Artificial intelligence approach on predicting current values of polymer interface Schottky diode based on temperature and voltage: An experimental study

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A B S T R A C T

In this study, an artificial neural network model has been developed to predict the current values of a 6H–SiC/MEH-PPV Schottky diode with polymer-interface, depending on temperature and voltage. In the training of the multi-layer perceptron network model with 13 neurons in its hidden layer, the experimentally measured current values between 100 and 250 K temperature and -3V to + 3V voltage range have been used. In the input layer of the model developed with a total of 244 experimental data, temperature, and voltage values have been defined and current values were obtained in the output layer. The mean square error value of the artificial neural network is 1.63E-08 and the R-value is 0.99999. The developed model has been able to predict the current values of the polymer-interfaced 6H–SiC/MEH-PPV Schottky diode with an average error rate of −0.15% depending on temperature and voltage, with high accuracy.

1. Introduction

Schottky diodes are one of the cornerstones of many advanced technological products, especially in today's electronics industry, due to their unique electronic properties [1,2]. This has made them electro-dynamic structures used in many fields from electronics to optics, from energy to healthy. At this point, silicon carbide (SiC) based Schottky diodes, one of these diodes, draws attention with their distinction from other conventional semiconductors due to their ability to operate in extreme conditions [3–6]. Especially the ability of these diodes to withstand high temperature and high power conditions makes them very special diodes [7,8]. Therefore, they have become an indispensable element of electronic devices that need to operate in harsh conditions, starting in the nuclear field, from electronics to space [7,9]. At present, the basic electronic properties of diodes, which are formed depending on the production parameters, determine the technological field in which they can be used. Therefore, researches on controlling the electronic properties of Schottky diodes are still important. One of the parameters affecting the electronic properties of Schottky diodes is the interface materials used during their production [10]. One of these materials is the conductive polymer known as Poly [2-methoxy-5- (2-ethyl) hexoxy-1,4-phenylenevinylene] (MEH-PPV). These polymers are used in the production of organic light-emitting LEDs (OLED), especially sensors and organic diodes due to their high environmental stability and easy conductivity control [11]. Therefore, it is very important to determine the effect of the material used on the interface on diode parameters. Therefore, current-voltage characteristics play an important role in determining the basic parameters (ideality factor, barrier height, and resistance) of Schottky diodes [1].

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Especially studies aimed at investigating the temperature-dependent electronic parameters of these diodes are still up-to-date. Today, methods known as an artificial neural network (ANN) have the potential to be used to understand such relationships [12,13]. Synthetic data of current-voltage characteristics that can be formed depending on the temperature, especially with the ANN system, can play an important role in understanding the electronic parameters of the Schottky barrier.

According to the literature, although there is no study within the scope of this study, there are similar studies. Olikh [14] investigated the use of algorithms to determine the basic parameters of the Schottky diode using various methods. He reported that a number of algorithms show promise in determining semiconductor parameters. Rabehi et al. [15] presented a new approach for predicting diode parameters with greater accuracy. They successfully demonstrated the utility of this new algorithm approach in parameter setting. Darwish et al. [16] showed that they were able to use the ANN system to optimize Schottky diode performance. They explained that with the ANN system, the diode performance can be increased by optimizing the temperature, current and voltage output. Rahmani et al. [17] performed Schottky diode modeling using the ANN system. They reported that they can optimize diode parameters with the ANN system. Zhu et al. [18] studied the current density-voltage and capacitance-voltage properties of MEH-PPV-based Schottky diodes. In the study, the temperature-dependent hole mobility of MEH-PPV is extracted from 300 to 400 K with space load limited transmission (SCLC) model and the use of SCLC model is investigated in a high electric field. The highest hole mobility measured is 0.013 cm^2/V at 353 K. It has been stated that the thickness of MEH-PPV in structures composed of ITO/MEH-PPV/Al greatly affects the performance of diodes and the thinner film shows better device performance. According to capacitance-voltage relationships, the effective carrier density of MEH-PPV and Schottky barrier height were obtained as 2.24×10^{17} cm^{-3} and 0.64 eV, respectively. Aydın et al. [19] studied the electrical characterization of the Al/poly MEH-PPV/p-Si structure by current-voltage and capacitance-voltage methods. The barrier height obtained from the I - V characteristic is lower than the barrier height obtained from the C - V characteristic. It was stated that the barrier height value for the Al/MEH-PPV film/p-Si/Al contact obtained at room temperature was significantly greater than the conventional Al/p-Si Schottky diode. The interface state density Nss is obtained as a result of the study where Al/MEH-PPV/p-Si varies from $3.84\ 10^{14}$ $cm^2\ eV^{-1}$ inch ($0.32-E_v$) eV to $1\ 10^{14}$ $cm^{-2}\ eV^{-1}$ inch ($0.68-E_v$) eV.

In this study, for the first time, the temperature-dependent current-voltage characteristics of the Schottky diode with a polymer interface, synthetic data have been created using the ANN system. The usability of the ANN system in determining the Schottky diode characteristics has been investigated by comparing these synthetically obtained current and voltage data with the experimentally obtained data. In addition, the results were discussed by comparing with each other and the literature.

2. Experimental

6H–SiC/MEH-PPV Schottky diode is produced by Cree Inc. A 280 μm thick n-type 6H–SiC semiconductor wafer, with a diameter of 2 inches (001), with a donor density of $2.6 10^{17}$ cm^{-3}, was used. The surface of the SiC wafer was cleaned using the clean method known as RCA (i.e. a 10 min boil in $NH_4 + H_2O_2 + 6H_2O$ followed by a 10 min boil in $HCl + H_2O_2 + 6H_2O$). Then, it was kept in HF/H_2O (1:10) solution for 20 s to remove the oxide layer formed on the surface. After this process, pure Au (99.995%) of 150 nm thickness was evaporated to the matte surface of the SiC wafer under 10^{-6} Torr pressure. To create ohmic contact, the sample was annealed at 500 °C for 5 min in the metal evaporation system. Then dissolved in toluene, MEH-PPV was coated with a spin coater on the polished surface of the SiC flake at 2000 rpm for 60 s. The coated SiC was annealed at 60 °C for 5 min to remove toluene from the wafer surface. After this process, pure aluminum (99.999%) of 140 nm thickness was evaporated to form rectifier(Schottky) contact. For this, a 1 mm diameter stainless steel mask is used. Experimentally produced 6H–SiC/MEH PPV Schottky diode is shown in Fig. 1. Keithley 2400 Sourcemeter was used for Current-Voltage (I–V) measurements. Measurements were carried out with the help of an IEEE-488 AC/DC converter card installed in the computer. Current-Voltage (I–V) was done with 0.05V increments in the voltage Range of -3V to + 3V. The layer thickness of the produced diode was measured using an optical profilometer.

3. Development of the ANN model

ANNs, which were developed in the middle of the twentieth century by taking the biological structure of the human brain as an example, are one of the prediction tools that are frequently used by researchers recently [20]. The most obvious advantage of ANNs compared to other traditional prediction tools is that they can learn the relationship between complex functions that do not have a
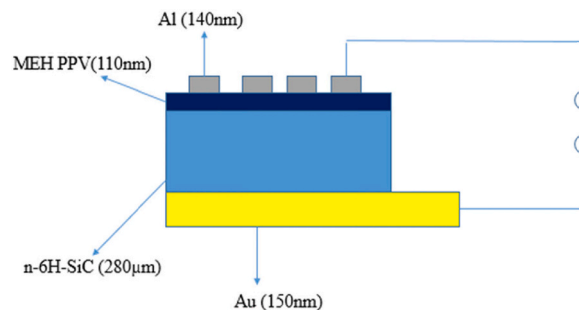

Fig. 1. Schematic diagram of 6H–SiC/MEH PPV Schottky diode.

linear correlation between them in the most ideal way and have high prediction performance [21]. MLP networks are one of the well-known models that are widely used by researchers in the literature in all kinds of science fields [22–25]. MLP networks have a strong structure that can learn and associate the relationship between the independent and dependent variables of complex and nonlinear functions that cannot be predicted with traditional prediction tools with a high success rate [26]. MLP networks consist of interconnected process elements varying according to the type of ANN model developed. The MLP network has an input layer, at least one hidden layer, and an output layer from which prediction data is obtained. The input, hidden and output layers are interconnected and consist of a computational element called a neuron. The neuron, which is the basic processing element used in modeling ANNs, is characterized by weight (w), bias (b), and an activation function (f). The weight values set using a random number generator are multiplied by the value of each neuron. By adding the results obtained with each other and with the bias value, the neuron output is obtained using Equation (1) [27].

$$Y_j = f\left(\sum_{i=1}^{n} W_{j,i} x_i + b_j \right) \tag{1}$$

In this study, an ANN model has been developed to predict the temperature-dependent current-voltage characteristics of a Schottky diode with a polymer interface. The developed model consists of a multilayer perceptron feed-forward back-propagation (FF-BP) multi-layer perceptron (MLP) network. Optimization of the amount of data to be used in ANN training is an important step that directly affects the prediction performance of ANN [28]. In the training of the ANN model developed in this study, a total of 244 experimental data were used. 146 of the data were used for the training phase, 61 for the validation phase, and 37 for the testing phase. In the input layer of the MLP model, temperature (T) and voltage (V) values are defined as input parameters, and current value (I) is obtained in the output layer. The basic configuration structure of the developed network model is shown in Fig. 2.

There is no definitive methodology developed for determining the number of neurons to be used in MLP network models [29]. For this reason, many different ANN models have been developed using different neuron numbers and different data groupings, their performances have been analyzed and the network model with 13 neuron numbers has been optimized. As the training algorithm, Levenberg-Marquardt training algorithm, which is frequently used in MLP models and has high performance, is used [30,31]. As the transfer functions to be used in the hidden layer and the output layer, the tangent sigmoid (Tan-Sig) and linear (Purelin) functions given in Equations (2) and (3), respectively, were preferred [32].

$$f(x) = \frac{1}{1 + \exp(-x)} \tag{2}$$

$$purelin(x) = x \tag{3}$$

The flow chart of the MLP model developed is shown in Fig. 3.

Analyzing the prediction performance of the ANN model is of great importance in understanding the consistency of the obtained outputs with the target values. For this purpose, MSE (Mean Square Error), R and MoD (Margin of Deviation) parameters have been used to evaluate the performance of the developed MLP model. The equations used in the calculation of performance parameters are given below [33].

$$MSE = \frac{1}{N} \sum_{i=1}^{N} \left(I_{exp(i)} - I_{ANN(i)} \right)^2 \tag{4}$$
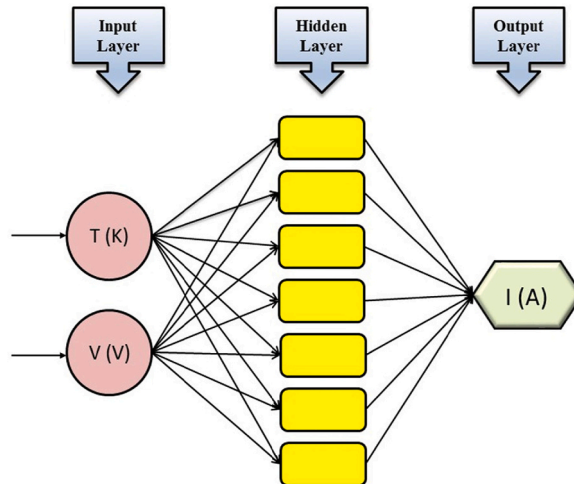

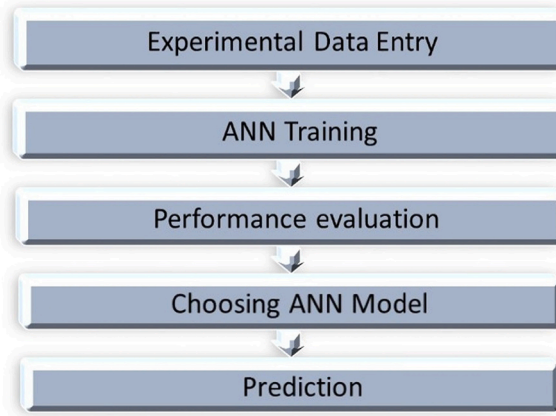**Fig. 2.** Basic configuration structure of the developed network model.

Fig. 3. The flow chart of the MLP model.

$$R = \sqrt{1 - \frac{\sum_{i=1}^{N} \left(I_{exp(i)} - I_{ANN(i)}\right)^2}{\sum_{i=1}^{N} \left(I_{exp(i)}\right)^2}} \tag{5}$$

$$MoD = \left[\frac{I_{exp} - I_{pred}}{I_{exp}}\right] x \ 100(\%) \tag{6}$$

4. Results and discussion

Current-voltage characteristics of the 6H–SiC/MEH PPV Schottky diode are shown in Fig. 4. These characteristics are the known diode characteristic. In Fig. 4, it can be seen that the forward parts of the breakdown voltage region become steeper at forward voltage as the temperature rises. This may be because the series resistance and interface states that changes with increasing temperature affect current transmission. If Fig. 4 'is examined carefully, it can be seen that the current starts after a certain voltage. This confirms the diode structure by showing the rectifier characteristic of the produced 6H–SiC/MEH-PPV structure. Additionally, the current and voltage characteristics of the 6H–SiC/MEH-PPV diode produced are compatible with the literature [18,34]. The training performance of ANN developed in Fig. 5 is shown. It is seen in the graph that the performance curves created with the data obtained from the train, validation and test stages of the ANN combined at the best point by reaching the lowest MSE value and the best validation performance value of 1.7811E-08 in the 49th epoch. The training of ANN has been finalised in this epoch, where the lowest MSE value has been reached and optimized in an ideal way. Error histogram graphics are one of the important data used in analysing the performance of ANNs. When the error histogram graph given in Fig. 6 is examined, it is seen that the numerical values of the error rates obtained from all three data sets are very low and the errors are located close to the zero error line. This situation confirms that the developed ANN has very low error values and is ideally designed.

In Fig. 7, the graph of the data obtained from the training phase of the developed ANN model is shown. Experimentally obtained
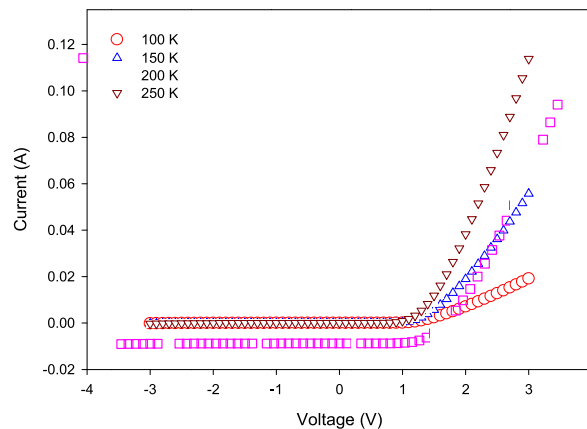

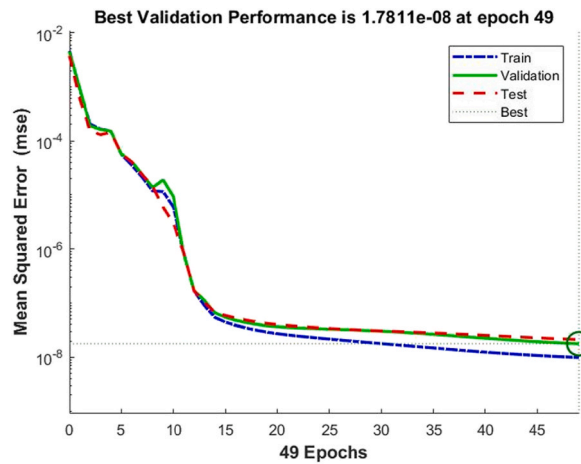**Fig. 4.** Current-voltage characteristics of the 6H–SiC/MEH PPV Schottky diode.

Fig. 5. Training performance of ANN according to epoch.
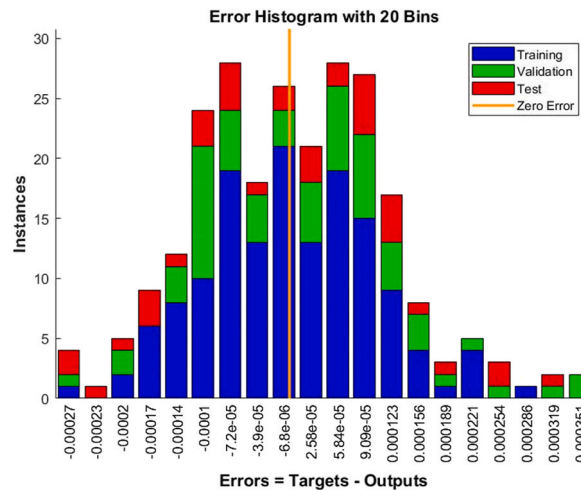

Fig. 6. Error histogram of the ANN model.

target values are located on the x-axis of the graph, and the predicted values obtained from the ANN model on the y-axis. When the graph is examined, it is seen that the data points obtained from the training stage are located on the equality line drawn in blue. However, the R-value obtained for the training phase is 0.99999. These results show that the training phase of the ANN model is ideally completed. Fig. 8 shows the data obtained from the validation stage of the MLP model. It should be noted that the data points in the graph are located on the equality line drawn in green. The R-value for the validation stage was calculated as 0.99997. The fact that the data points are located on the equality line and the R-value obtained show that the validation phase of the network model has been completed with high accuracy.

The data obtained from the test phase of the ANN model is shown in Fig. 9. In the graphic, it is clearly seen that the data points obtained from the test phase are located on the equality line drawn in red. The R-value calculated for the test phase is 0.99997. These results show that the testing phase of the MLP model has been completed with a very low error rate.

The points obtained from all of the data used in the training phase of the MLP network with 244 data are shown in Fig. 10. When attention is paid to the position of all data points on the equality line, it is seen that all of them are on the full line. The R-value calculated for all data has been found 0.99999. When all these data obtained are evaluated, It is seen that the developed ANN model has been designed in such a way that it can predict the current values of a polymer interface Schottky diode with a high accuracy depending on temperature and voltage.

The numerical values of the performance parameters of the ANN model developed are given in Table 1.

In Fig. 11, experimental data and ANN outputs are shown at each data point. While there are data numbers on the x-axis of the graph, there are experimental and ANN outputs on the y axis. When the graph is examined, it is seen that the data points obtained from ANN and the experimental data points are in perfect harmony. This perfect match of ANN outputs with experimental data confirms that the MLP network has been developed in such a way that it can predict the current values of a Schottky diode with a polymer interface
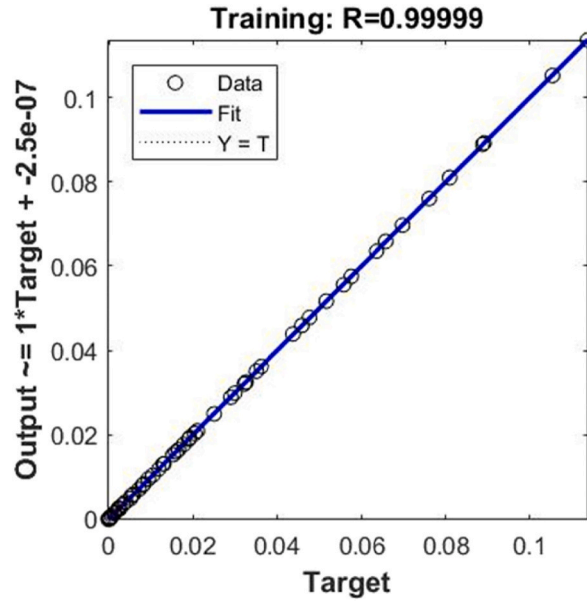
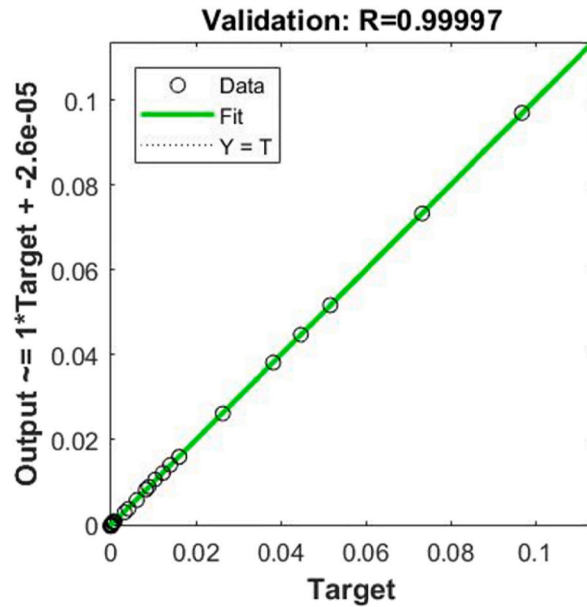**Fig. 7.** Training phase of the ANN.

Fig. 8. Validation phase of the ANN.

with a very low error rate depending on temperature and voltage.

In Fig. 12, MoD values calculated using Equation (6) are given for each data point. When the positions of the data points expressing the MoD values at each point are examined, it is seen that the MoD values are very low, and also close to the zero error line. The designed ANN model can predict the current value of a Schottky diode with polymer interface at rates varying from 2.96% to −3.02% and with an average error of −0.15%.

Fig. 13 shows the voltage-dependent current values of a polymer interface Schottky diode at a constant temperature. When the values given for the temperatures of 100, 150, 200, and 250 K are examined, it is clearly seen that the prediction results obtained from the ANN model are in perfect harmony with the experimental data. This situation, which has been evaluated separately for each temperature, can be interpreted as another proof that the MLP network is designed in an ideal way.

Experimental data on the x-axis of Fig. 14, and ANN outputs on the y-axis. It is clearly seen in the graph that red data points are located on the equality line expressed in blue rank. This location of the data points is another proof that the ANN model has been
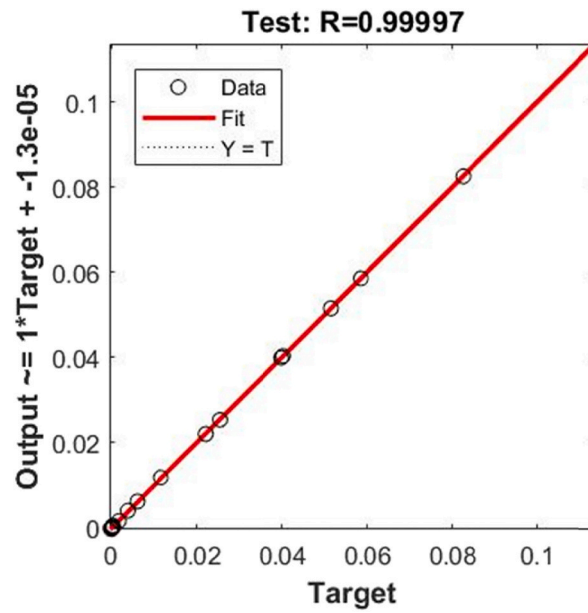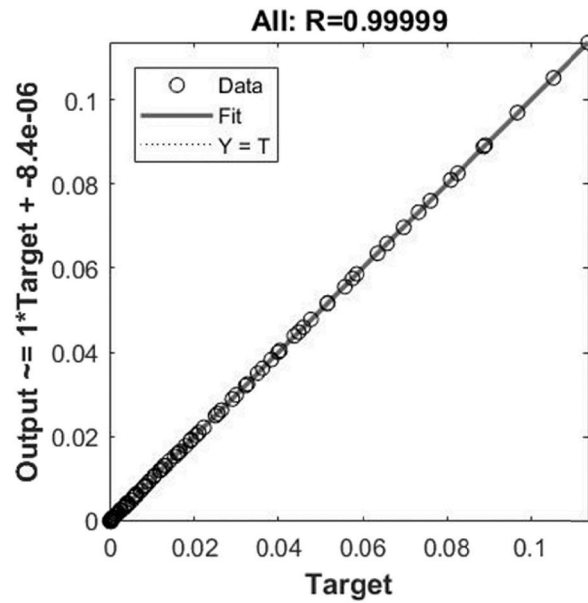
Fig. 9. Test phase of the ANN.

Fig. 10. Overall data of the ANN.

Table 1
The numerical values of the performance parameters of the ANN.

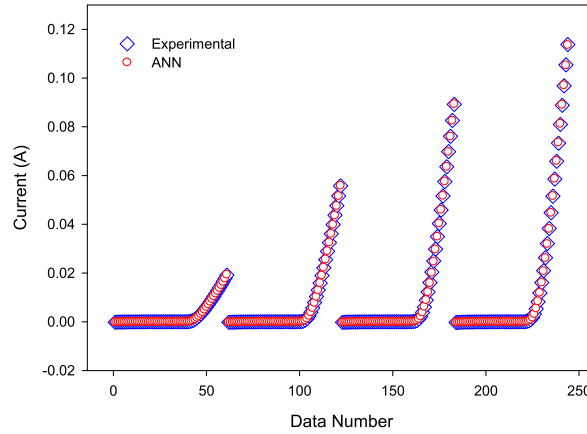| Data Set	MSE	R	Number of Data
Training	9.91E-09	0.99999	146
Validation	1.78E-08	0.99997	61
Test	2.13E-08	0.99997	37
All	1.63E-08	0.99999	244

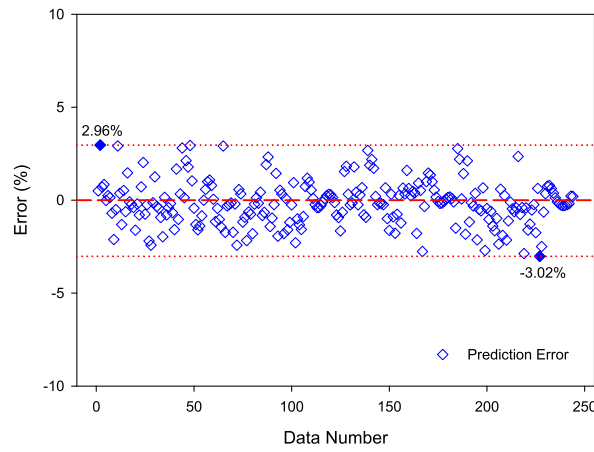**Fig. 11.** Experimental data and ANN outputs according to data numbers.

Fig. 12. MoD values of the ANN according to data numbers.

developed in such a way that it can predict the current values of a polymer-interfaced Schottky diode with very high accuracy and an acceptable error rate depending on the temperature and voltage.

5. Conclusion

In this study, a model has been developed to predict the current values of a polymer-interfaced 6H–SiC/MEH-PPV Schottky diode with an artificial intelligence approach, depending on temperature and voltage. As the simulation model, a feed-forward multi-layer perceptron artificial neural network is preferred. In the training of the artificial neural network, the experimentally measured current values of the 6H–SiC/MEH-PPV Schottky diode with polymer-interface in the temperature range of 100–250 K and voltage range -3V to + 3V have been used. Of the total 244 experimental data used in the network model developed with 13 neurons in the hidden layer, 146 have been reserved for training, 61 for validation, and 37 for testing. For the artificial neural network model, the MSE value is 1.63E-08 and the R-value is 0.99999. The developed model has been able to predict the current values of the polymer-interfaced 6H–SiC/MEH-PPV Schottky diode, depending on the temperature and voltage, with error rates between 2.96% and −3.02%. The results obtained show that artificial neural networks are an ideal tool to be used to predict the current values of the polymer-interfaced 6H–SiC/MEH-PPV Schottky diode depending on temperature and voltage.
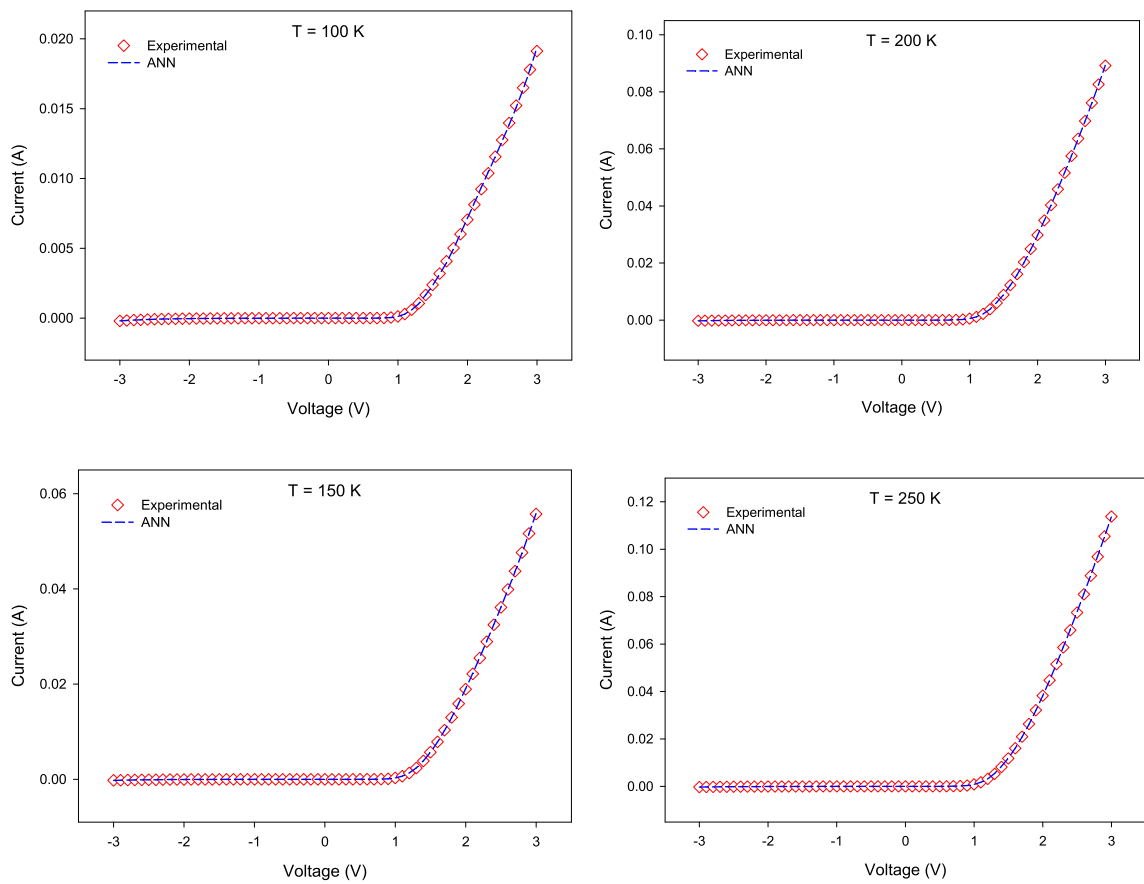
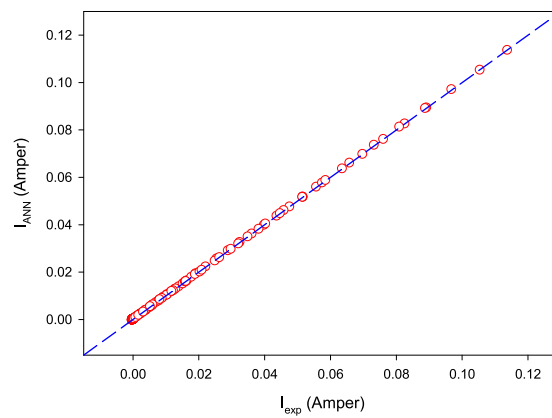**Fig. 13.** Voltage-dependent current values at constant temperature.

Fig. 14. Experimental data vs ANN output.

Declaration of competing interest

We declare that there is no conflict of interest.

Nomenclature

ANN	Artificial Neural Network
FF-BP	Feed-forward back-propagation
I	Current (Amper)
LED	Light Emitting Diode
MEH-PPV	Methoxy Ethyl Hexoxy - Phenylenevinylene
MLP	Multi-layer perceptron
MSE	Mean Square Error
OLED	Organic Light Emitting Diode
SiC	Silicon carbide
SCLC	Space Load Limited Transmission
T	Temperature (K)
V	Voltage (Volt)

Credit author statement

Tamer Güzel: Conceptualization, Writing – original draft, review and editing. Andaç Batur Çolak: Investigation, Methodology, Writing – original draft and editing.

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