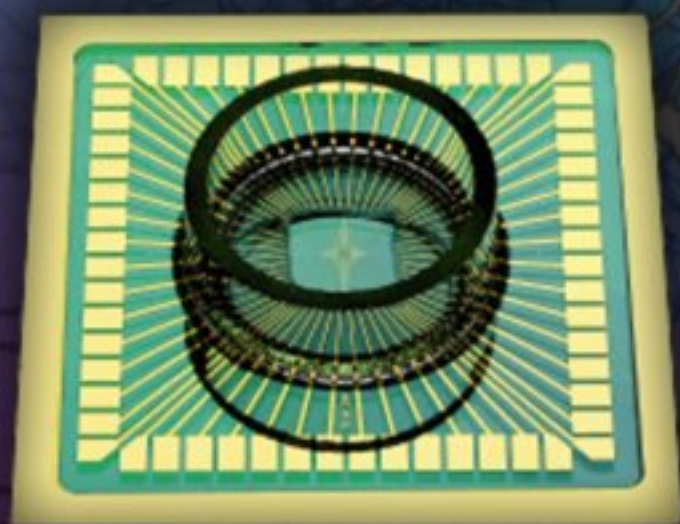


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ANN Modeling of a Chemical Humidity Sensing Mechanism

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Abstract: This work aims to achieve a modeling of a resistive-type humidity sensing mechanism (RHSM). This model takes into account the parameters of non-linearity, hysteresis, temperature, frequency, substrate type. Furthermore, we investigated the TiO₂ and PMAPTAC concentrations effects on the humidity sensing properties in our model. Using neuronal networks and Matlab environment, we have done the training to realize an analytical model ANN and create a component, accurately express the above parameters variations, for our sensing mechanism model in the PSPICE simulator library. Simulation has been used to evaluate the effect of variations of non-linearity, hysteresis, temperature, frequency, substrate type and TiO₂ and PMAPTAC concentrations effects, where the output of this model is identical to the output of the chemical humidity sensing mechanism used. *Copyright © 2010 IFSA.*

Keywords: Resistive humidity sensor, Sensing mechanism, Neuronal network, MLP, TiO₂ PMAPTAC.

1. Introduction

Humidity is a significant parameter as the pressure or the temperature. It changes the electric characteristics of materials and acts on the response of the systems carried out. Humidity measurement is one of the important tasks in many industrial processes for manufacturing of products such as textiles, food, paper, semiconductors and petrochemical [1-3].

There are various types of humidity sensors based on the sensing principle they use, such as resistive, mechanical, gravimetric, capacitive, and thermal humidity sensors [4-5]. In the current paper we

modeled a new chemical humidity sensing mechanism. The sensing design of the sensor is optimized by the TiO₂ and PMAPTAC concentrations effects on the humidity sensing properties, which are employed in our model.

Recently, artificial neural networks (ANNs) have emerged as a highly effective learning technique suitable to perform nonlinear, complex, and dynamic tasks with high degree of accuracy [6]. However, complex nonlinear and cross sensitivity modeling has been successfully tackled by (ANNs) [7]. Neural models are, therefore, much faster than physics/electro-mechanical models and have a higher accuracy than analytical and empirical models. Furthermore, they are easy to develop for a new device or technology [8-9].

In this paper, we propose an ANNs model for a resistive humidity sensing mechanism (SM) operated under dynamic environment. It provides accurate readout of the applied humidity; we have designed and established on SPICE software this SM. The SM model carried out take into account the non linearity response, the hysteresis, the temperature and frequency effects in a dynamic environment and TiO₂ and PMAPTAC concentrations.

2. Resistive Humidity Sensor Mechanism (RHSM) Design

The sensing mechanism measures the change in electrical impedance, it absorbs the water vapor then ionic functional groups are dissociated, resulting in an increase in electrical conductivity. The impedance range of typical resistive elements varies from 100 to 100,000,000 Ohms.

The resistive-type humidity sensing mechanism used for this modeling was fabricated by the *in situ* photopolymerization of TiO₂ nanoparticles/polypyrrole (TiO₂ NPs/PPy) and TiO₂ nanoparticles/polypyrrole/poly-[3-(methacrylamino)propyl] trimethylammonium chloride (TiO₂ NPs/PPy/PMAPTAC) composite thin films, our model contain tow mechanisms of this composite, the first is fabricated on a polyester (PET) substrate and the second on an alumina substrate. The effect of the TiO₂ and PMAPTAC concentrations on the humidity sensing properties are investigated.

The various compositions are shown in Table 1. The composite solution is coated, on an alumina and onto a PET substrate, with a pair of comb-like electrodes. Thus, a humidity sensor of the resistive-type was obtained (Fig.1).

Table 1. Composition of the composite films used to prepare humidity sensors [data taken from 10-11].

Substrate	Sample number	Pyrrole (g)	AgNO3 (g)	TiO ₂ (g)	PMAPTAC (g)
Alumina	1	0.125	0.0314	0	0
	2	0.125	0.0314	0.0012	0
	3	0.125	0.0314	0.0118	0
	4	0.125	0.0314	0.0480	0
PET	5	0.125	0.0314	0.0012	0
	6	0.125	0.0314	0.0118	0
	7	0.125	0.0314	0.048	0
	8	0.125	0.0314	0.048	0.008
	9	0.125	0.0314	0.048	0.08

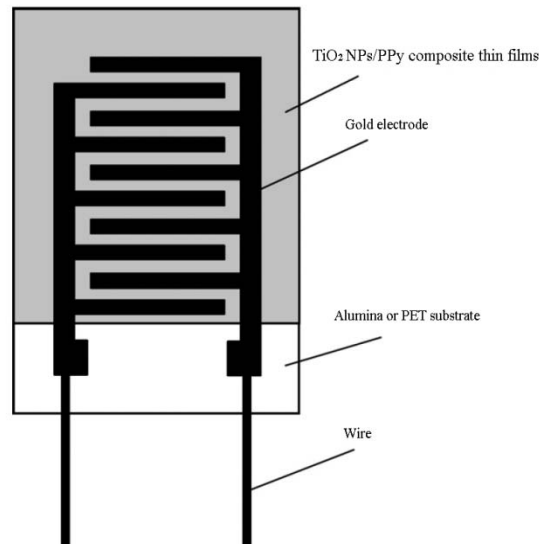


Fig. 1. Structure of humidity sensor.

In order to determine the humidity sensitivity of the humidity sensors, the resistance was measured as the humidity was increased from 30 % RH to 90 % RH at a constant temperature of 40 °C and a constant frequency of 1 kHz. Fig. 2 (a) represents responses curves of the humidity sensor samples 1-2-3-4, (b) represents responses curves of the humidity sensor samples 5-6-7 and (c) represents responses curves of the humidity sensor samples 8-9 [10-11].

3. Analytical Model SM

The experimental results were used [10-11] to create a database arranged as (Sub, Hys, T, F, TiO₂, PMA, H, Z), where Sub is the substrate sensing mechanism type, Hys is the hysteresis, T is the environment temperature in the measurement point, F is the applied frequency, TiO₂ is the TiO₂ concentration, PMA is the PMAPTAC concentration, H is the humidity applied to the SM, and Z is the SM response. Note here that, in our model, the input Sub takes the value of 0 for the alumina substrate and the value 1 for the PET substrate and the input Hys takes the value 0 for humidification and the value 1 for desiccation. In a second step we arrange the data into training, validation, and test subsets. One-fourth of the data are taken for the validation set, one-fourth for the test set, and half for the training set. The sets are picked as equally spaced points throughout the original data. It is important not to use any element of the test base and validation base throughout all training. These bases are reserved only for the final performance measurement [12].

3.1. Training

The training phase requires a database, selecting the network architecture and finding the numbers of layers and neurons in each layer. However, since the neuron numbers in the input and output layers are determined by the input and output numbers of the system to be modeled, the SM has 7 inputs and only one output Z “Resistance”, the input layer has 7 neurons and only one neuron for the output layer. So that the ANN model accurately expresses the SM response variation, it is a question of finding the optimal parameters (number of the hidden layers, number of neurons by layer and transfer functions), so we proceed as follows:

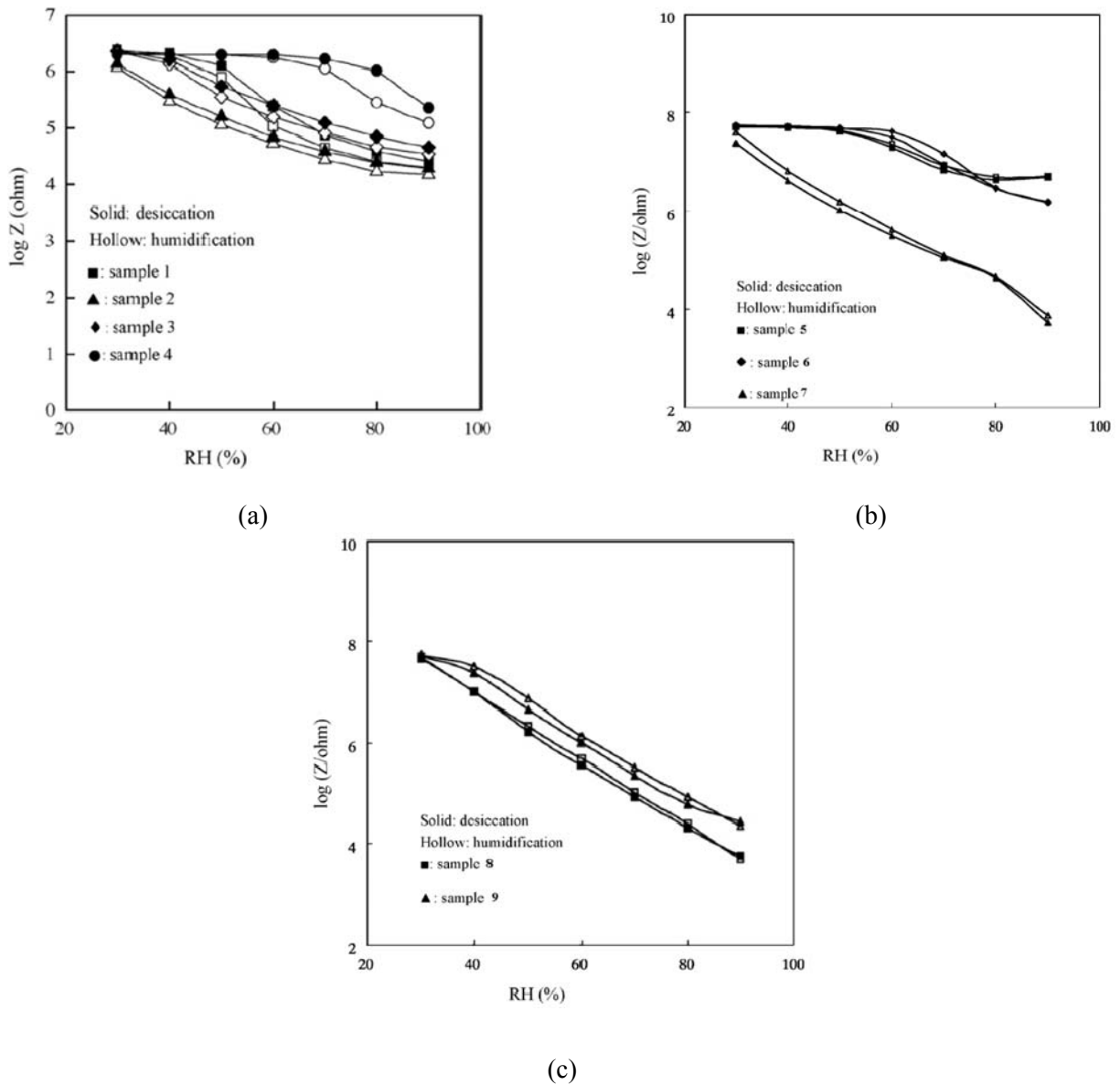


Fig. 2. Impedance vs. relative humidity (a) for samples 1–4 (b) for samples 5–7 (c) for samples 8–9 (compositions are shown in Table 1), measured at 1 kHz (Inset) The result of the sensor of Ref. [10, 11].

1. Divide the available data into training, validation and test set
2. Select architecture and training parameters
3. Train the model using the training set
4. Evaluate the model using the validation set
5. Repeat steps 2 through 4 using different architectures and training parameters
6. Select the best model and train it using data from the training and validation set
7. Assess this final model using the test set.

After many tests of different ANN models we considered MLP with two hidden layers, 13 neurons and the transfer function Logsig for the first layer, 17 neurons and the Transfer function Logsig for the second layer and the Transfer function Linear for the output layer. Fig. 3 (a) shows the symbolic notation of ANN optimized model and Table 1 summarized those parameters.

We have made the neuronal network training for the database with the back propagation (BP) algorithm; Fig. 3 (b) shows the program flowchart.

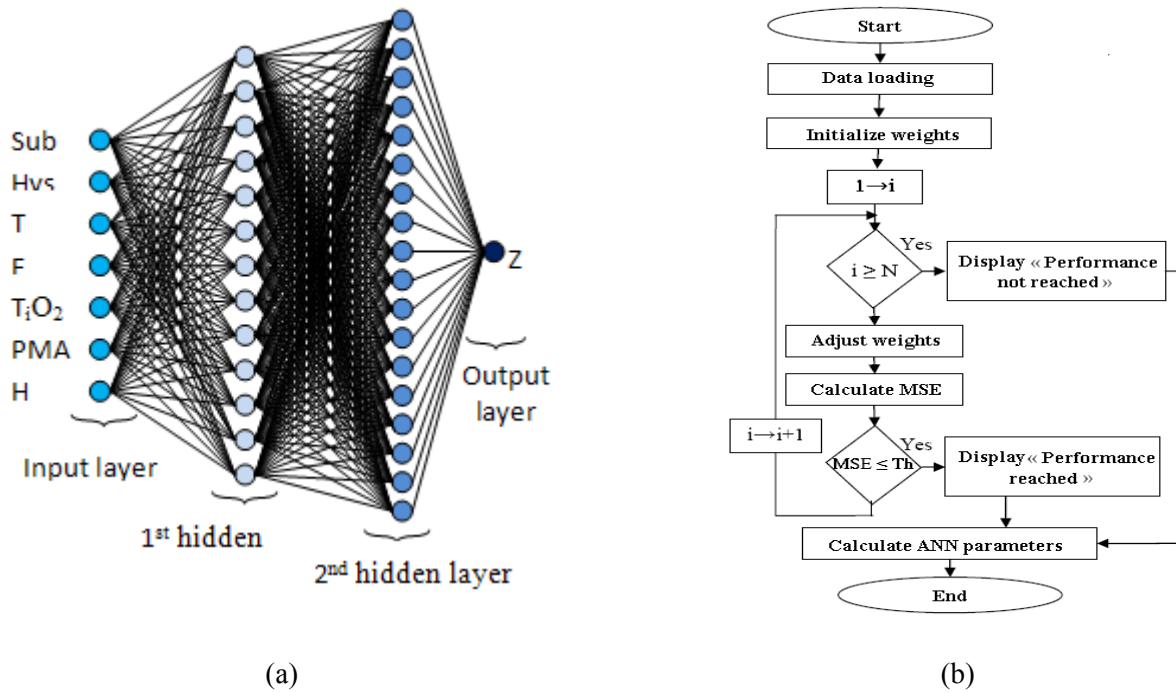


Fig 3. Symbolic notation of the ANN optimized model (a); Training program flowchart (b).

Note that the data loading is: training base, test base, number of layers and neurons, type of the transfer functions, number of iteration and estimate threshold. N is the number of iterations, MSE is the mean square error, T_h is the estimate threshold “Test MSE” and the ANN parameters are the neuronal network element (B_{ni} the bias matrix and W_{nji} the weights matrix). Finally we measure the model performance obtained with the test base.

Table 2. Optimized parameters of the neural networks model.

Database		Training base					21,600
		Test base					10,368
		Validation base					10,368
Number of Neurons		Input layer					7
		1 st hidden layer					13
		2 nd hidden layer					17
		Output layer					1
Transfer function		1 st hidden layer					Logsig
		2 nd hidden layer					Logsig
		Output layer					Linear
Input	In (unit)	T (°C)	F (kHz)	TiO ₂ (g)	PMA (g)	H (%)	
	Max	35	100	0.048	0.08	90	
	Min	15	1	0	0	30	
Output		log (Z/Ω)					
		Max					7.7598
		Min					1.9983
Training MSE		10 ⁻⁴ (chosen by the user)					
Test MSE		9.589 10 ⁻⁴ (given by the Matlab)					

3.2. Model Test

The comparison between the initial database and that obtained after the training, using the test base, indicates that our model expresses accurately the response variation of the RHSM. Fig. 4 presents the model performance obtained for the sample 1, measured at 1 kHz at fixed temperatures 15, 25 and 35 °C.

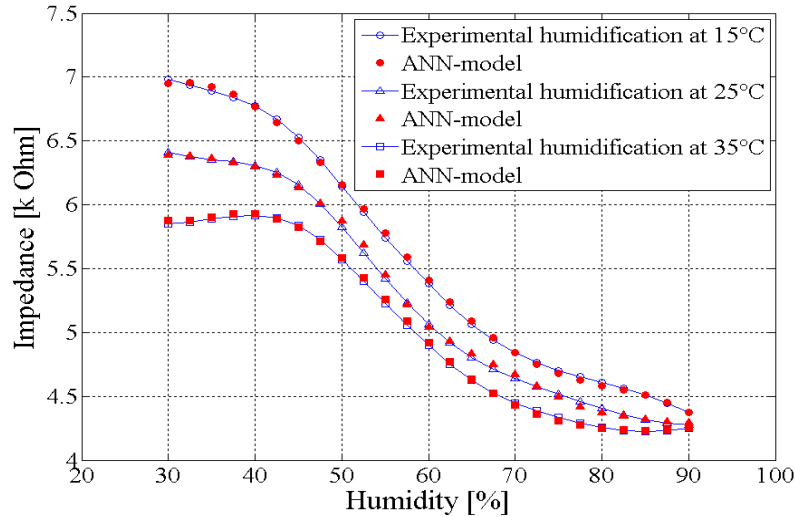


Fig. 4. ANN model performance for the sample 1, measured at 1 kHz at fixed temperatures 15, 25 and 35 °C.

4. Implementation ANN in PSPICE

The SM was modeled using the ABM (Analog Behavioral Modeling) of the PSPICE library, each neuron of the ANN is replaced by one ABM which is characterized by the neuron equation, for example, the ABM 1 equation is:

$$\text{out} = \frac{1}{1 + \exp\left(-\left(B_{11} + W_{111} \cdot V(\text{sub}) + W_{112} \cdot V(\text{Hys}) + W_{113} \cdot V(\text{T}) + W_{114} \cdot V(\text{F}) + W_{115} \cdot V(\text{PMA}) + W_{116} \cdot V(\text{TiO}_2) + W_{117} \cdot V(\text{H})\right)\right)} \quad (1)$$

The equation exponential form is due to the choice of the transfer function in the first hidden layer, B_{11} is the first bias of the first hidden layer in the bias matrix “ B_{ni} ”, W_{111} - W_{117} are respectively the first-the seventh weight for the first hidden layer in the weights matrix “ W_{nij} ”.

5. SM Validation

In order to validate the sensor introduced on PSPICE simulator, the SM is implemented in the electrical circuit as shown in Fig. 5(a) and the measurement circuit of sensor resistance is shown in Fig. 5(b). The sensor resistance R_s may be calculated with the equation:

$$R_s = \left(\frac{V - V_{RL}}{V_{RL}}\right) \times R_L = \frac{(V - V_{RL})}{I_{RL}} \quad (2)$$

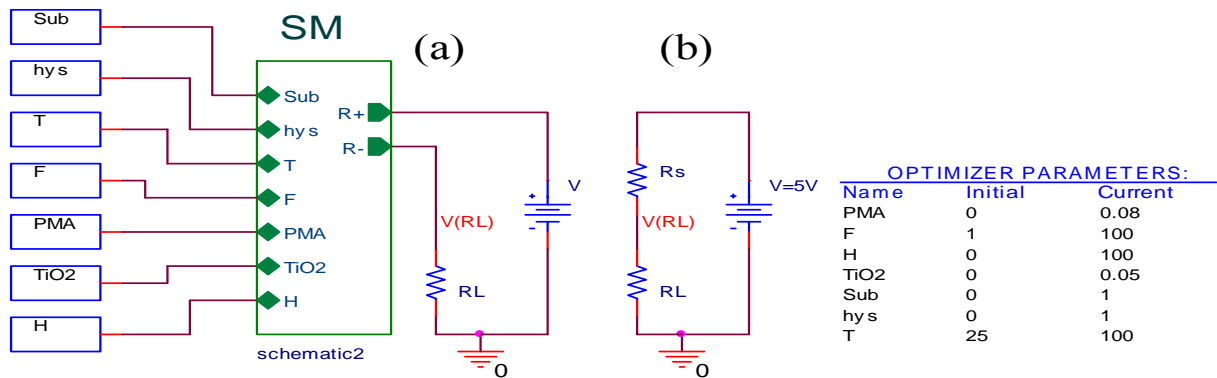


Fig. 5. The humidity sensor electrical circuit (a); the measurement circuit of the sensor resistance (b).

The temperature, the frequency and the PMA are fixed at 25 °C, 1 kHz and 0 (g) respectively when humidity is varying within the range 30 % to 90 %, for humidification (Hys=0) in the alumina substrate (Sub=0). A parametric SWEEP analysis, for the four concentrations values of TiO₂ 0, 0.0012, 0.0118 and 0.048 (g) (concentrations values of samples 1-4) gives the results represented Fig. 6(a).

A parametric SWEEP analysis, for the three temperatures 15, 25 and 35 °C, at fixed frequency of 1 kHz when humidity is varying within the range 30% to 90%, for the sample 1 in humidification, gives the results represented in Fig. 6(b).

The temperature, the frequency and the TiO₂ are fixed at 25 °C, 1 kHz and 0.048 (g) respectively when humidity is varying within the range 30 % to 90 %, for (Hys=1) in the PET substrate (Sub=1). A parametric SWEEP analysis, for the tow PMA concentrations values of 0.008 and 0.08 (g) (concentrations values of samples 8-9) gives the results represented Fig. 6 (c).

A parametric SWEEP analysis, for the three frequencies 1, 11 and 100 kHz, at fixed temperatures of 25 °C when humidity is varying within the range 30 % to 90 %, for the sample 9 in humidification, gives the results represented in Fig. 6(d).

These simulations indicate that our component, introduced in PSPICE simulator, expresses accurately the response variation of the SM compared to the [10-11] experimental results. Furthermore, this component can predict the responses for all temperature, frequency, hysteresis and different concentrations of TiO₂ and PMAPTAC.

6. Conclusions

In this paper, we have proposed an electrical circuit used to optimize the TiO₂ and PMAPTAC concentrations of a resistive humidity sensing mechanism. When the ambient temperature changes over a wide range, the nonlinear response characteristics of the SM undergo change in a complex manner. At different concentrations of TiO₂ and PMAPTAC, a data points from the sensor characteristics were obtained. Those data were then used to train the MLP model using the back propagation algorithm. After training, the MLP, our model is able to estimate the sensor's response for each substrate and hysteresis type, different TiO₂ and PMAPTAC concentrations, temperature values and frequency values. It accurately expresses the SM nonlinear characteristics and its dependence on temperature. After that we use the bias matrix and the weights matrix obtained by training to establish our models on PSPICE simulator, which verified the sensors responses, by simulations results. This model can also predict the SM responses, for different temperature, frequency, hysteresis and concentrations of TiO₂ and PMAPTAC.

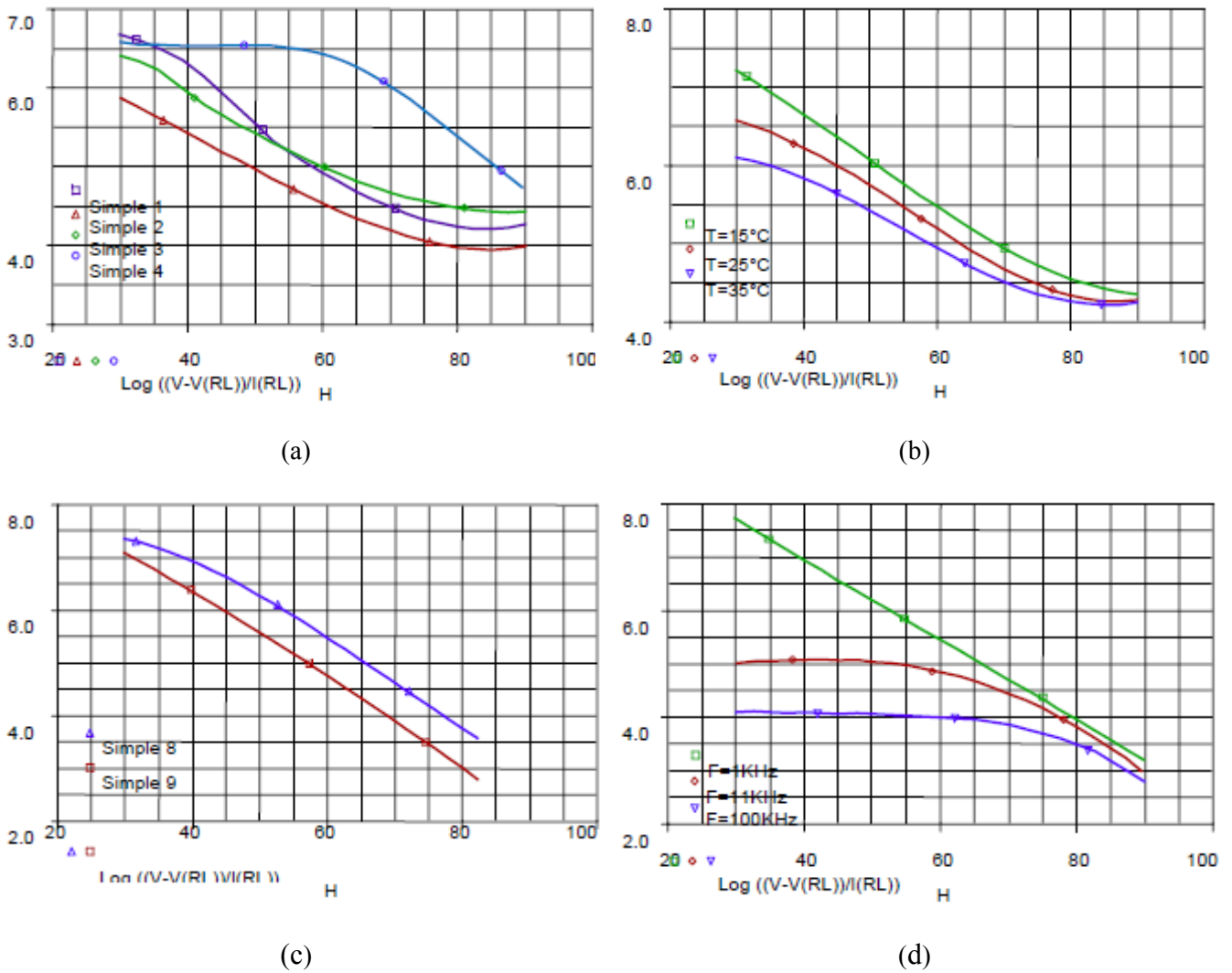


Fig 6. (a) SM output for a parametric SWEEP analysis for sample 1-4 at fixed temperature and frequency 25 °C, 1 kHz respectively (b) SM output for a parametric SWEEP analysis for the sample 1 at fixed frequency 1 kHz, for the temperatures 15, 25 and 35 °C (c) SM output for a parametric SWEEP analysis for sample 8-9 at fixed temperature and frequency 25 °C, 1 kHz respectively (d) SM output for a parametric SWEEP analysis for the sample 1 at fixed temperature 25 °C, for the frequencies 1, 10 and 100 kHz.

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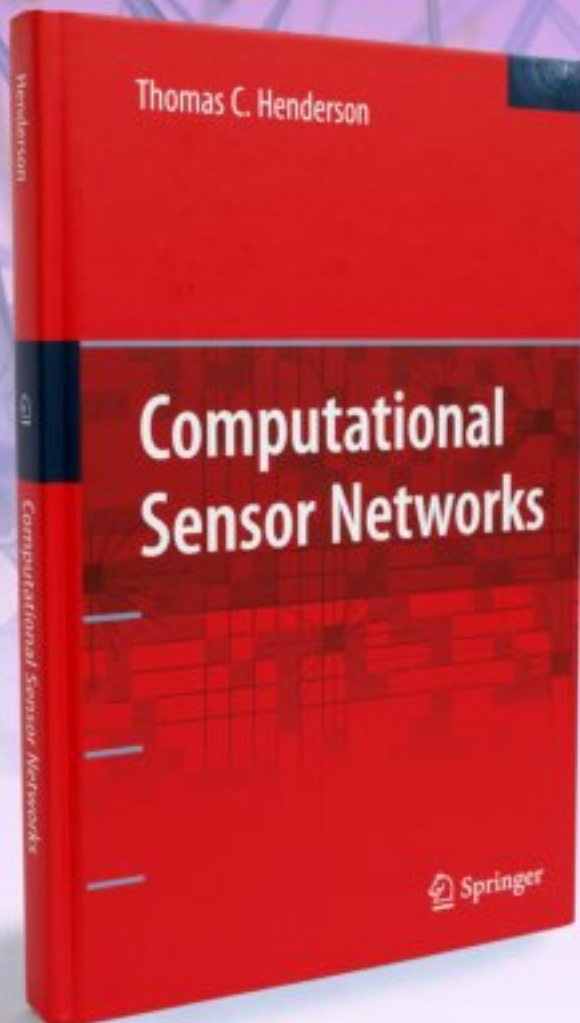
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