Expert Systems with Applications 39 (2012) 4094–4101

Contents lists available at SciVerse ScienceDirect

Expert Systems with Applications

journal homepage: www.elsevier.com/locate/eswa

Exploration of artificial neural network to predict morphology of TiO_2 nanotube

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ARTICLE INFO

Keywords:
TiO_2 nanotube
Artificial neural network
Anodization
Prediction
Morphology

ABSTRACT

Artificial neural network (ANN) was developed to predict the morphology of TiO_2 nanotube prepared by anodization. The collected experimental data was simplified in an innovative approach and used as training and validation data, and the morphology of TiO_2 nanotube was considered as three parameters including the degree of order, diameter and length. Applying radial basis function neural network to predict TiO_2 nanotube degree of order and back propagation artificial neural network to predict the nanotube diameter and length were emphasized in this paper. Some important problems such as the selection of training data, the structure and parameters of the networks were discussed in detail. It was proved in this paper that ANN technique was effective in the prediction work of TiO_2nanotube fabrication process.

1. Introduction

Titanium dioxide (TiO_2) nanotube has attracted great attention in recent years owing to its remarkable potential applications in the areas of electronics, gas-sensing materials, optics, and biotemplating (Mor, Varghese, Paulose, Shankar, & Grimes, 2006; Varghese et al., 2003). Some experiments indicated that the geometrical feature of the nanotube affects its photocatalysis and sensing properties impressively which are crucial for applications (Valota et al., 2009; Vega et al., 2007). DC current electrochemical anodization is widely used to fabricate highly ordered TiO_2 nanotube (Mor et al., 2006; Varghese et al., 2003). In order to optimize its properties in applications, a lot of theoretical and experimental works have been carried out to investigate the relation between anodization conditions and geometrical parameters of the nanotube. Works focusing on the mechanistic aspects successfully explained the formation process of the tube in general, but failed in predicting the geometrical parameters of the tube at a certain anodization condition precisely (Macak et al., 2007; Yasuda, Macak, Berger, Ghicov, & Schmuki, 2007). The influence of some important anodic conditions on the structure and morphology of TiO_2 nanotube was investigated through experiment (Oh, Lee, Kim, Suh, & Chi, 2008; Prakasam, Shankar, Paulose, Varghese, & Grimes, 2007), but the result was unsatisfied and the process was both costly and time-consuming. Till now there are still lack of descriptions in detail about the relationship between anodization parameters and morphology of TiO_2 nanotube.

Artificial neural network (ANN), a powerful tool for modeling complex processes, is finding growing acceptance in the field of aerospace, automotive, electronic, manufacturing, robotics, telecommunication, etc. (Guessasma & Coddet, 2004; Parthiban, Ravi, & Kalaiselvi, 2007). ANN method can reveal certain correlations based on analyzing experimental data in biological mode without knowing their underlying physical mechanism. It can handle nonlinearity, imprecise and fuzzy information and simulate the input/output mapping at any accuracy in theory (Zhang, Yang, & Evans, 2008). Most importantly, ANN method can provide users the prediction power but not being confined to input/output fitting. Now it is almost a standard modeling technique based on statistical approach. ANN has been successfully applied to simulate the structures (Khanmohammadi, Garmarudi, Khoddami, Shabani, & Khanlari, 2010) and physical properties (Dutta, Parsons, Bhattacharjee, Bandhyopadhyay, & Datta, 2010; Kandjani, Salehpoor, Tabriz, Arefian, & Vaezi, 2010), such as adsorption efficiency, photocatalytic efficiency, for various kinds of nanostructures. As to the formation process of self-organized TiO_2 nanotube, which contains plenty of experimental data and lacks precise physical model, ANN method is considered to be suitable for the prediction work.

In this paper, two different ANN models was innovatively employed to the prediction work of TiO_2 nanotube preparation process with the aim for architecting suitable ANNs to simulate morphology of TiO_2 nanotube under a certain fabricating condition. Some data simplification and network training process were discussed in detail. Finally, optimized network structures and mature networks with satisfied prediction accuracy were obtained, and some further usages were also discussed.

2. Artificial neural network

A typical structure of ANN can be seen in Fig. 1. The basic unit in ANN is the neurons which are distributed in the neural network

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doi:10.1016/j.eswa.2011.09.081

layers. Neurons in adjacent layers are connected to each other and each connection is corresponding to a weight, which can regulate the influence of the received data. The input/output data are linked with a set of basic functions. Each layer corresponds to a bias and a specific transfer function (Shen, Chan, Lo, & Chau, 2002). After processed by the weight, bias and transfer function, the input data are delivered layer by layer and finally formed the output data. Apparently, the simulation accuracy depends on the network parameters, but there is no standard method to determine them (Guessasma & Coddet, 2004; Parthiban et al., 2007). Trial and error method is applied in this paper to choose all these network parameters step by step.

Back propagation artificial neural network (BPANN) is the most important and frequently used ANN, which is a kind of multi-layered feed-forward network trained with the back-propagation learning algorithm. While radial basis function (RBF) network is another kind of important ANN, which is a kind of multi-layer feed-forward error-back propagation networks with three-layers, and it runs faster than BPANN. There are some other types of ANN such as Hopfield networks, Kohonen networks, adaptive resonance theory (ART) networks, et al. Each of them has their own characteristics and special applications, and the selection of a certain kind of ANN depends on the type of the problem.

3. Experimental procedure and ANN training approach

3.1. Preparation of TiO_2 nanotube

Titanium foils (20 mm × 15 mm, 0.2 mm thick, 99.6% purity) were used to prepare TiO_2 nanotube arrays. The foils were cleaned with acetone solution in ultrasonic bath, followed by rinsing in deionized water and finally dried in air. The anodization process was conducted in a two-electrode configuration under constant potential, in which titanium foil acted as the anode and platinum foil in the same size as the cathode. The two electrodes with a distance of 2 cm were submerged into an electrolyte containing fluoride ions and the oxidation time was ranging from 3 min to several hours. Morphologies of the nanotube arrays were characterized by the scanning electron microscopy (Philips XL30). All experiment was carried out at room temperature of approximately 22 °C.

3.2. Input data simplification

A set of input and output should to be determined before the simulation process. Morphology of the nanotube array was intensely affected by the electrochemical condition and electrolyte parameters. The electrolyte used in the anodization could be HF electrolytes, acidic HF mixtures, buffered neutral electrolytes or water free electrolytes (Macak et al., 2007). So the initial experimental conditions or the input data were defined as the solute and solvent in the electrolyte, the anodization voltage and reaction time. In this paper, four kinds of commonly used solute and six kinds of solvent were considered. To record the electrolyte in a numeric way, "1" was placed under the applied solvent and "0" under the others. At the same time, values in the solute part meant the mass fraction of the corresponding materials. If the solvent was water, the value of water content in the solute should be recorded as "0", otherwise it could be non-zero. The original input data contained 12 different kinds of parameters which can be seen in the left side in Fig. 2 for example. In order to describe morphology of the resulting nanotube arrays, the degree of order, diameter and length of the nanotube were used as experimental results. Furthermore, the degree of order was defined as five degree (Fig. 2), in which "1" stood for highly ordered while "5" for the highly order less distribution, and "2"–"4" corresponded to a gradually weakening degree of order.

It was too complex for the original data to be used as ANN's input, and a new way to represent the electrolyte parameters was developed for simplification. The simplified data contained information about the quantity of solute (one quantity parameter) and the type of solute and solvent (two type parameters) but were more compact. The two type parameters were obtained in a way which was similar to the decimal to binary conversion. At first, the four kinds of solvent and six kinds of solute were arranged in a certain sequence, and all the non-zero values under them were recorded as "1" (Fig. 3, Step 2) to obtain the binary style data. Then the solvent and solute parts were regarded as two binary numbers and converted to decimal numbers (Fig. 3, Steps 3 and 4) to obtain the two type parameters. The non-zero values of the original solute data (at most two in this paper) were record in the same order to form the quantity parameters (Fig. 3, Step 5). Keeping the anodization voltage and time unchanged (Fig. 3, Step 1), the simplified data (Fig. 3, the right part) were finally obtained. They contained six kinds of parameters and could be used as ANN input.

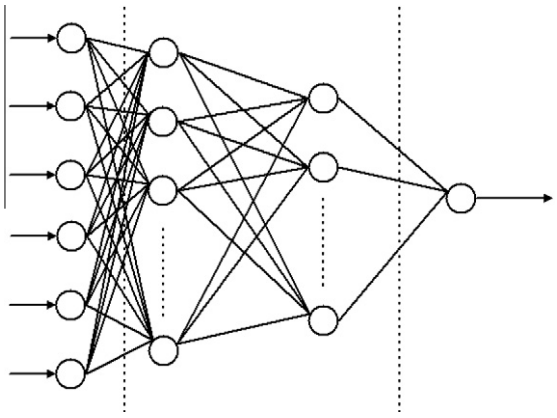

Fig. 1. Schematic illustration of a feed-forward hierarchical artificial neural network.

3.3. Deployment of RBF network for prediction work of the degree of order

Among the three output parameters, the degree of order was a discrete variable and radial basis function (RBF) network was suitable for its simulation (Pal & Srimani, 1996); nanotube diameter and length were continuous variables and back propagation artificial neural network (BPANN) was chosen for the simulation work.

For radial basis function (RBF) neural network, the methods to select the training datasets and the spread of radial basis functions affect the simulation results greatly. In this paper, five different training data selection methods were compared to achieve the best simulation results. The spread factor was adjusted during the comparison to achieve a satisfied network in a certain specific condition. The trained networks corresponding to different training data selection methods were tested by all data sets. If the predictive values of the best-performed network achieved excellent agreements with the experimental ones, a mature network and a suitable training data selection method would be obtained, otherwise an in-depth design of the RBF network should be carried out. The specific of the five training data set selection methods were as follows:

1. 20 randomly selected data sets.
2. 23 randomly selected data sets.
3. 27 randomly selected data sets.