Microelectronics Reliability 147 (2023) 115040

Contents lists available at ScienceDirect

Microelectronics Reliability

journal homepage: www.elsevier.com/locate/microrel

Performance prediction of current-voltage characteristics of Schottky diodes at low temperatures using artificial intelligence

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ARTICLE INFO

Keywords:
Semiconductor
Diode
Schottky
Machine learning
Artificial Neural Network

ABSTRACT

Schottky diodes are still one of the most important elements of electronics. Therefore, investigating the properties of diodes is very important in determining their usage areas. In this study, the performance of the artificial neural network model trained using high temperature data in predicting the current-voltage properties at low temperatures was investigated. An artificial neural network is modeled using the experimentally measured current and voltage values at the temperature range of 80 and 375 K. In the developed network model, temperature and voltage values are defined as input parameters and current values are estimated. Levenberg-Marquardt training algorithm was used as the training algorithm in the neural network, which was developed using a total of 1584 data. The current values obtained from the artificial neural network were compared with the experimental current values, and the prediction performance of the network model was extensively analyzed by using various performance parameters. The results showed that the developed artificial neural network can predict current values at low temperatures with high accuracy depending on voltage. In addition, it was found that the current-voltage characteristics of the Schottky diode at low temperatures could be predicted with an error rate of approximately ±7 %. On the other hand, the error rates in the prediction of diode characteristics by artificial intelligence were determined to be independent of temperature.

1. Introduction

Semiconductors are one of the milestones in the development of civilization. Since their invention, it has been made significant progress in electronics science. Nowadays, electronics and electronic applications are taking place more and more daily in human life. Undoubtedly, one of the most significant shares in this belongs to the diodes. Diodes are one of the key circuit elements in the management and orientation of electrons. Today, diodes are used in many areas from health to defense and even energy production [1,2]. Semiconductor materials form the basic building blocks of diodes. Among them, gallium phosphate has a special place with its indirect band structure [3–5]. Gallium phosphate-based diodes have a wide range of uses, from optoelectronics to power generation [6–8]. The variety of production methods of diodes and the differences in semiconductor materials used in their production determine the electronic performance of diodes. In fact, one of these factors is the temperature range in which the diodes will be used [9]. A wide range of operational temperatures are available for diodes [10,11]. They are available for use in many temperatures range from very high to very low temperatures [12,13]. At this point, it is very important to determine the diode performance in a certain temperature range. One of the methods to determine the diode characteristics is to measure the current-voltage values [14–16]. Accordingly, the use of machine learning has recently begun to increase in the determination of these characteristics [17,18]. One of these is that the characteristics of semiconductors can be determined depending on the temperature [19,20]. In this case, the use of machine learning in the determination of electronic properties at low temperatures has the potential to provide great benefits to researchers in terms of time and cost.

According to the literature, new studies have been yet started to determine the electrical parameters of semiconductors by the machine learning method. However, the low-temperature data prediction of artificial intelligence trained using high-temperature data has been reported for the first time. Doğan [21] investigated the performance of different algorithms used to determine the electrical parameters of the Schottky diode. She used meta-heuristic optimization algorithms for this. She reported that some of these algorithms perform much better than others in determining the electrical character of the barrier diode.

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https://doi.org/10.1016/j.microrel.2023.115040
Received 24 March 2023; Received in revised form 26 May 2023; Accepted 30 May 2023
Available online 7 June 2023

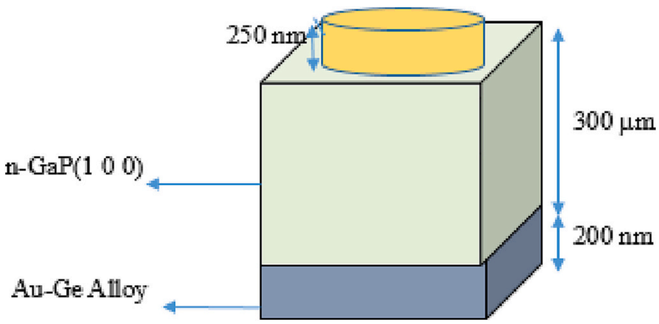

Fig. 1. Schematic representation of Au-Ge/n-GaP/Au Schottky diode.

Güzel et al. [22] researched the usability of artificial intelligence data in determining the electrical characteristics of Schottky diodes. They calculated and compared electrical parameters such as ideality, barrier height, and resistance using data obtained from artificial intelligence outputs and experimental results at certain temperatures. They showed that artificial intelligence data can be used to calculate in electrical parameters. Hao et al. [23] showed the performance of artificial intelligence in finding diode performance. For this, they obtained a variety of sample data including diode structure and performance parameters. They stated that artificial intelligence's reverse breakdown voltage and open circuit resistance estimation were also quite well. Torun et al. [24] used some commonly used machine learning methods to determine the temperature-dependent current-voltage characteristics of Schottky diodes. They explained that the ANFIS and RMSE algorithms outperform the others in estimating the temperature-dependent current-voltage characteristics. Doğan et al. [19] proposed an Artificial Neural Network (ANN) model to characterize the annealed and annealed Schottky diode. They used experimental data over a wide temperature range for this. They reported that the modeling performance of the current-voltage characteristics of the annealed diode is lower than that of the fabricated one. Rabehi et al. [25] investigated the usability of artificial intelligence algorithms in the extraction of some basic electrical parameters of Schottky barrier diodes. For this, they compared the parameters obtained by machine learning with the results calculated analytically. They reported that the features calculated by some proposed algorithms are in good agreement with the parameters calculated by the analytical method. Çolak et al. [26] researched the determination of temperature-dependent current-voltage characteristics using an ANN. For this, they compared the current-voltage properties experimentally measured at some temperatures and predicted by the ANN method. They explained that ANNs are quite successful in determining temperature-dependent current-voltage characteristics.

When the literature studies are examined, it is seen that there is no study on the estimation of the critical parameters of Schottky diodes at low temperatures with machine learning approach. In this study, the high-temperature current-voltage experimental data of the diode produced were used in the training of artificial intelligence. Then, the performance of artificial intelligence was investigated by providing the

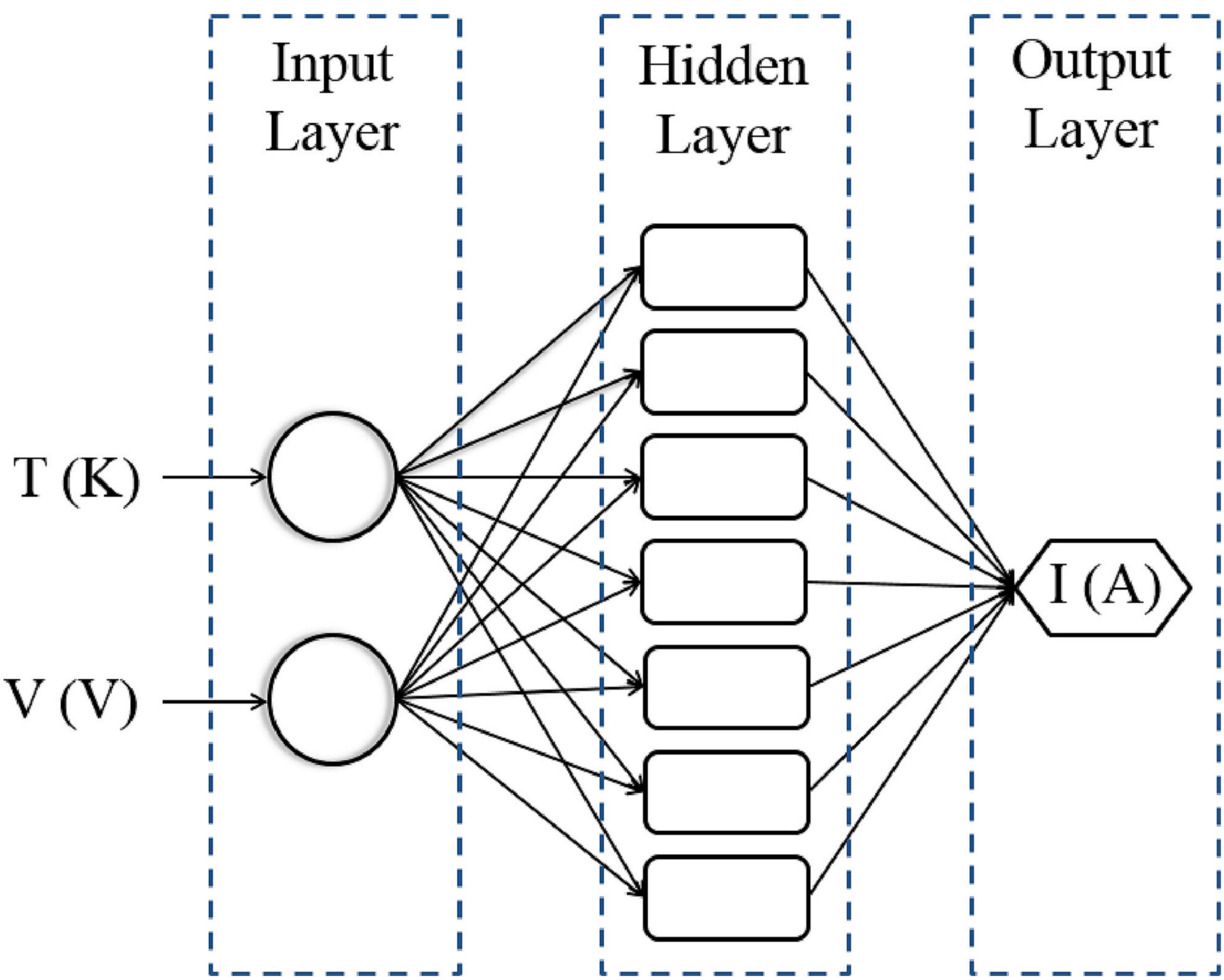

Fig. 2. The structural configuration model of the developed MLP network.

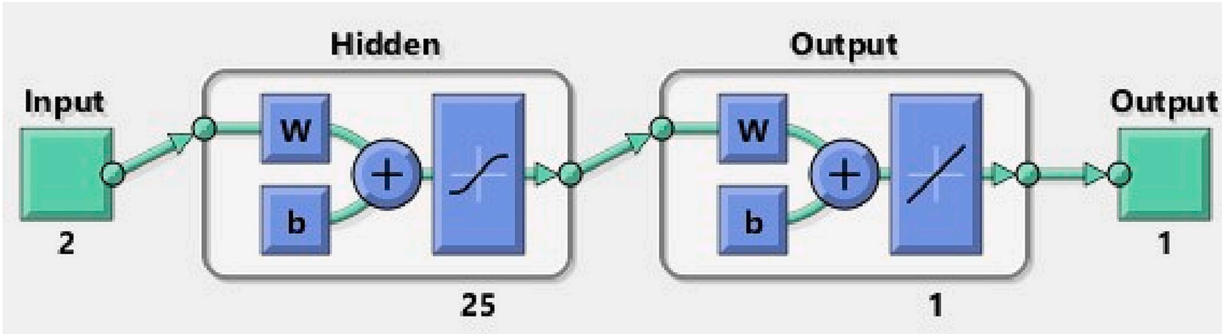

Fig. 3. The main structural features of the developed network model.

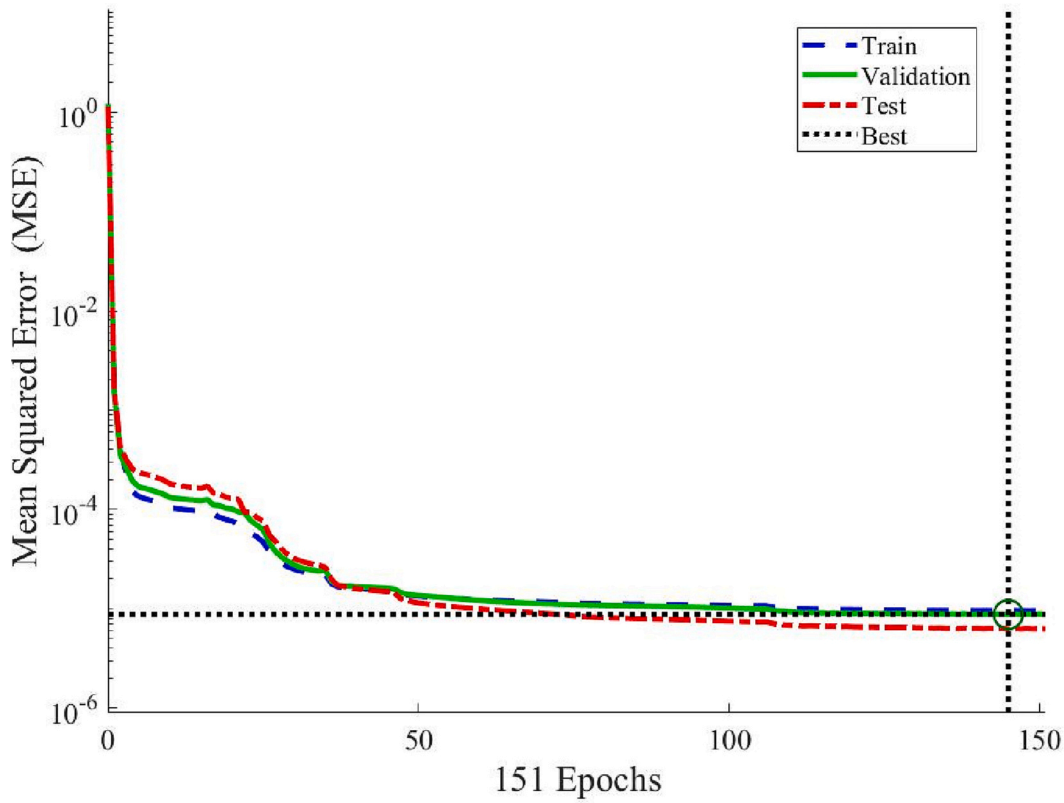

Fig. 4. The training performance of the MLP model.

estimation of the current-voltage characteristics at low temperatures and comparing the characteristics determined as a result of both experimental and artificial intelligence estimation. The results were discussed and compared with each other and with the literature. This study can be considered as a pioneering study aiming to close an important gap in the literature.

2. Experimental set-up

The produced Au-Ge/n-GaP/Au diode is shown in Fig. 1. For the fabrication of the Au-Ge/n-GaP/Au diode, an n-type gallium phosphate (GaP) crystal with a thickness of 300 μm and a carrier density of 1×10^{18} cm^{-3} in the (100) orientation was used. First of all, they were cleaned in an ultrasonic bath containing ethylene, acetone, and methanol solutions, respectively, for 5 min and dried in N_2 environment in order to clean the organic and other heavy metal contaminants on the surfaces of the semiconductor. After cleaning, the matte surface of the semiconductor was coated with a 200 nm thick gold-germanium (Au—Ge, 88:12 wt%) alloy at 10^{-6} Torr pressure to form the Ohmic contact. Then, the Au-Ge/n-GaP ohmic contact was formed by annealing the sample at 400 °C for 3 min. After this process, using a 1 mm diameter steel mask, 250 nm thick Au was evaporated to the surface at 10^{-6} Torr pressure, and a rectifying contact was composed. Keithley 2400 Sourcemeter was used for Current-Voltage (I-V) measurements. Voltage-dependent current measurements of the produced diodes were carried out in the range of 80-375 K in 25 K increments.

3. Development of the ANN model

An ANN model has been developed to analyze the machine learning performance of Schottky diodes in determining the current-voltage characteristics at low temperatures. ANNs are one of the widely used machine learning tools, thanks to their high predictive capabilities. Multilayer sensor (MLP) architecture was used in the ANN model, which was developed using the current-voltage data of the experimentally obtained Schottky diode. MLP networks are a network model consisting

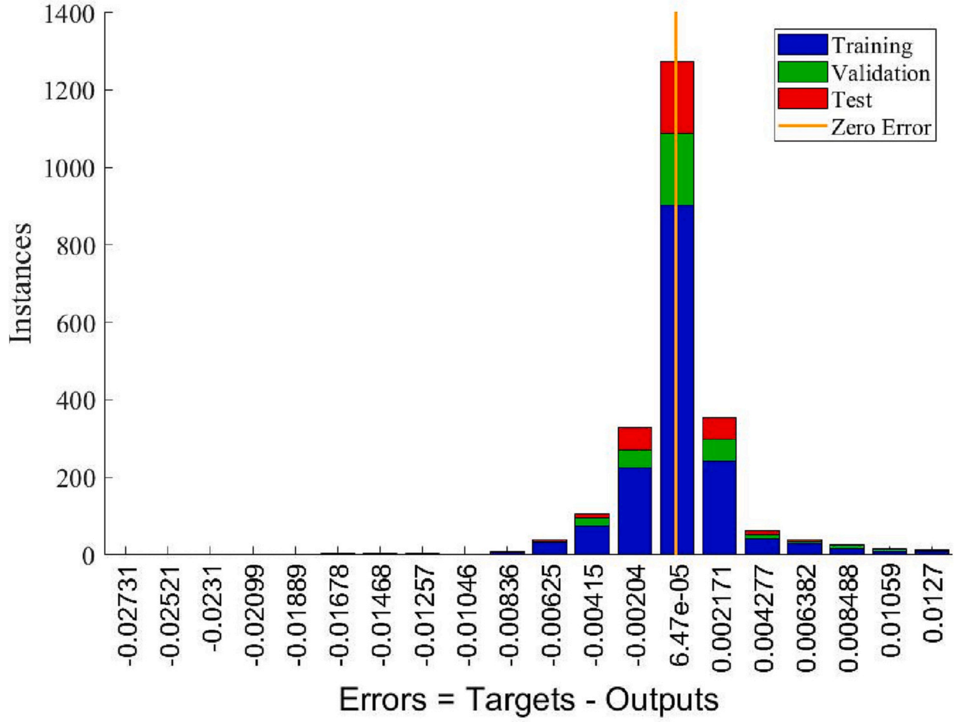

Fig. 5. The error histogram created with the data obtained from the training stages.

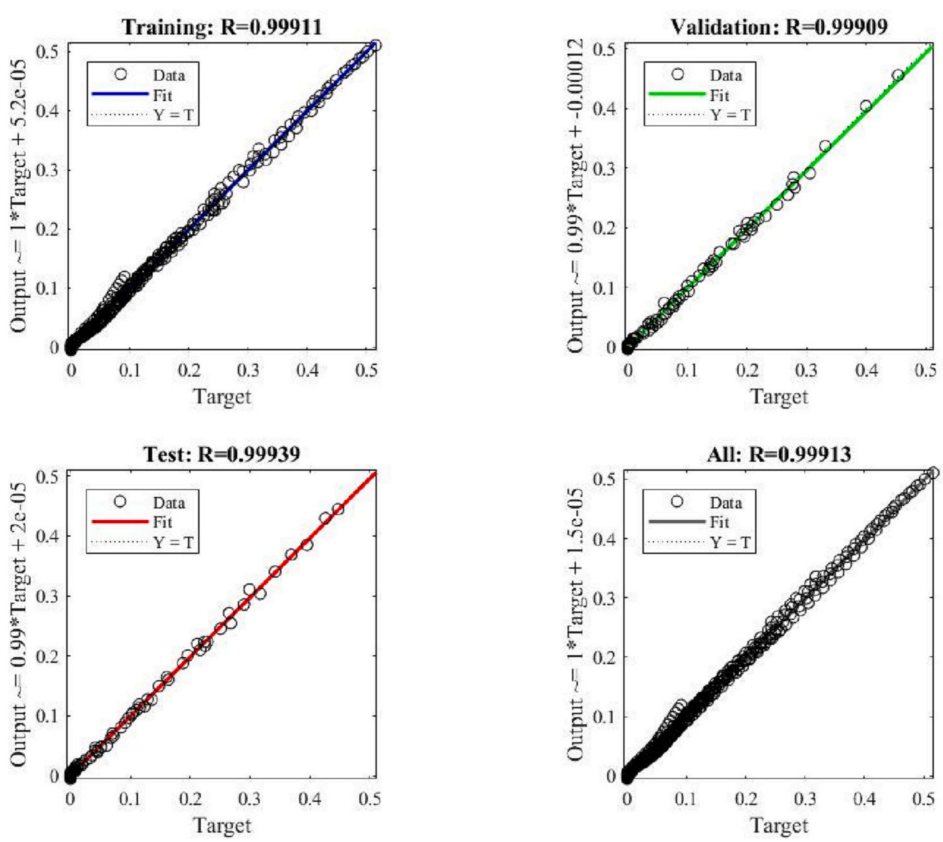

Fig. 6. The fit of the target and output data.

of three basic layers directly connected to each other. In the input layer of the developed MLP network, voltage and temperature values are defined as input parameters and current values are obtained in the output layer. The structural configuration model of the developed MLP network is shown in Fig. 2.

It is important to ideally group the training data to be used in MLP

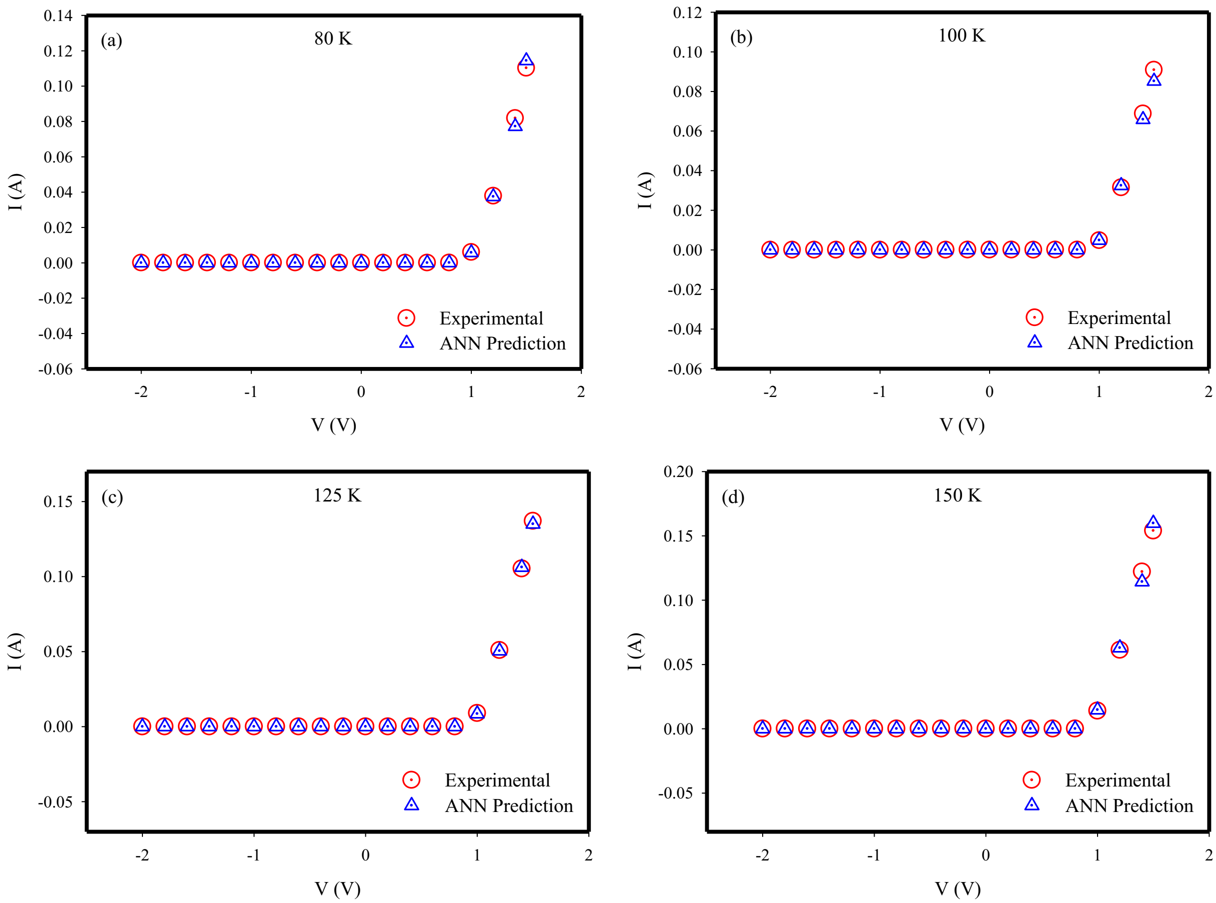

Fig. 7. I-V plots at each 80, 100, 125 and 150 K temperatures.

networks. In the network model, which was trained using a total of 1584 experimental data of the Schottky diode obtained at high temperatures, 1108 of the data were reserved for the training of the model, 238 for the validation of the model and 238 for the testing phase of the model. Determining the number of neurons in the hidden layer of MLP networks is one of the major challenges and a clear methodology is not yet available. In order to overcome this difficulty, the performances of MLP networks developed with different neuron numbers were analyzed and the network model with 25 neurons in the hidden layer was determined as the most ideal model. The main structural features of the developed network model are shown in Fig. 3.

The MLP network model is trained using the widely used Levenberg-Marquardt training algorithm, which has strong learning capabilities. Tan-Sig and Purelin transfer functions are used in the hidden and output layers, respectively. Equations of transfer functions are given below:

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

$$purelin(x) = x \tag{2}$$

Examining the training, learning and prediction performances of ANN models is an important step in terms of the reliability of the models. In order to be used in the performance analysis, a literature review was conducted and the performance parameters that are widely used by the researchers were determined. The mathematical expressions used in the calculation of coefficient of determination (R), mean squared error (MSE), and margin of deviation (MoD) parameters used in the performance analysis are given below:

$$R = \sqrt{1 - \frac{\sum_{i=1}^{N} \left(X_{exp(i)} - X_{ANN(i)}\right)^2}{\sum_{i=1}^{N} \left(X_{exp(i)}\right)^2}} \tag{3}$$

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

$$MoD = \left[\frac{X_{exp} - X_{ANN}}{X_{exp}}\right] x\ 100\ (\%) \tag{5}$$

4. Results and discussion

The investigation of the critical parameters of Schottky diodes, which is an important electronic component, is one of the serious studies in the field of electronics. The fact that sensitive characteristics can be obtained with reliable accuracy without the need for experimental studies brings important advantages such as time and financial issues. Obtaining the current values of Schottky diodes at low temperatures depending on temperature and voltage is a serious issue that can overcome important difficulties in a short time. The learning, training and prediction performance of the MLP model, which was developed using experimentally obtained current-voltage values at high temperature, was extensively investigated and the accuracy of the proposed model was examined in detail.

In order to ensure that the training phase of the ANN model is completed in an ideal way, the MSE values obtained from the training phase are shown in the training performance graph in Fig. 4. In MLP networks, voltage and temperature values, which are the input

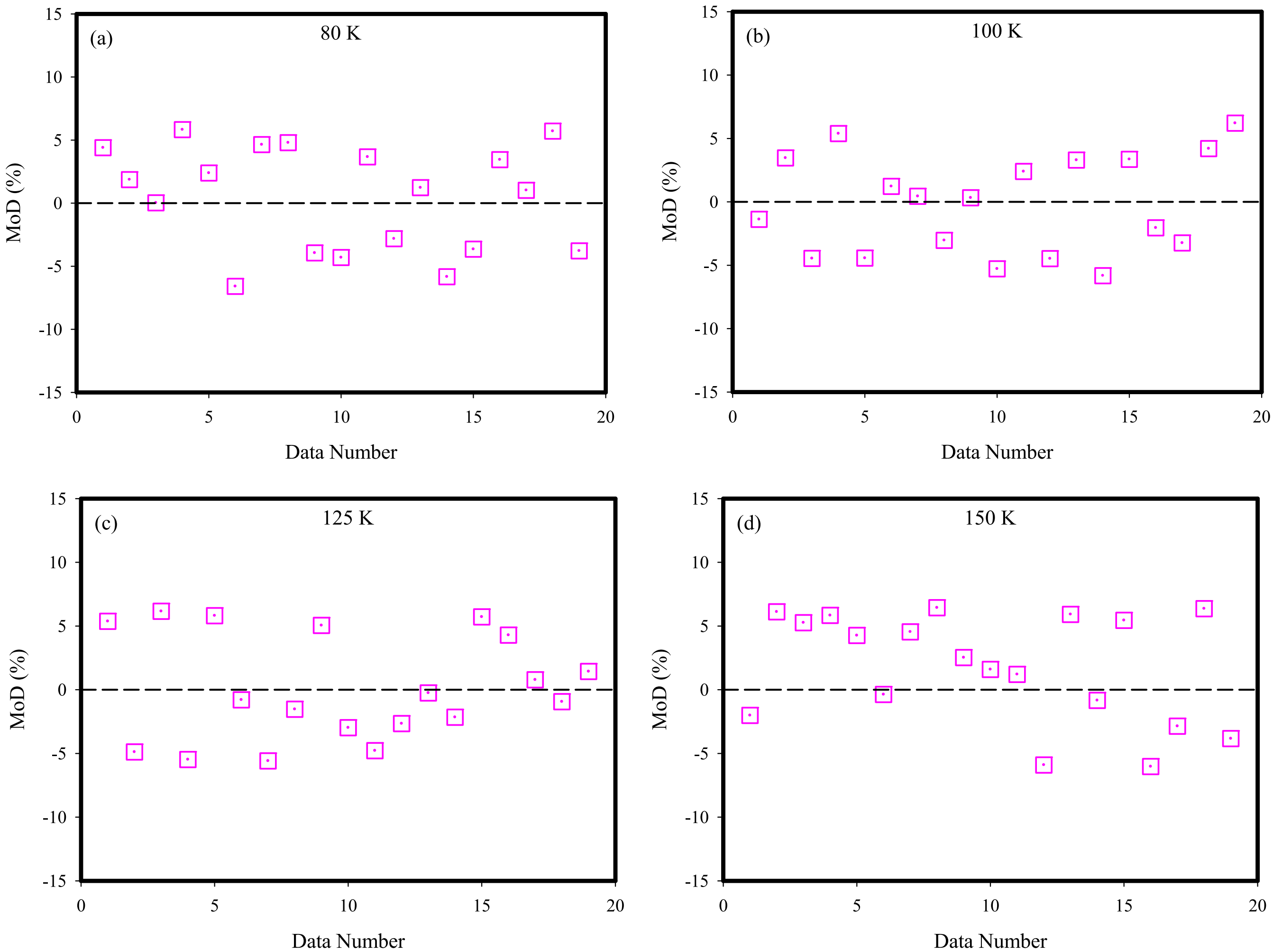

Fig. 8. MoD values according to data number.

Table 1
Temperature-dependent margin of deviation in determining current-voltage characteristics.

	T(K)	MoD (%)	
Data group used in the training of ANN (175-375K)	375	-6,98	6,89
	350	-6.90	6.57
	325	-7.00	6.92
	300	-7.00	6.90
	275	-6.99	6.80
	250	-6.99	6.82
	225	-6.93	6.87
	200	-6.93	6.87
	175	-6.95	6.91
Data group predicted by ANN (80-150K)	**150**	**-6.99**	**6.87**
	125	**-6.91**	**6.88**
	100	**-6.81**	**6.46**
	80	**-6.99**	**6.89**

parameters introduced to the system in the input layer, move towards the hidden and output layer that follows it. The current value obtained in the output layer is compared with the experimentally obtained current value and the data is sent back from the output layer to the input layer in order to eliminate the errors in between. For each epoch that occurs, the MSE values are calculated and the MSE values are decreased with each cycle. The decrease in MSE values means that the error value in the output layer also decreases. In Fig. 4, it can be seen that the MSE values, which were high for each data set at the beginning of the training phase, decrease at each epoch. Upon reaching the ideal validation value, the lowest MSE values were obtained and the training phase of the model was completed by minimizing the difference between the current value obtained in the output layer and the experimental current value.

In Fig. 5, the error histogram created with the data obtained from the training stages is given. In error histograms, it is aimed to analyze the errors in the training phase of the model by examining the errors that occur between the target and the actual data. When the errors obtained for each grouped data set are examined, it is seen that they are generally concentrated around the zero error line. In addition, it should be noted that the numerical values of the errors are also very low. These results obtained from the error histogram prove that the training phase of the developed ANN model is completed ideally with very low errors.

Fig. 6 shows the fit of the target and forecast data given separately for each of the datasets allocated for the training, validation and testing phases. Afterwards, comparisons of the entire data set are presented. When attention is paid to the positions of the data points, it is generally seen that all of them are located on the zero error line. However, it is seen that fitted line and zero error line are also located on top of each other. When the R values calculated for each data set are examined, it is seen that each of them is higher than 0.999. The MSE value, another performance parameter calculated for the ANN model, was obtained as 9.59E-06. The closeness of the R values to the value of 1 and the closeness of the MSE value to the zero value indicate that the training

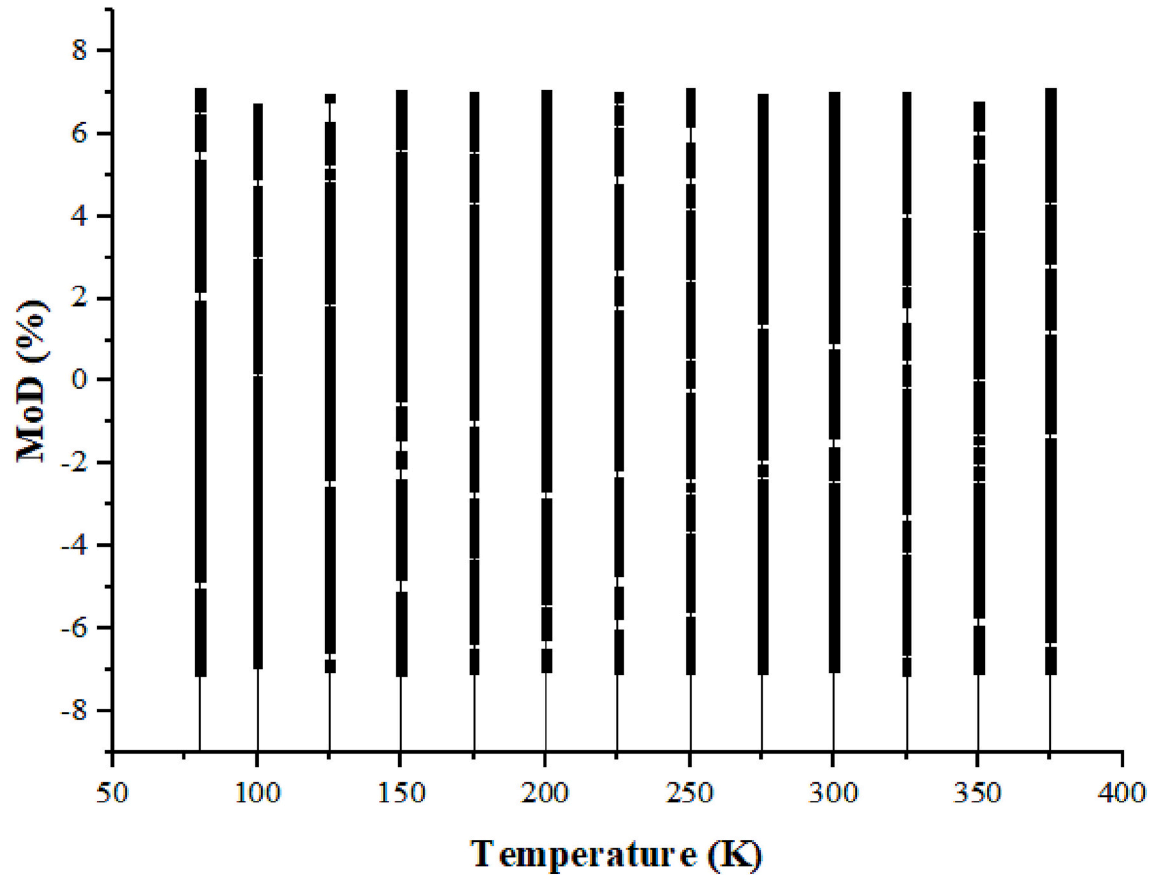

Fig. 9. The margin of deviation in the temperature-dependent estimation of the current-voltage characteristics of the Au-Ge/n-GaP/Au Schottky diode by ANN.

phase of the developed ANN model is ideally completed.

In order to evaluate the prediction performance of the ANN model, the compatibility of the prediction and experimental data has been extensively examined. Fig. 7 shows the I-V plots at each 80, 100, 125 and 150 K temperatures. When the data points shown in the graphs are examined, it is seen that the flow values obtained from the ANN model are in excellent agreement with the experimental flow values. This perfect match of current values for each voltage value shows that the developed ANN model can predict low temperature current values with high accuracy and ideally depending on temperature.

In order to analyze the deviation ratios between the flow values obtained from the ANN model and the experimental flow values, the MoD values were calculated and shown in Fig. 8. When the graphs presented for each data point at 80, 100, 125 and 150 K temperatures are examined, it is seen that the data points expressing the MoD values are generally located close to the line expressing the zero deviation value. In Table 1, the MoD in the determination of current-voltage characteristics of machine learning depending on temperature was given. According to the table, the current-voltage characteristics of the diode were found to be approximately ±7 % at all temperatures, including low temperatures, within the limitation of the prediction algorithm used in this study. In fact, this situation can be seen much more clearly in Fig. 9. According to the figure, it can be clearly understood that the error rate in the prediction does not change at all temperatures.

In fact, this shows that the MoD value, which can be considered as a performance indicator in determining the current-voltage characteristics of machine learning in the context of diodes, is independent of temperature. This situation is quite interesting. Because, according to the literature, different current conduction mechanisms are dominant at low temperatures [27]. Some of the reasons for the change in the current conduction mechanism are Interface states and increased trap density. Especially at low temperatures, temperatures below 200 K degrees are considered low temperatures according to the literature, these situations become more dominant and affect the current-voltage properties [28–33]. On the other hand, In Schottky diodes, the thermionic current-conduction mechanism, which is valid at high temperatures replaced by conduction mechanisms such as thermionic field emission, field emission, minority carrier injection, and generation-recombination at low temperatures. These transmission mechanisms become the dominant current mechanism, either alone or in combination. In this case, high deviations are observed in the ideality factor, which is one of the characteristics of Schottky diodes. In this case, it affects the experimentally measured voltage-dependent current values [34,37]. As a result, deviations occur from the thermionic theory proposed to explain the current conduction mechanism of diodes [38]. However, the fact that the MoD value is independent of temperature, although different mechanisms affecting the current occur at low temperatures, the fact that the artificial intelligence prediction performance is the same with high temperatures shows that artificial intelligence can tolerate the factors that may affect the current conduction mechanisms at low temperature. This result also showed that the developed ANN model is an ideal mathematical tool that can be used to predict current-voltage characteristics in the specified temperature range.

5. Conclusion

One of the turning points in the history of civilization was the invention of semiconductors. Since their inception, it has been made tremendous advances in electronics research. Electronics and electronic applications are used in more and more aspects of everyday life nowadays. The diodes unquestionably have one of the largest percentages in this. One of the most important circuit components for managing and directing electrons is the diode. Diodes are employed in a variety of applications today, including energy generation, defense, and even health. The estimation of some important parameters, which can be obtained in experimental studies carried out in the field of electronics, especially diodes, with machine learning algorithms is one of the issues that have been increasing in importance recently.

In this study, the voltage-dependent currents of a manufactured Schottky diode at 150, 125, 100 and 80 K temperatures were experimentally measured in the 375-150 K temperature range. An ANN was developed using the current-voltage characteristics obtained. Temperature and voltage values are defined in the input layer of the network model with MLP architecture and current values are obtained in the output layer. In the ANN model developed with a total of 1584 experimentally obtained data, 1108 of the data were used for the training of the model, 238 for the validation and 238 for the testing phase. Levenberg-Marquardt training algorithm was used as the training algorithm in the ANN model with 25 neurons in the hidden layer. The results obtained from the ANN model were compared with the experimental results. The study findings showed that the flow values obtained from the ANN model were in ideal agreement with the experimental flow values. Among the parameters determined for the performance analysis of the ANN model, the MSE value was calculated as 9.59E-06 and the R value as 0.99913. The MoD values for the current values obtained from the ANN model remained in the range of ± 7 %. These results show that the developed ANN model can predict the current values of the Schottky diode at low temperatures with high accuracy depending on the voltage. In addition, since the margin of deviation is approximately similar at all temperatures, it has been determined that MoD is independent of temperature in the estimation of electrical properties in this study.

CRediT authorship contribution statement

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

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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