available at www.sciencedirect.com

ScienceDirect

journal homepage: www.intl.elsevierhealth.com/journals/dema

Estimation of chemical resistance of dental ceramics by neural network

Jasenka Živko-Babić[a], *Dragutin Lisjak*[b], *Lidija Ćurković*[b], *Marko Jakovac*[a,*]

[a] *Department of Prosthodontics, School of Dental Medicine, University of Zagreb, Gundulićeva 5, 10000 Zagreb, Croatia*
[b] *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia*

ARTICLE INFO

Article history:
Received 23 January 2006
Received in revised form
11 January 2007
Accepted 19 January 2007

Keywords:
Dental ceramics
Neural network
Chemical resistance

ABSTRACT

Objectives. The purpose of this research was to determine the mass concentrations of ions eluted from dental ceramic after an exposure to hydrochloric acid and, drawing on those results, to develop a *feedforward backpropagation* neural network (NN).

Materials and methods. Four dental ceramics were selected for this study. The experimental measurement was conducted after 1, 2, 3, 6 and 12 months of exposure to hydrochloric acid. The results of the 1, 2, 6 and 12 months of immersion were used for training a 13-13-5 model of NN. For evaluating NN efficiency, the regression analysis of input variables obtained by the experiment and output variables provided by the trained network was used.

Results. The measured data from the 3-month acid exposure and data obtained by the neural network estimation were compared.

High correlation coefficient (R) and low *normalized root mean square error* (NRMSE) between the measured and estimated output values were observed.

Conclusions. It could be concluded that the artificial neural network has a great potential as an additional method in investigating the properties of dental materials.

1. Introduction

Dental materials have to satisfy strict criteria because of their long therapeutic durability in the oral cavity. One of the most important properties of all restorative dental materials is their chemical resistance. Chemical resistance or chemical durability depends on the structure and composition of the material, laboratory conditions, and environment, which is in this case the oral cavity.

There are several methods for testing the chemical resistance of restorative materials. ISO [1] and ADA [2] standards are usually recommended. Both methods use a 4% acetic acid as a solution medium for faster degradation of dental ceramics. The goal of these methods is to find out the weight loss of ceramic samples after an exposure to the mentioned acid. There are also methods that test chemical resistance of ceramic in more detail, in different media, for a longer period, etc. [3–11]. However, technical literature does not mention any method which could predict the amount of chemical degradation of ceramic material after the measuring interval and at all points during the interval. For this reason a neural network is developed. A neural network is a computer simulation of the behavior of a material based on the experimental research of its properties. This method has been used for testing materials in mechanical engineering [12]. However, neural networks are rarely used for testing dental materials and never for evaluating the chemical resistance of dental ceramics [13,14]. The purpose of this research was to determine the mass concen-

* *Corresponding author*. Tel.: +385 14802135; fax: +385 14802159.
E-mail address: jakovac@sfzg.hr (M. Jakovac).
0109-5641/$ – see front matter © 2007 Academy of Dental Materials. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.dental.2007.01.008

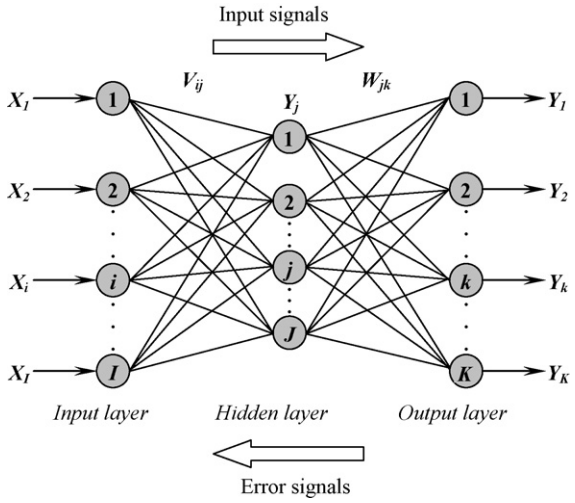

Fig. 1 – Principle of the *feedforward backpropagation* training algorithm.

trations of ions eluted from a dental ceramic after an exposure to hydrochloric acid and, drawing on those results, to develop a *feedforward backpropagation* neural network.

2. Artificial neural network

Artificial neural networks (ANN) are inspired by the biological neural system and its ability to learn through example. Instead of following a group of well-defined rules specified by the user, neural networks learn through intrinsic rules obtained from presented samples. The most commonly used ANN architecture is the multilayer *backpropagation neural network*. Backpropagation was created by generalizing the *Widrow-Hoff* learning rule to multiple-layer networks and nonlinear differentiable transfer functions [15]. Input vectors and the corresponding target vectors are used to train the network until it can approximate a function, associate input vectors with specific output vectors. Standard backpropagation is a gradient descent algorithm, as is the *Widrow-Hoff* learning rule, in which the network weights are moved along the negative of the gradient of the performance function. The term *backpropagation* refers to the manner in which the gradient is computed for nonlinear multilayer networks. *Backpropagation* neural networks often have one or more hidden layers of sigmoid neurons followed by an output layer of linear neurons. Multiple layers of neurons with nonlinear transfer functions allow the network to learn nonlinear and linear relationships between input and output vectors. There are numerous variations of the basic algorithm that are based on other standard optimization techniques, such as conjugate gradient and Newton methods [15]. The one used in this paper is the *feedforward backpropagation* training algorithm designed to minimize the *mean square error* (MSE) between the actual (estimation) output (a, A) and the desired (target) output (d, T). Fig. 1 shows the principle of the *feedforward backpropagation* training algorithm. The basic learning algorithm can be summarized as follows:

Step 1. Set the initial values of weights V_{ij} and W_{jk}.

Step 2. Compute the outputs of all neurons layer-by-layer, starting with the input layer as shown below:

$$\mathrm{net}_j = \sum_{i=1}^{I} \mathrm{V_{ij}X_i}, \quad j = 1, 2, \ldots, J-1, \quad i = 1, 2 \ldots, I \tag{1}$$

$$\mathrm{Y}_j = f(\mathrm{net}_j) \tag{2}$$

$$\mathrm{net}_k = \sum_{j=1}^{J} \mathrm{W_{jk}Y}_j, \quad j = 1, 2, \ldots, J-1, \quad k = 1, 2, \ldots, K \tag{3}$$

$$\mathrm{Y}_k = f(\mathrm{net}_k) \tag{4}$$

where V_{ij} is the weight between the input layer and the hidden layer, W_{jk} the weight between the hidden layer and the output layer, X_i the input signals (value of chemical composition), i the number of neurons of the input layer, I the number of inputs of neuron j in the hidden layer, Y_j the output of the hidden neurons, j the number of neurons of the hidden layer, J the number of inputs of neuron k in the output layer. Y_k the output signals (mass of eluted ions per gram of samples), and k is the number of neurons of the output layer. In the case of sigmoidal transfer function of the hidden layer, the following equation applies:

$$f(x) = \frac{2}{1 + e^{-x}} - 1 \tag{5}$$

Step 3. Compute system error E:

$$E = \frac{1}{2}\sum_{k=1}^{K}(d_k - a_k)^2 \tag{6}$$

where K represents the total number of patterns, d_k the desired outputs (experimental values) and a_k the actual outputs.

Step 4. If E is small enough or learning iteration is too big, stop learning.

Step 5. Compute learning errors for every neuron layer-by-layer:

$$\delta_k = (d_k - a_k)f'(\mathrm{net}_k), \quad k = 1, 2, \ldots, K \tag{7}$$

$$\delta_k = \sum_{k=1}^{K} \mathrm{W_{jk}}\delta_k f'(\mathrm{net}_j), \quad j = 1, 2, \ldots, J-1, \quad k = 1, 2, \ldots, K \tag{8}$$

Step 6. Update weights along negative gradient of E:

$$\mathrm{W_{jk}}(n+1) = \mathrm{W_{jk}}(n) + l_r\delta_k \mathrm{Y}_j + \alpha(\mathrm{W_{ij}}(n) - \mathrm{W_{ij}}(n-1)) \tag{9}$$

$$\mathrm{V_{ji}}(n+1) = \mathrm{V_{ji}}(n) + l_r\delta_j \mathrm{X}_i + \alpha(\mathrm{V_{ji}}(n) - \mathrm{V_{ji}}(n-1)) \tag{10}$$

where l_r is the learning rate, α the momentum, and n is the current iteration step.

Step 7. Repeat from Step 2.