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Modeling of In_2O_3-10 wt% ZnO thin film properties for transparent conductive oxide using neural networks

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ABSTRACT

Effects of deposition process parameters on the deposition rate and the electrical properties of In_2O_3–10 wt% ZnO (IZO) thin films were modeled and analyzed by using the error back-propagation neural networks (BPNN). Output models were represented by response surface plots and the fitness of models was estimated by calculating the root mean square error (RMSE). The deposition rate of IZO thin films is affected by the RF power and the substrate temperature. The electrical properties of the IZO thin films are mainly controlled by O_2 ratio and the substrate temperature. The predicted output characteristics by BPNN can sufficiently explain the mechanism of IZO deposition process. Thus, neural network models can provide the reliable explanation of IZO film deposition.

1. Introduction

Transparent conductive oxide (TCO) films have been widely used for electrodes in optoelectronic devices such as solar cell, organic light emitting diodes and flat panel display [1]. Sn-doped indium oxide (ITO) has been applied to practical manufacturing process due to its high transparency and low resistivity [2,3]. However, new TCO materials such as impurity doped ZnO and multicomponent oxides have been investigated to replace ITO because of thermal stability and cost reduction [4,5]. Among them, In_2O_3–ZnO (IZO) is expected to be a new candidate for TCO by reason of its thermal stability and high conductivity [6,7]. Many groups reported electrical and structural properties of IZO thin films with process parameters [8–10]. However, process modeling on IZO thin films has not been reported yet.

Due to the complexity and nonlinear relationship in system, modeling methodology using artificial intelligence, such as a neural network (NNet), has been developed to analyze the process which is difficult to characterize by using classical methodology [11,12]. Recently, the NNet was adopted to characterize the semiconductor manufacturing processes such as plasma-enhanced chemical vapor deposition [13], molecular beam epitaxy [14] and plasma etch [15]. NNet can perform the highly complex mapping between input variables and output responses to draw the nonlinear relationships between input and output factors of a process. In addition, NNet can generalize the whole tendencies in functional relationships using a limited number of processing data. In this paper, the modeling of processing effect on the electrical properties and the deposition rate of IZO thin films using NNet based on error back-propagation algorithm is introduced.

2. Experiments

IZO thin films were deposited on SiO_2 (3000 Å)/SiN_x (1000 Å)/glass substrates (corning 1737) by RF magnetron sputtering with target composed of In_2O_3–10 wt% ZnO ceramics. The base pressure in the chamber and the deposition pressure were maintained below 5×10^{-6} Torr and at 3.5×10^{-3} Torr, respectively. The RF power and the substrate temperature were in the range of 30–80 W and room temperature (27 °C)–400 °C. The O_2 ratio in sputter gas was varied from 0% to 2%. The film thicknesses of IZO thin films were measured using the alpha step. Resistivity, carrier concentrations and mobility of IZO thin films were also measured by Hall measurements using Van der Pauw method. Structural properties of thin films were examined with X-ray diffraction (XRD) where a Ni-filtered Kα (λ = 1.54056 Å) was used.

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The process modeling of IZO thin films was characterized by D-optimal experimental design with additional 1 center point. D-optimal experimental design is one of the computer-generated designs, which is mainly applied in the experiments that the region of interest for experiments is irregular or the model is complicated [16]. It can reduce the number of experimental runs required by modeling. The order of experiments was randomized to balance out the effect of any irrelevant effects. The 8 experiments were trained by NNet which had one hidden layer trained by the error back-propagation algorithm. The additional 2 experiments were performed to verify the predicted NNet models. The NNet has 3-4-1 structure indicating that the hidden layer is composed of 4 neurons. The learning rate and momentum were 0.005 and 0.04, respectively. The output models on deposition rate, carrier concentrations, mobility and resistivity of IZO thin films trained by NNet were represented by the response surface plots. In order to measure fitness of models constructed by using NNet, the RMSE of training and testing experiments were calculated.

3. Theory

In order to characterize the semiconductor manufacturing process, neural network based model has been widely used recently [13–15]. A NNet is composed of input layer, hidden layer, and output layer. The each input unit in input layer is fully connected to the each hidden unit in hidden layer with the weight (w_{ih}), which in turn is sequentially connected to the each output unit with the weight (w_{ho}). The back-propagation algorithm is the training algorithm of NNet and searches for weight values that minimize the error of the NNet model over the set of training inputs [17]. In this algorithm, NNet begins with random weights and biases. When input vector is entered into the NNet, the output is calculated by summing the weighted input and filtering with the activation function. After the calculated output value is compared with the measured value, the NNet model error is acquired as the sum of square errors of the two values. The error is then back-propagated to the NNet to minimize the error by adjusting the weights of the NNet.

4. Results and discussion

The modeling results for deposition rate, carrier concentrations, mobility and resistivity of IZO thin films appear in Fig. 1, where the squares (■) represent the training data and the circles (○) represent the testing data of NNet models. In the modeling scheme, neural network begins with weights and biases initialized with random values. Process variables are entered into the network by coding as high level (+1) or low level (−1) and the output is calculated by summing the weighted inputs and filtering with the activation function. The calculated output is then compared with the measured output and the network error is defined as the sum of squared errors of these two outputs. After adjusting the weights of NNet by using the gradient descent approach to minimize the error, the process models are obtained. Fig. 1 shows the linear relationship between the measured data and the predicted model out-

Table 1
The RMSE of training and testing experiments.

	RMSE of training	RMSE of testing
Deposition rate	0.046	0.039
Carrier concentrations	0.020	0.110
Mobility	0.090	0.249
Resistivity	0.196	0.289

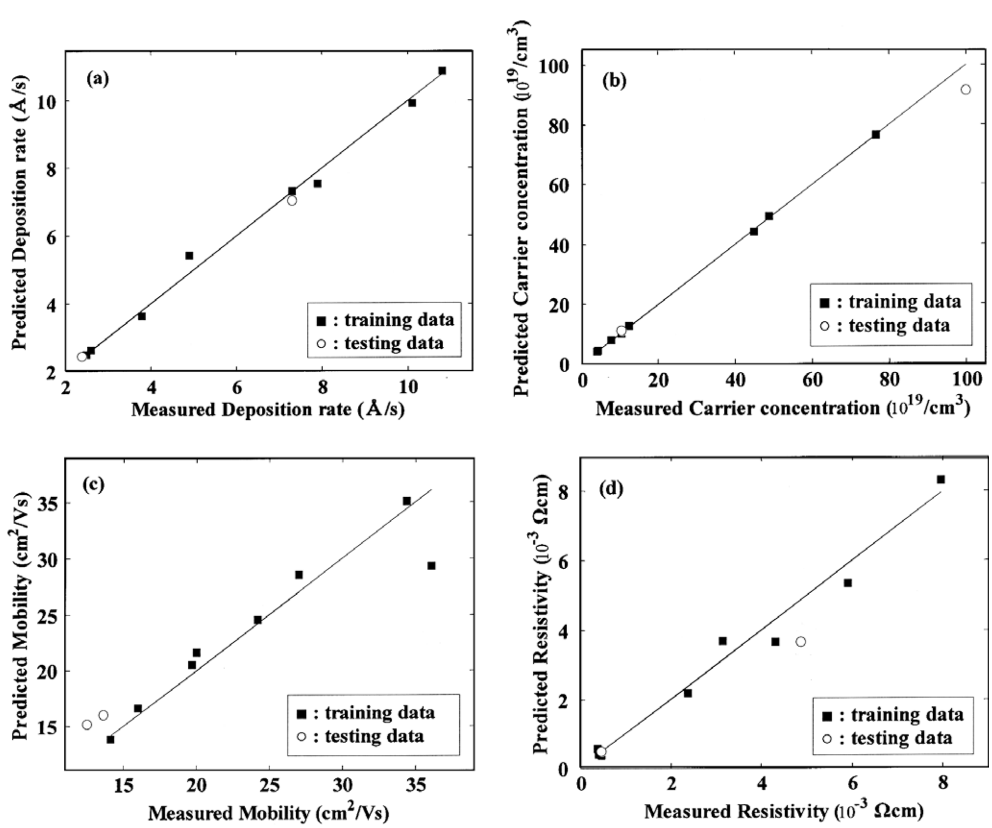

Fig. 1. The neural network modeling results for (a) deposition rate, (b) carrier concentrations, (c) mobility, and (d) resistivity of IZO thin films.