Neural Network Model for Predicting the Electrical Properties of Nano-Structure Materials

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ABSTRACT

This paper focuses on the development of a knowledge-based system in nano-material and nanotechnology research areas. The developed system is used to study the electrical properties of nano structures, which are made by using Zinc (Zn), Oxide (O) and Cadmium (Cd) nano particles. This system represents the relationships between the physical parameters of Preparatory Time Temperature, Applied Voltage, Thickness, Type of mixed particles and predicts the electrical parameter of Current (I) in nano materials using Zn, O and Cd. The Artificial Neural Network (ANN) technology is used to develop the knowledge based system and the system is trained using Back Propagation method. The system is predicted the desired property of Current under the different types of property variables as input, which are not experimentally investigated in laboratory yet. This knowledge based system helps to research people to study and develop new nano devices using Zn, O and Cd nano materials.

Keywords
Nano material, Knowledge Based System, Artificial Neural Network, Back Propagation Algorithm.

1. INTRODUCTION

Nano materials have a broad spectrum of applications. Today, they are contained in many products and used in various technologies. Nano materials are emerging family of novel materials that could be designed for specific properties. The various properties of nano materials are optical, physical, chemical and electrical, which could be tailored for specific applications. Nano structured semiconductors have greatest attraction among the research community due to their excellent physical and chemical properties compared to their bulk counterparts. In particular, composite nano structures are essential for nano devices like solar cell, light emitting diodes, thin film transistors etc. Among the many type nano structures, the nano particles Zinc (Zn), Cadmium (Cd) and Oxide (O) based nano structures are played a major role in the field of optoelectronic devices, due to their interesting properties of optical, electrical and its wide band gap [1] [2]. The characteristic of this material can be synthesized by sol-gel [3].

At the time of constructing new optoelectronic devices and in the development of thin films, the properties of Current, which is produced by the nano structure under the condition of different physical parameters should be observed, measured and manipulated in experimental. One of the critical challenge faced currently by the researchers in the nano technology and nano science fields are the inability and lack of instruments to study the properties at the nano-meter level to find the new one [4]. These difficulties can be overcome by creating a knowledge based system using Artificial Neural Network (ANN). The knowledge base contains all interactions and relations between all variables of the object and it allows calculating the values of one part of variables through others. In other words, the relation between the properties will allow to find the properties of new composite structure that have not been investigated yet. In this present work, the relations between the properties of temperature, thickness, number of elements, voltage and current are trained by already existing values for nano structures, which are made by using Zn, Cd and O particles, which are reported earlier [5] [6]. Then by making use of these trained values by the neural network, the electrical property of the current will be predicted for the nano structures, which are made by using either mono or poly composite materials of Zn, Cd and O.
2. METHODOLOGY

The proposed ANN models are based on experimental measurements of electrical characteristics of Zing (Zn), Cadmium (Cd) and Oxide (O) materials with embedded into Zing Oxide, Cadmium-Oxide and Zing-Cadmium-Oxide. The activities involved the construction of ANN model can be defined in two steps. Firstly, the properties of preparatory time temperature, voltage, thickness of material, combination of elements and its corresponding Current levels are collected and formed as a data base with cleared of mistakes, anomalies, duplicates and inconsistencies. The prepared table for the modeling is shown in the Table-I as training data set. In data base, the number of elements mixed in a nano structure is represented as a integer, which is generated based on binary weight value, which is shown in the Table-II. Secondly, ANN architecture corresponding to the size of database collected (5 column and 552 rows) was chosen, and ANN training was executed. During training the different sets of data installed to the input layer of the ANN from the columns 2 to 5 and the corresponding values of Electric current (column 6) is installed in the ANN output layer. The ANN model obtained can be used to predict the electric current for different combinations of input factors.

### Table I

**TRAINING DATA SET**

<table>
<thead>
<tr>
<th>Query</th>
<th>Thickness</th>
<th>Current</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0000</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0.0000</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0.0000</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>0.0000</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>0.0000</td>
<td>1</td>
</tr>
</tbody>
</table>

### Table II

**CODING FOR NUMBER OF ELEMENTS**

<table>
<thead>
<tr>
<th>O</th>
<th>Zn</th>
<th>Cd</th>
<th>Number</th>
<th>Element(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>Cd</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>Zn</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>4</td>
<td>O</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>3</td>
<td>Zn and Cd</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>5</td>
<td>O and Cd</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>6</td>
<td>O and Zn</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>7</td>
<td>O, Zn and Cd</td>
</tr>
</tbody>
</table>
3. DESIGN OF ANN MODEL:
The proposed ANN model is designed using the JNN (Just Neural Network) tool, it supports exclusively to back propagation based learning phase. The success of ANNs depends on the architecture, the learning algorithm and its parameters, the transfer function, the number of layers and processing elements (neurons). Back propagation Neural Networks is one of the most common neural networks and they are simple and effective tool [7]. The Architecture of Neural Network with Back Propagation Algorithm consists of Input layer with 4 neurons, hidden layer with 5 neurons and output layer with one neuron as shown in Figure-1.

![Diagram of ANN model](image)

**Figure 1: Typical neural network model using ‘JustNN’**

The learning process forms the interconnection between neurons and is accomplished by known inputs and output, and presenting these to the ANN in some ordered manner. Due to the interconnection, signals are sent from the input layer to the output layer through the hidden layer. The intensity of the transmitted signal is determined by the weight of the interconnections. It is used to properly obtain the model by iteratively adjusting the values of interconnections between the neurons while the sum of squared residuals between calculated and expected values are minimized. The Back Propagation Algorithm (BPA) uses sigmoid activation function $f(x) = 1/(1+e^{-x})$ [8] [9]. The BPA is a supervised learning algorithm that aims at reducing overall system error to a minimum. In this learning procedure, an initial weight vectors $w0$ is updated using the relation

$$w_i (k+1) = w_i (k) + \mu (T_i-O_i)f'(w_ix_i)x_i$$

Where, $w_i$ = The weight matrix associated with $i^{th}$ neuron; $x_i$ = Input of the $i^{th}$ neuron; $O_i$ = Actual output of the $i^{th}$ neuron; $T_i$ = Target output of the $i^{th}$ neuron, and $\mu$ is the learning rate parameter. The specific parameters for learning algorithm are the learning rate ($\mu$) and momentum ($\alpha$), which took the values of 0.02 and 0.01 respectively.
4. RESULT AND DISCUSSIONS
The designed system is used for the computation of current property for mono or composite nano material using Zn, Cd and O particles. An extensive training phase has to be performed before the testing started. When the training is completed using Back Propagation Algorithm, the system is tested with the known Input and known output. The tested values are group into three groups and its current property, studied. First group is mono type material, which consists of either Zn or Cd or O, second group is aimed for dual composite material with the combination of ZnCd or CdO or ZnO, the triple bond nano particles of ZnCdO is under third group. The various type of required preparatory time temperature, thickness, group code are given to input values and measured the output of current (i) value. The difference between the trained values and measured values are well coincided with each other irrespective of all three groups. The performance of the knowledge system is studied and finds the accuracy. To find the accuracy, the results obtained using the knowledge system is compared with that of the experimental values. It is found that the regression equation (-124.34+1.008X) arrived gives the unity slope (0.9968) and the intercept (0.3168) closes to the zero value which is shown in Figure-2. The Correlation Coefficient R=0.99, shows that the data predicted is well correlated with that of the estimated results. Figure-3 shows the performance of the neural network for both the outputs for training data and actual value. In the graph a solid line is generated, in which the values of simulated and measured are fitted with each other.

5. CONCLUSION
The benefits of knowledge based system are, which is best method to solve the direct and inverse problem. It also suitable to predict the result of experiments which is not carried out. The developed knowledge based system contains the all relationships between variables of nano materials based on Zn, O and Cd. It allows us
to compute the values of one part of variables through others. This type of knowledge based system can expand to other types of nano structures and predict its desired characteristics. The integration of all experimental data base for various type nano particles, which are developed by various research people will lead to construction of data ware house and the acquired knowledge can get by anyone from anywhere using cloud computing technology. This work is trusted about the usage of artificial neural networks in creation of knowledge based system.

REFERENCES


