses started by mixing of powders and their heating in quartz or quartz-glass ampoule went on while the transparent melt was gained. Then the melt was spilled at the brass plate [9]. Preparing glass by heating original carbonates ($PbCO_3$, Na_2CO_3, K_2CO_3, Li_2CO_3) one can notice their decomposition on CO_2 and the formation oxides, which create glasses [7, 8]. Temperature used during the glasses preparation depended on their composition and was from the interval (900 – 1100) °C.

A specific data file designed to create artificial neural networks included 13428 cases. Indeed 7 of the total number of variables were used as inputs to the artificial neural networks. As the input variables were identified concentrations of source substances Sb_2O_3, $PbCl_2$ $PbCO_3$, Na_2CO_3, K_2CO_3, Li_2CO_3 and wavelength. One output variable has been marked as the transmittance. Scheme of input and output variables related to the neural network is shown in Fig. 2.

Software Statistica – Neural Networks was used for the creation of artificial neural networks. Data file had to be modified before the creation of artificial neural networks so that it could be used in mentioned software (Statistica). Total amount of data were randomly divided into three parts: training, testing and validation. This is necessary for a proper learning and verification of the accuracy of the prediction of created artificial neural network. Several artificial neural networks with varying structure and parameters were created on the basis of adjusted data. The one that had the best results of learning has been selected for the prediction of defects. It was three-layer network with topology 7-10-1. This means that the input layer contains 7 neurons, hidden layer 10 and the output layer one neuron [9].

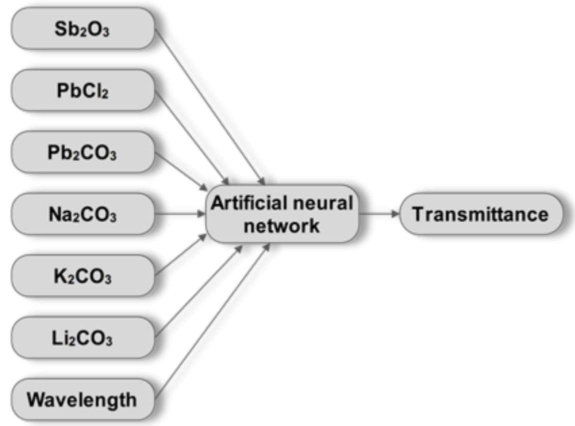

Fig. 2 Structure of input and output data

The rate of inaccuracy between predicted and actual output represent a prediction error. In technical applications the error is mainly represented by following relations:

The relation for RMS error calculation (Root Mean Squared) – it does not compensate for units used

$$\mathrm{RMS} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - o_i)^2}{n-1}} \tag{3}$$

The relation for REL_RMS error calculation – it compensates for units used

$$\mathrm{REL\_RMS} = \sqrt{\frac{\sum_{i=0}^{i=n-1}(y_i - o_i)^2}{\sum_{i=0}^{i=n-1}(y_i)^2}} \tag{4}$$

where: n - number of patterns of a training or test set, y_i - predicted outputs, o_i - measured outputs.

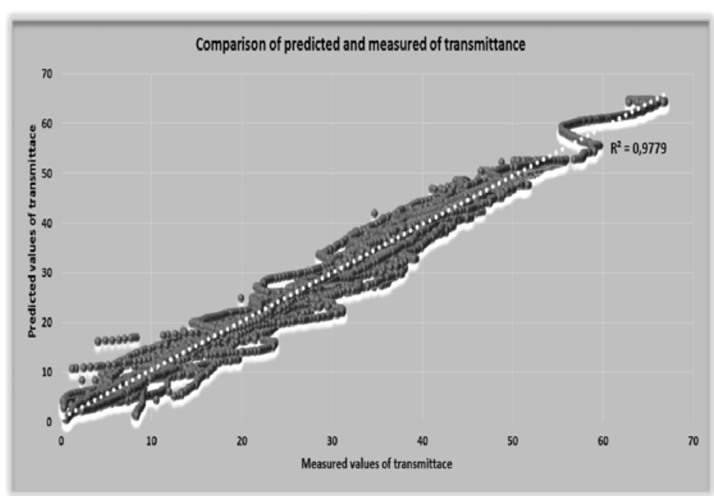

Fig. 3 Comparison of measured and predicted data

Prediction errors of the chosen neural network model calculated according to relations (3) a (4) are RMS = 2.28 and REL_RMS = 0.068. Comparison of measured and predicted data is represented on Fig. 3. Figure 4 shows a histogram of the residues, expressing also the quality of the learning. Selected neural network enables to predict the optical transmittance with sufficiently small error (7%).

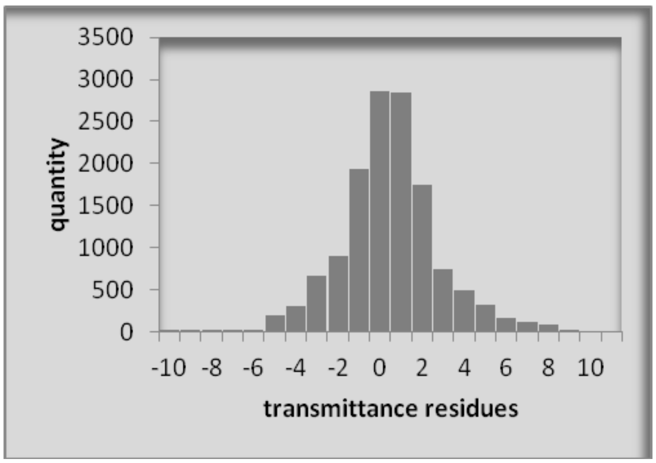

Fig. 4 Histogram of residues

Furthermore, sensitivity analysis was realized for this neural network. This analysis reflects the influence of individual input variables on a given system. Sensitivity analysis showed that $PbCl_2$, Sb_2O_3 were variables with the greatest influence on the system. Conversely, wavelength and $PbCO_3$, Li_2CO_3, K_2CO_3 are variables, which have a relatively small effect on the system. The overview of sensitivity analysis and the significances is in the Table 1.

Table 1 Sensitive analysis

Variable	**Relative importance of the variables**	**Sequence**
$PbCl_2$	119,62	1
Sb_2O_3	103,10	2
$PbCO_3$	70,10	3
Na_2CO_3	59,91	4
K_2CO_3	49,77	5
Wavelength	27,22	6
Li_2CO_3	25,11	7

In terms of conclusions about the plausibility of the ANN analysis, it is important to find out how the contents of individual components of used modifiers affect properties of glasses. The realized ANN analysis (Table 1) showed a new possibility for the determination of the relative importance which is in good agreement with the assumptions. High relative importance of starting substances containing Pb ($PbCl_2$, $PbCO_3$) is a given by the fact, that atom of Pb in the role of modifier interrupts structural units given by the Sb_2O_3. With regard to the coordination number 6 and the size of an atom of Pb in this arrangement it can be expected significant change of optical properties after the addition of the substances based on lead. The most significant relative importance at $PbCl_2$ is given by the fact that the chlorine atom may also participate in the interruption of bindings between structural units by the occupying positions of oxygen atoms in the structural units. The relatively small impact of the substances bringing alkali metals oxides (K_2CO_3, Li_2CO_3, Na_2CO_3) is associated with a small radius of the alkali metals. The relative lowest importance of Li_2CO_3 on the optical properties of the glasses is connected with radius of Li which atoms occupy in the glass network primary interstitial positions. If we start from Table 1, we can say that the wavelength is also a low important factor, which is in accordance with the assumptions.

For the use of the results of the learned artificial neural network parameters and the structure of the selected network were implemented to a custom program created in the development software environment for C++. This program is independent on the software Statistica, i.e. program in which the neural networks were created and tested. This program can be used for prediction of defects on the basis of the entering of input parameters to all required variables.

III. Conclusion

A model of neural network for prediction of optical transmittance of the chosen glass systems was created. The model enables to predict the optical transmittance with an adequately small relative error (7 %). After evaluation of achieved results we can state that exploitation of neural networks is advantageous, if it is necessary to express complex mutual relations among different sensor-based data. It was verified that usage of artificial neural networks for prediction of for prediction of optical transmittance of the glass systems is very perspective.

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