

Prediction of optical parameters of Sn doped CdO films using neural network

K. ERTURK, S. KOSE^a, F. ATAY^a, V. BILGIN^a, I. AKYUZ^a, M. C. HACHISMAILOGLU, I. KUCUK*, N. DEREBAŞI
Uludağ University, Department of Physics, 16059 Gorukle, Bursa, Turkey
^aOsmangazi University, Department of Physics, 26480 Eskisehir, Turkey

In recent years, there was great interest and demand for the production and investigation of low cost and novel transparent conducting oxide films. CdO is a promising material among these films for future applications with its unique properties. A learning and generalization ability, real-time operation, and ease of implementation have made an artificial neural network popular in recent years. In this work we have produced CdO:Sn films by the ultrasonic spray pyrolysis technique which is economical and simple to process. Optical parameters of Sn doped CdO films with developed, have been estimated by the artificial neural network using experimental results as a training data. The correlation obtain from the artificial neural network was found to be 99% with the experimental results.

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1. Introduction

There has been a lot of work on the growth and physical properties of transparent conducting oxides (TCO) which have recently had increasing applications [1, 2]. These films have low electrical resistivity and high transparency in the visible and near-IR regions of the electromagnetic spectrum and consist of wide band gap semiconductor materials [3,4]. These electro-optical properties make the TCO films common materials for photovoltaic solar cells, electroluminescence circuits, liquid crystal displays, detectors and gas sensors [5–10]. The most commonly used TCO materials are tin oxide (SnO₂), indium oxide (In₂O₃), indium tin oxide (ITO), zinc oxide (ZnO) and cadmium oxide (CdO) [11]. Among these materials, there had been limited work on CdO until the last decade. But the studies made on photovoltaic solar cells and gas sensors [12] showed that the CdO is an important material for the fabrication of these devices.

The special features of CdO, such as high conductivity, high transmission and a narrow band gap as compared with other TCOs, make it applicable in photodiodes, phototransistors, photovoltaics, transparent electrodes, liquid crystal displays, IR detectors and anti-reflecting coatings. It is a candidate for CdTe and CIS hetero-junctions as the window material [13,14]. The CdO thin films are produced by different techniques such as sputtering, spray pyrolysis, chemical deposition, sol-gel and metalorganic chemical vapour deposition [12,15,16]. Among these techniques, spray pyrolysis is the most economic and simple technique and allows film deposition on large areas. The films produced by this technique have a polycrystalline structure [17–22]. An ultrasonic spray pyrolysis (USP) technique includes an ultrasonic atomizer which is connected to an oscillator. This enables the solution to be sprayed with better atomizing using

ultrasonic waves and this results in decreasing of the droplet size and production of more homogeneous materials [23,24].

Learning and generalization ability, real-time operation, and ease of implementation have made artificial neural networks (ANNs) popular in the last years [25]. ANNs have been applied in many areas [26–29] because of these features.

In this paper, the optical transmittance (T) of Sn incorporation of CdO films are modelled using genetic algorithm (GA), artificial neural network (ANN) and experimental data. The proposed model is not time consuming and more accurately and easily predicted the optical properties of Sn doped CdO films.

2. Experimental

2.1 Experimental procedure

CdO:Sn films were produced with different Sn incorporation percentages (1, 2, 3 and 4 at %) using the USP technique at the substrate temperature of 200 ± 5 °C. Details of the USP technique were given in our previous works [30,31]. The ultrasonic frequency was 100 kHz, while the droplet size was 20 μm . A 100 ml of solution was totally prepared by dissolving the appropriate volume of $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.1 M) and $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (0.1 M) solutions. A deionized water was used as a solvent. So the solution was sprayed during 20 mins, while the solution flow rate was controlled by a flowmeter and kept at 5 $\text{ml} \cdot \text{min}^{-1}$. A compressed purified air was used as the carrier gas (1 bar). The substrates were heated up using an electrical heater, and the substrate temperature was measured by an iron-constantan type thermocouple. The distance between the nozzle and substrate was maintained

at 30 cm. The thicknesses of the films were measured as 0.53 μm , 0.71 μm , 0.68 μm , 0.78 μm and 0.75 μm , respectively depending on the increasing Sn incorporation using Metallurgical Optical Microscope. The Optical transmissions and absorptions of the films were recorded by a Perkin Elmer UV/VIS Lambda 2S spectrometer (double-beam).

2.2 Multilayered perceptron Neural Networks

There are many types of neural networks for various applications available in the literature. Multilayered perceptrons (MLPs) are feed-forward networks and universal approximators. The MLPs are the simplest and therefore most commonly used neural network architectures [25]. In this paper, they have been adapted for the calculation of the optical transmittance of Sn incorporation of CdO films

The MLP used in this work is trained by the genetic algorithm (GA). An MLP consists of three layers: an input, an output, and an intermediate or hidden layers. Processing elements (PE) or neurons in the input layer only act as buffers for distributing the input signals x_i (i show the i -th input PE) to the PEs in the hidden layer. Each PE j (j show the j -th PE in the hidden layer and output layers) in the hidden layer sums up its input signals x_i after weighting with the values of the respective connections w_{ji} from the input layer and computes its output y_j as a function f of the sum,

$$y_j = f\left(\sum w_{ji}x_i\right) \quad (1)$$

where f can be a simple threshold function, which is a sigmoid or hyperbolic tangent function. The output of PEs in the output layer is computed similarly. Training of network consists of adjusting its weights using a training algorithm. The training algorithms adopted in this study optimize the weights by attempting to minimize the sum of squared differences between the desired and actual values of the output neurons [25], namely:

$$E = \frac{1}{2} \sum_j (y_{dj} - y_j)^2 \quad (2)$$

where y_{dj} is the desired value of output neuron j and y_j is the actual output of that neuron. Each weight w_{ji} is adjusted by adding an increment Δw_{ji} to it. Δw_{ji} is selected to reduce E as rapidly as possible. The adjustment is carried out over several training iterations until a satisfactorily small value of E is obtained or a given number of iterations is reached. How Δw_{ji} is computed depends on the training algorithm adopted. There are a number of training algorithms used to train a MLP [25].

In this work target transmittance for the MLP have been determined by the GA. The computation process is carried out with a set of measurements.

2.3 Genetic algorithm

The GA method is based on a computer simulation of biological evolution and initially works with a randomly generated population with several variables to be estimated [32]. The population size is usually related to the problem under consideration and can be determined by a number of variables. Each member or individual of the population is usually called a chromosome or a string consisting of genes or bits, and encoded into one variable (T) for this work. A new population is built up by selecting individuals among members of the initial population according to their fitnesses through fundamental genetic process of selection criterion based on the roulette wheel. The fitness function(ff) is calculated by

$$ff = \frac{1}{\sum_{k=1}^n (T_{d,k} - T_{c,k})^2} \quad (3)$$

where n is the population size, T_d and T_c are the desired and calculated transmittance, respectively.

Fitness value for each string was calculated using the fitness function, hence new members were chosen for reproduction according to their fitness based on the specified selection criterion. Thus, the fittest had a greater chance to be selected for next population. Once the reproduction was completed crossover operation was implemented by simply exchanging bits between two randomly selected members in the population. The final genetic process was mutation that randomly changes a particular bit in a particular string, that is, a zero bit may change to a one or vice versa.

2.4 ANN applications to transmittance of Sn doped CdO films

The proposed technique involves training an MLP to calculate transmittance (T) when the values are thickness of films (ω), incorporation rate of Sn (%), wave length (λ) absorbance (A). The ranges of training data set were $53 \mu\text{m} \leq \omega \leq 78 \mu\text{m}$ at 5 points, $0 \leq \% \leq 4$ at 5 points, $450 \text{ nm} \leq \lambda \leq 1100 \text{ nm}$ at 651 points, $0.2 \text{ mm} \leq A \leq 4.3 \text{ mm}$ at 2600 points. The training of MLP using the GA to compute T involves presenting them with different sets ($\omega, \%, \lambda$ and A) sequentially and/or randomly and corresponding calculated values T . Differences between the target outputs (T) and the actual outputs (T_{ANN}) of the MLP are calculated through the network to adapt its weights using Eq. (3). The adaptation is carried out after the presentation of each set ($\omega, \%, \lambda$ and A) until the calculation accuracy of the network is deemed satisfactory according to some criterion (for example, when the errors between T and T_{ANN} for all the training set fall below a given threshold) or the maximum allowable number of epochs is reached. The epoch is the time period that encompasses all the iterations performed after all the patterns are presented to the network.

In order to understand the MLPs prediction accuracy

and generalization capacity of the networks were also trained by the training set, cross-validation set and checked by test data. The network memorizes the training set and does not generalize well when the network is trained too much [33]. The training holds the key to an accurate solution, so the criterion to stop training must be very well described. Cross-validation is a highly recommended criterion for stopping the training of a network. When the error in the cross validation increases the training should be stopped. A practical way to find a point of better generalization is to use a small percentage (around 10%) of the training set for cross-validation. For obtaining a better generalization of the networks presented in this work 260 of training data, which were selected randomly, were used as cross validation set.

Total 2640 data sets were used in training and test phases, 450 data sets were used to test the network. For the validation, untrained experimental data are also used to test the neural model as well. The number of hidden layers and neurons in each layer were determined through trial and error to be optimal including with different transfer functions as hyperbolic tangent, sigmoid and hybrid. After several trials, a better result was obtained by a three-layered network. In this network the hyperbolic tangent function is used in the hidden layer, and output layers. The number of epochs was 1000 for training, and the most suitable network configuration found was $4 \times 10 \times 1$. It means that the number of neurons were 10 for the hidden layer.

3. Results

In the proposed model 5 different incorporation rate Sn of CdO films were used. The estimates of T were found to be in the range of 0 to 59.52, by use of measured transmittance results in the CdO films at wave lengths varying from 450 to 1100 nm.

All tested CdO films in the range of training data have high correlation coefficients. Fig. 1 shows the variation of T obtained from the neural network model and experimental data. The values of transmittance achieved from the proposed model are in 99% agreement with the experimental values of transmittance. The model was assessed by 3% Sn doped CdO films which is outside the range of the training data. The variation of the optical transmittance for %3 Sn incorporation of CdO films with wave length given in Fig. 2 also shows good correlation between measured and predicted results.

4. Discussion

This results show that the neural network model is potentially useful for designers in predicting the optical transmittance in cases when measurements and production may be time consuming. If the training data set contains a large range of CdO film parameters then the accuracy of the model can be improved. However the accuracy in the prediction of transmittance with the field of the training set

given in this work is sufficient for many applications.

Since the neural model presented in this work has accuracy and requires no tremendous computational efforts and less background information about the optical properties of CdO films, it can be used to predict more accurately and easily the optical transmittance.

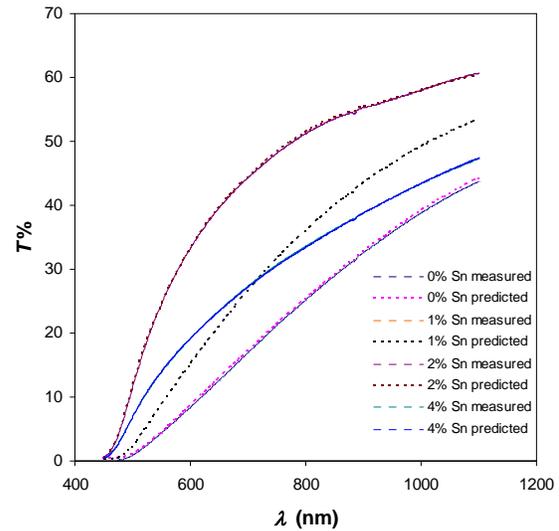


Fig. 1. The variation of predicted and measured transmittance with wave length in Sn doped CdO films.

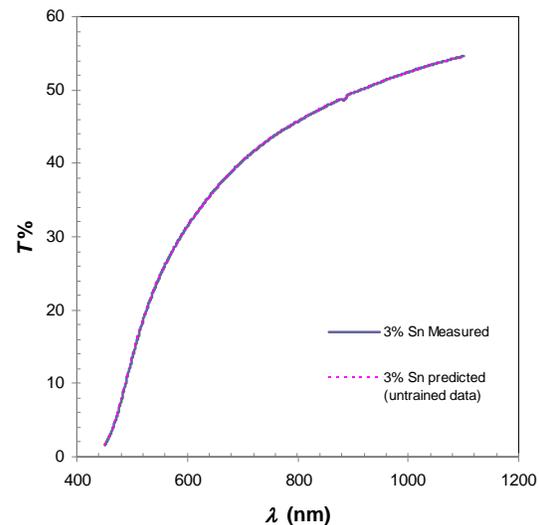


Fig. 2. Comparisons of experimental and predicted transmittance in 3% doped CdO films.

7. Conclusions

The predicted results from the neural network

approach sound very satisfactory and in agreement with experimental results concerning the Sn doped CdO films. The proposed model is fast and allows the application of standard learning algorithm for the neural network. Finally, the model capable of more accurately predicting optical transmittance is also very useful to producers working in this field.

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*Corresponding author: ikucuk@uludag.edu.tr