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# Modeling the electrical resistivity of Zn–Mn–S nanocrystalline semiconductors

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ABSTRACT

In this paper, a feed-forward multilayer perceptron artificial neural network model is used to simulate the electrical resistivity of nanocrystalline diluted magnetic semiconductors. Variations in the concentrations of Zn, Mn and temperature were used as the model inputs and the resulting electrical resistivity of the nanocrystalline semiconductors as the output of the model. Comparison between the model predictions and the experimental observations predicted a remarkable agreement between them.
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## 1. Introduction

Large extensions in development of the production of the nanostructures and nanocrystalline materials require the application of different evaluation methods as well as different prediction models for their behavior. Artificial neural networks (ANNs) that possess massive parallel computing capability and can map the input–output relationships have attracted significant attention in research on material processing and properties. This modeling framework has been recently used by many authors in various fields, for example, microstructure modeling [1], kinetics analysis of non-isothermal oxidation of ceramic nanocomposites [2], mechanical properties of metals [3–5], physical [6] and mechanical [7] properties of composites, thermomechanical processing [8–10], casting properties [11,12] and phase transformation [13]. However, to the knowledge of the authors, application of this framework to determine the electrical resistivity of $Zn_{1-X}Mn_XS$ magnetic semiconductor nanocrystalline films is scarce.

The objective of this research was to simulate the effect of the variations in the concentrations of Mn and Zn and temperature on the electrical resistivity of magnetic semiconductors of Zn–Mn–S nanocrystalline films. In order to do that, an artificial neural network with several hidden layers was used and the model predictions were compared with the previously published results in [14].

## 2. Model setup

Artificial neural network is a network with nodes or neurons analogous to the biological neurons. The nodes are interconnected to weighted links [11–13]. The weights are usually adjustable and can be trained through a learning process and training example. ANNs have different layers, interconnected through a complex network. Fig. 1 shows the structure of ANN model with various layers. The number of used hidden units determines the complexity of neural network and predicted values are more accurate with increasing the number of hidden units. However, with increasing the number of hidden units, there may be an overriding in data. Therefore, the optimum number of the hidden layers and neurons should be determined and applied before using the predictions of the model.

In this study, the feed-forward multilayer perceptron was used and trained with back propagation algorithm. The concentrations of Zn and Mn and formation temperature were used as inputs and resulting electrical resistivity was the output of the neural network model. The inputs and outputs were first normalized within the range of 0–1 [11–13,15]. The output $y_i$ produced by the neuron $i$ in the layer $L$ is given by the following relationship:

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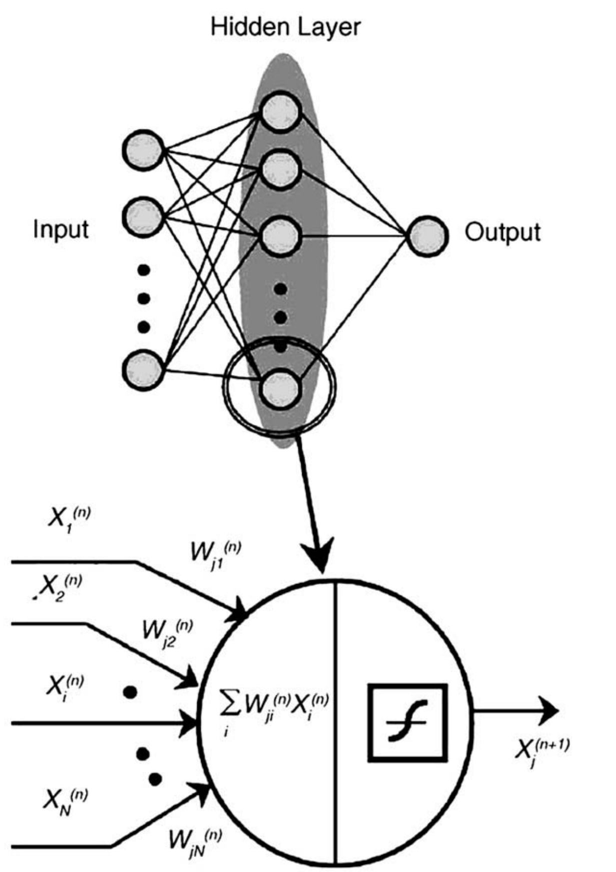


**Fig. 1.** A schematic description of artificial neural network configuration (upper part). The lower part gives the relationships between the input and output vectors of one neuron [11–13].

$$y_i = f\left(\sum_{j=1}^{n} w_{ij} + b\right) \quad (1)$$

where $f$ is the activation function, $n$ the number of elements in the layer $L-1$, $w_{ij}$ the weight associated with the connection between the neuron $i$ in the layer $L$ and the neuron j in the layer $L-1$, whose output is $w_i$, and $b$ is the offset or bias where shifts the activation function along the basic axis. An iterative algorithm adjusts the weights of connection while $y$ responses to the input patterns generated at output neurons, according to Eq. (1). The $y$ values given by Eq. (1) are as close as possible to their respective desired responses $d$, which can be tested by minimizing the learning error, defined by mean square error (MSE):

$$\text{MSE} = \frac{1}{QN_0}\sum_{m=1}^{Q}\sum_{n=1}^{N_0}[d_n(m) - y_n(m)]^2 \quad (2)$$

where $N_0$ is the number of output, $Q$ the number of training sets, $d$ the desired output, and $y$ the network output. The performance of the developed network was evaluated with the help of:

1. Drawing a scatter diagram of estimated versus target values.
2. Computing mean absolute error (MAE) using:

$$\text{MAE} = \frac{\sum |x - y|}{n} \quad (3)$$

where $x = X - X'$; $X$ is the target output, $X'$ the mean of $X$, $y = Y - Y'$; $Y$ is the network output and $Y'$ the mean of $Y$.

## 3. Materials and data collection

The initial data used for this study have been selected from a published work by Sreekantha Reddy et al. [14], in which the electrical properties of diluted magnetic semiconductor $Zn_{1-X}Mn_XS$ nanocrystalline films at different compositions has been investigated [14]. Fig. 2 shows the variation of resistivity with temperature for samples of all compositions studied in the mentioned work [14]. A decrease in resistivity is observed with increase in temperature showing semiconducting behavior [14]. Further the resistivity showed a definite decrease with increasing Mn concentration [14]. In that investigation [14] 135 samples have been produced. Among these data, 108 samples

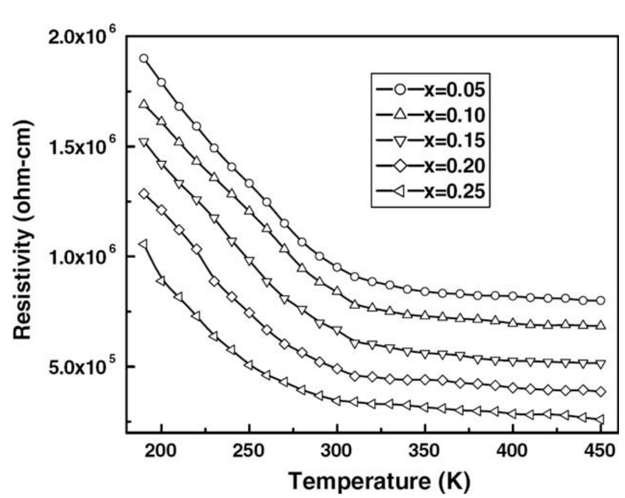


**Fig. 2.** Variation of electrical resistivity of $Zn_{1-x}Mn_xS$ films with temperature [14].

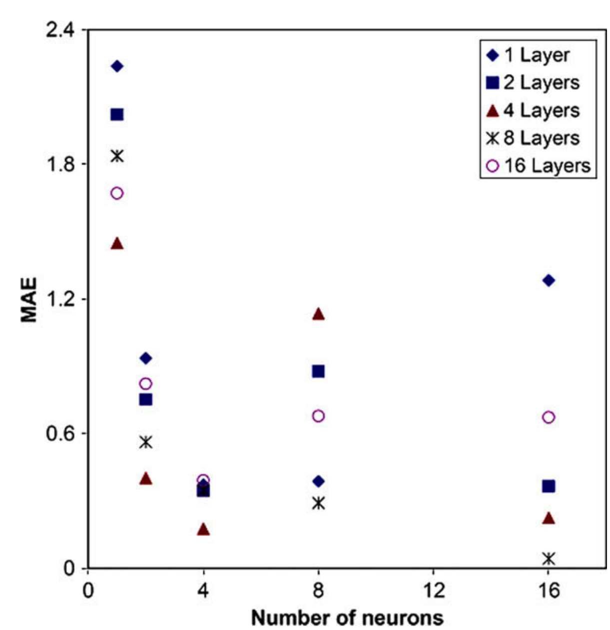


**Fig. 3.** MAE for different hidden layers and neuron numbers.

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