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Optimization of tubelength in TiO_2 nanotube – a computational approach

S.HarshaVarthan[1], V. Saravanakannan[2], R. Chandiramouli[2]

[1]School of Mechanical Engineering, SASTRA University, Tirumalaisamudram, Thanjavur -613 401, India
[1]School of Electrical & Electronics Engineering, SASTRA University, Tirumalaisamudram, Thanjavur -613 401, India

Abstract: In the present work, TiO_2 nanotube length is optimized using artificial neural network. The length of TiO_2 nanotube can be varied with the parameters such as applied voltage and anodization time inanodization of Ti foil method. Various range of tube length from 0.400 -10.998µm can be grown when voltage is kept at 10V and the anodization time is adjusted from 1 - 45 hours. The tube length of 0.400-11µm can be synthesized, when the voltage is kept at 20 V and the anodization time is adjusted from 1 -70 hours. The computed results of the tube length are found to be in close agreement with the experimental results with an error of 0.00403. The optimization process of TiO_2 nanotube length reduces the strain and effort of researchers while synthesizing TiO_2 nanotubes.
Keywords:titanium oxide; nanotube; anodization; tubelength.

1. Introduction

Transition metal oxides (TMO) are mainly used as chemical sensors, catalyst and in solar cells. One among the transition metal oxides is titanium oxide (TiO_2).TiO_2 exhibits three polymorphism namely, rutile, anatase and brookite phase. TiO_2naturally occurs as a rutile in some acid igneous rocks and metamorphic rocks and is also in sedimentary rocks &beach sands. The metastable anatase and brookite phases convert irreversibly to the equilibrium rutile phase upon heating above temperatures in the range 600°-800°C.TiO_2 have tremendous applications in various fields such as in photo catalytic applications [1], gas sensing [2], photo electrolysis [3], polymer based bulk heterogeneous photovoltaics [4], energy storage devices such as Li – ion batteries and super capacitor [5]. 1-D nanowire and nanotube of TiO_2 with high surface to volume ratio possess significant useful and unique properties. Moreover, the morphology of TiO_2 nanostructures gives rise to numerous applications. TiO_2 can be synthesized by many methods such as sol gel transcription process using organo gelato templates [6], pulsed laser deposition[7], hydrothermal techniques [8] andanodization of titanium in fluid based electrolyte leads to controlled dimension of nanotube synthesis [9].The thickness of TiO_2nanostructures plays an important role in deciding different properties such as physical, chemical, electrical and mechanical properties. Meiling et al synthesized TiO_2 nanotubes by anodic oxidation and electro deposition methods[10].Pei et al prepared TiO_2 nanotubes by a hydrothermal method [11]. Tang et al synthesized TiO_2 nanotubes by anodization of Ti films at room temperature[12].Yuren et al reported the synthesis of TiO_2 nanotubes using a hybrid synthetic strategy [13]. Cui synthesized TiO_2 nanotubes by facile microwave-assisted hydrothermal method [14].

The artificial neural network (ANN) find its applications in time series prediction [15], fitness approximation [16], robotics [17], control including computer numerical control [18], generation of conductivity map on the ground [19], reliability analysis of steel structures [20] and thermal analysis of heat exchangers [21].The motivation behind the present work is to fine-tune the nanotube dimension of TiO_2 using the artificial neural network and to optimize the nanotube length during. From the literature survey, it is known that not much work is done to optimize TiO_2 nanotube dimension using ANN. In the present work, the nanotube anodization of Ti sheetslength of TiO_2 is optimized using ANN and the results are reported.

2. Computational details

The success of the artificial neural network depends on their architecture, learning algorithm, which is used in the transfer function and the number of neurons. In this present work, back propagation algorithm (BPA)neural networkis used to estimate the length of TiO_2. A simple architecture of neural network is shown in Figure 1, which has two input neurons in the input layer, three neurons in the hidden layer and two neurons in the output layer. Usually BPA is a supervised learning algorithm, which reduces over all systems to minimum and it uses the sigmoid activation function $f(x)=1/1+e^{-x}$.Usually during the learning or training process, an interconnection between the input, hidden and output layers are established. This interconnection between the layers enables the signal transfer between the layers. The intensity of the signals can be determined with the help of the weights of the corresponding signals. This can be done by iteratively changing the weights of the corresponding signals between the neurons and the sum of the squared errors between the calculated weights and expected weights can be minimized by the model selected.

During the learning process, the initial weight vectors W_0 are updated using the following equation,

$$W_i(k+1)=W_i(k)+\mu(T_i-O_i)f'(W_ix_i)x_i$$

where W_i is the weight matrix associated with i^{th} neuron , x_i is the input of i^{th} neuron,O_i is the actual output of the i^{th} neuron, T_i is the target output of the i^{th}neuron and μ is the learning rate parameter.

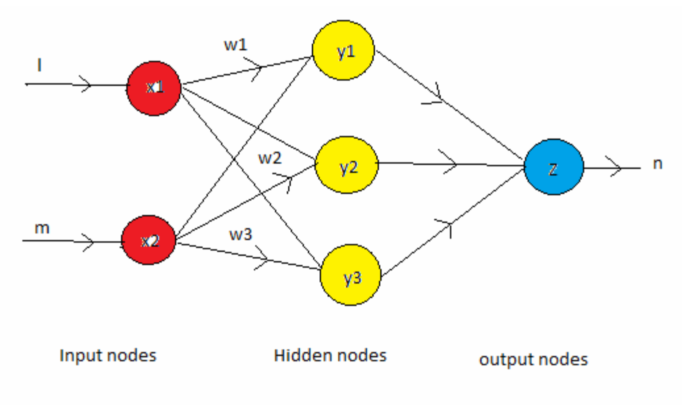

Fig. 1 Basic Neural Network Model

In the present work, the data obtained from the experiments [22] are given as input. The modelled network consists of two input nodes with voltage between the electrodes and the anodization time as inputs. Finally the result of the tube length is obtained when the voltage between the electrodes and the anodization time is given as input. For the number of training cycles being 1.82 x 10^9, the mean error obtained is 0.000403. Thecycle learning rate is 0.6000 with the momentum of 0.8000.After the running cycles for several time with voltage being 10,20 and 25 V,wide range of tube length are calculated.

3. Results and discussion

Usually in anodization of Ti foils, titanium anode and a platinum cathode is immersed in an aqueous electrolyte of dilute acid to which a small dc voltage is applied. The surface layer is sufficiently resistive to prevent current flow. Electrolyte composition also primarily decides whether the oxide film is porous or it forms a barrier.Initially, pits are formed on the TiO_2 layer, then poresstarts growingto form the ordered nanotube arrays in the substrate. On anodization, the pore growth takes place, after certain time dissolution occurs along the inter pore region,finally ordered nanotube arrays are formed.It is observed that TiO_2nanotube structure is grown on increasing the voltage beyond 23V and by adding 0.5% hydrofluoric acid electrolyte in a ratio of 1:7,mechanically strongernanotubes can be synthesized.Fig. 2 represents the anodization process of Ti foils to form TiO_2 nanotubes.The input data are given from the reported work and the optimization of TiO_2 nanotube are calculated using ANN [22]. Finally querying rows has been added for testimony of the artificial neural network and the errorsare minimized as stated above and the data are verified.

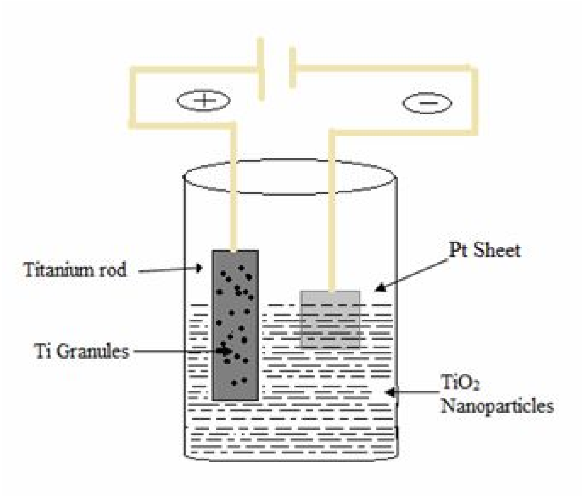

Fig. 2 Anodization of Ti foils to form TiO_2 nanotubes

Training process

The result obtained from the experiment[22] is used in the growing the network.The voltage and anodization time are given as the input in the two input nodes and the tube length is obtained as output. Fig. 3 illustrates the reported TiO_2 nanotubes synthesized at different voltage for various time duration.

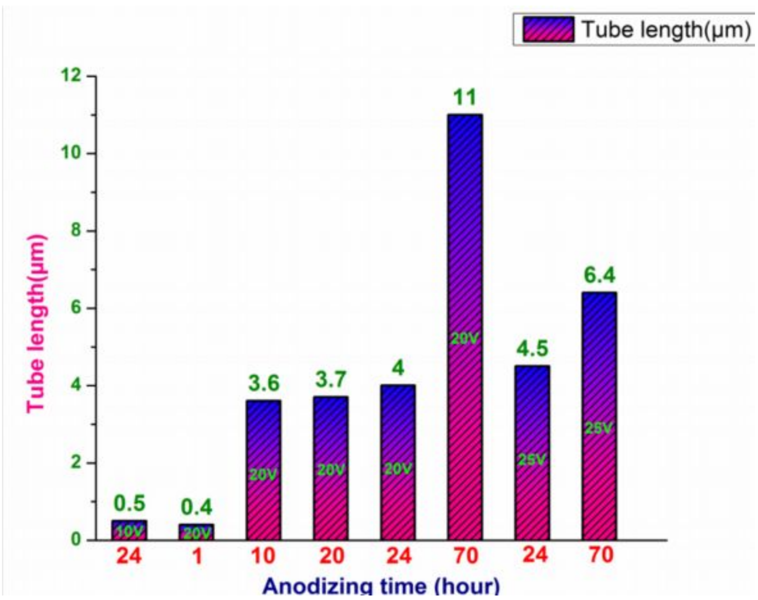

Fig. 3 Reported TiO_2 nanotubes synthesized at different voltage -ref [22]

Testing process

After training the back propagation neural network with the data obtained from the anodization experiment, test rows are generated, then the correctness of the neural network is tested by giving input and the training ANN once again. The resultsobtained have error of 0.000403 and the correctness of the results are validated as in Fig. 4.

O:0	I:1	I:2
4.3559	25.0000	65.0000
4.5023	25.0000	66.0000
4.6037	25.0000	66.5000
4.7299	25.0000	67.0000
4.8871	25.0000	67.5000
5.0825	25.0000	68.0000
5.3244	25.0000	68.5000
5.6224	25.0000	69.0000
5.9859	25.0000	69.5000
0.8421	20.0000	3.0000
2.2909	20.0000	6.0000
3.3596	20.0000	9.0000
3.8201	20.0000	12.0000
3.9929	20.0000	15.0000
4.0554	20.0000	18.0000
4.0777	20.0000	21.0000
4.0885	20.0000	27.0000
4.0895	20.0000	30.0000
4.0899	20.0000	33.0000
4.0902	20.0000	36.0000
4.0906	20.0000	39.0000
4.0922	20.0000	42.0000
4.0980	20.0000	45.0000
4.1193	20.0000	48.0000
4.1985	20.0000	51.0000
4.4936	20.0000	54.0000
5.5907	20.0000	57.0000
8.7324	20.0000	60.0000
10.8766	20.0000	63.0000

O:0	I:1	I:2
4.0900	25.0000	25.0000
4.0900	25.0000	26.0000
4.0901	25.0000	29.0000
4.0901	25.0000	31.0000
4.0901	25.0000	33.0000
4.0902	25.0000	46.0000
4.0901	25.0000	35.5000
4.0902	25.0000	47.0000
4.0903	25.0000	49.0000
3.9994	25.0000	4.0000
4.0910	25.0000	52.0000
4.0915	25.0000	53.0000
4.0923	25.0000	54.0000
4.0935	25.0000	55.0000
4.0953	25.0000	56.0000
4.0982	25.0000	57.0000
4.1026	25.0000	58.0000
4.1094	25.0000	59.0000
4.1200	25.0000	60.0000
4.1363	25.0000	61.0000
4.1616	25.0000	62.0000
4.2008	25.0000	63.0000
4.2616	25.0000	64.0000
4.3559	25.0000	65.0000
4.5023	25.0000	66.0000
4.6037	25.0000	66.5000
4.7299	25.0000	67.0000
4.8871	25.0000	67.5000
5.0825	25.0000	68.0000

O:0	I:1	I:2
3.7889	10.0000	31.0000
5.9411	10.0000	34.0000
9.7262	10.0000	37.0000
10.9633	10.0000	40.0000
0.4022	10.0000	22.0000
0.4202	10.0000	23.0000
1.1004	10.0000	26.0000
2.7433	10.0000	29.0000
0.5003	10.0000	24.0000
0.4000	10.0000	1.0000
2.7433	10.0000	29.0000
0.5000	10.0000	24.0000
0.4000	20.0000	1.0000
3.6000	20.0000	10.0000
3.7000	20.0000	20.0000
4.0000	20.0000	24.0000
11.0000	20.0000	70.0000

Fig. 4 Training data set given for the neural network

Optimization of TiO_2 tube length

Thirty three data have been generated by keeping 10V as input voltage and varying anodization time, thirty four data have been generated keeping 20V as input voltage and varying anodization time, thirty three data have been generated keeping 25V as input voltage and varying anodization time.Fig. 5 represents the growth process of TiO_2 nanotubes. Various range of tube length from 0.400 -10.998µm is observed when voltage is kept at 10V and the anodization time is adjusted from 1-45 hours.The tube length of 0.400-11µm can be grown, when the voltage is kept at 20 V and the anodization time is adjusted from 1 -70 hours.When the voltage is kept at 25 V, 4.5 -6.4 µm can be synthesized. From the results, it is inferred that for anodization time of 24-70 hours, tube length of 4.500 -6.400 µm can be synthesized.Fig. 6 illustrates the optimized growth prediction of TiO_2 nanotube length for various voltages. Moreover, the higher conductivity of electrolyte is the influencing factor for the growth of TiO_2 nanotubes. Initially, the growth of TiO_2 nanotube increases. However, for the time period of 10 hours to 20 hours, the chemical etching leads to improved conductivity of electrolyte [22]. Meanwhile, the top debris results in the breakage of nanotube length, which gives rise to decrease in the tube length for higher voltages as shown in the Fig. 6.The importance of the present work is a wide range of results can be generated, which is hard to obtain experimentally and is also time consuming process.

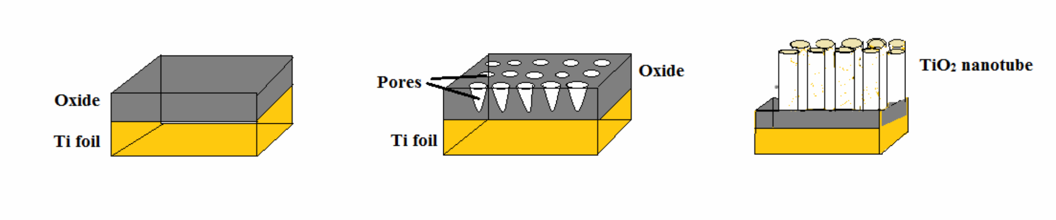

Fig. 5. Growth process of TiO_2 nanotubes

From the above results it is clear that by varying the voltage and anodization time TiO_2 nanotubes of different lengths ranging from 0.4 to 11 µm can be obtained and the parameter for different length can be obtained using ANN. Although many methods of diagnosis have been reported, the preparation of TiO_2nanotubes by anodization in electrolytic solution have proven to be one of the efficient method. Furthermore, incorporating the experimental results with the artificial neural network gives the accurate and optimized result. Besides, the work proves that it is legitimate to use artificial neural network in obtaining the results.

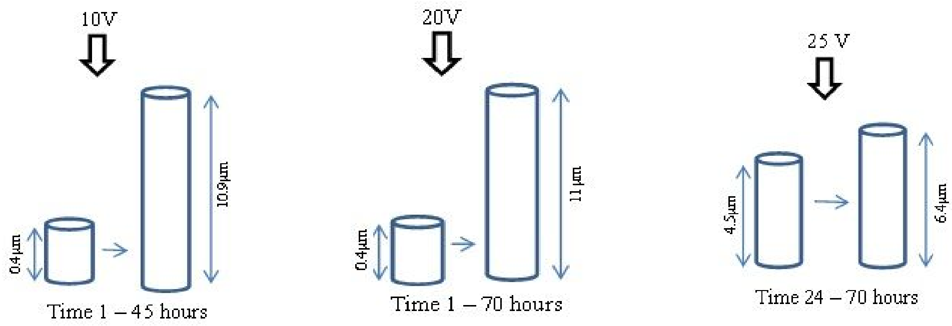

Fig. 6. Optimized growth prediction of TiO_2 nanotube length for various voltages

5. Conclusion

In summary, the tube length of TiO_2 nanotubes is optimized using ANN. Even though there are number of experimental procedures to synthesis TiO_2 nanotube of various sizes, researchers still find it difficult to adjust the parameters to obtain the desired length of TiO_2 nanotube. Moreover, ANN is a reliable method to optimize TiO_2 nanotube tubelength by feeding the experimental data and generating the tubelength without going for the tedious experimental methods. In the present work, an attempt has been made to optimize the tube length of TiO_2 nanotubes. The desired tubelength of TiO_2 nanotubes can be obtained byanodization method using this approach. It also reduces the strain and effort of the researchers for obtaining the correct parameters to get the desired TiO_2 nanotube length.

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