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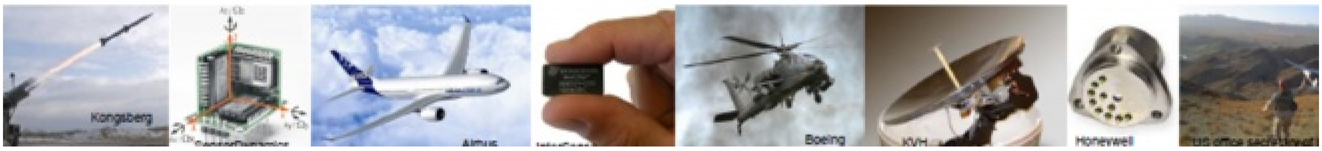
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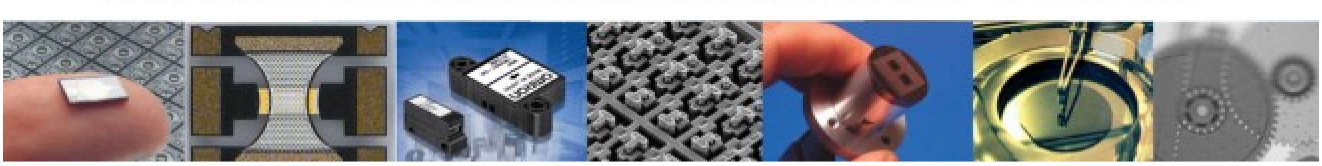

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Prediction of the Surface Oxidation Process of AlCuFe Quasicrystals by Using Artificial Neural Network Techniques

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Abstract: In this paper, we present a method to determine the inputs of a manufacturing process used in Microelectromechanical System (MEMS) that will drive its output to desired targets. This method uses a combination of artificial neural network (ANN) modeling and the inverse control together with optimization techniques in order to obtain the minimum error between the neural net results and the desired values. The problem aims to find the depth of thin film layer that we needed for the surface oxidation for the preparation of i-AlCuFe quasicrystals, which is the output of the process, by giving the percentage of oxygen concentration and temperature, which are the inputs of the process. The outputs are related to the inputs of the process by an artificial neural net model which is trained and tested with historical input-output data. The final results of the developed neural net model and the inverse control techniques show high level of the accuracy of the results. *Copyright © 2011 IFSA.*

Keywords: Artificial Neural Network, MEMS, Oxidation, Optimization, Quasicrystals, i-AlCuFe, Inverse control.

1. Introduction

Quasicrystal (QCs) are alloys whose structure is atomically well organized but not periodic [1]. Although the first quasicrystalline phase discovered in 1984 was metastable [2], Thermodynamically stable quasicrystalline have been obtained in 1986 [3]. Today, there are hundreds of quasicrystalline alloys have been discovered many of them contain aluminum and are of icosahedral phase, such as i-AlCuFe, where i noted to icosahedral phase. Also, nickel, titanium and zirconium are considered the basic element of the quasicrystalline alloys. Toxic and the cost play the important rule when selecting these elements in alloys. Cheap and absence of toxicity is the important factors of the choice of AlCuFe alloys.

The icosahedral phase of the AlCuFe alloy $(Al_{70}Cu_{20}Fe_{10})$ was identified in 1987 [4]. The i-AlCuFe alloy is considered as one of the reference material to understand and describe the position of the atoms in the bulk or on the surface of icosahedral structure. The quasicrystal alloys which are rich in aluminium have low electrical conductivity compared with the ordinary aluminum alloys at room temperature. Also, this conductivity is decreased with temperature, contrary to the behavior of metals [5]. They are considered as an excellent heat insulator. They are considered very brittle in bulk form low temperature up to a few hundred degrees below their melting point [6]. The brittleness is due to alloy structure, which is made up of clusters, and these clusters cannot be deformed. The preparation of quasicrystalline surfaces and the detailed steps for the oxidation are explained in [1] and [7] respectively.

In this paper we applied neural network techniques on the historical date, which is related to our studies, is obtained manually from [1], training and testing region are introduced for the data and the normalized data. We normalized data to improve accuracy. The normalized results are regenerated again to deal with the original data. We apply the neural net model again in order to improve the equality of the result. The inverse control technique is applied on the trained neural net model in order to predict input data by driving output. The inverse control method and optimization techniques are applied together to minimization the least square error between the neural net results and the desired values. The artificial neural networks (ANN) are a powerful method for modeling nonlinear system. System identification with neural networks has been applied to highly non linear industrial process [10]. The availability of an input-output ANN model for a complex process permits the design of a control law for that process as shown in the reference.

2 Process Used for Preparation of AlCuFe

The chemical vapor deposition (CVD), etching, and oxidation process are process for Microelectromechanical system (MEMS) fabrication which is used for preparation the i-AlCuFe$(Al_{70}Cu_{20}Fe_{10})$ alloys. The chemical vapor deposition process is based on the principle of initiating a chemical reaction in a vacuum chamber, resulting in the deposition of a reacted species on a heated substrate. The etching process is used to selectively remove material using imaged photo resist as a masking template [8].

The surface of the i-AlCuFe$(Al_{70}Cu_{20}Fe_{10})$ alloys performed on the ultra high vacuum (UHV) analysis chamber with introducing O_2 gas and controlling the temperature for the sample used. The rough cleaved surface resulted is polished by an etching and annealing procedure. This process must be carried out very carefully due to the instability of the surfaces and the sensitivity of the surface to the contamination. Thus optimal treatment conditions must be done. These conditions are limited ion etching energy, annealing temperature to avoid a surface recrystalization into a cubic phase at too low temperature or too high temperature. The ion etching is used in order to obtain chemically clean surface. Special techniques are used to satisfy it which is explained in [1]. Also, annealing after etching is necessarily to obtain a quasicrystalline surface with high quality surface. So, there is an optimum annealing temperature.

2. Growth of Oxide on i-AlCuFe Quasicrystal

The successive stages for the oxidation are summarized in [1] in three stages. First the chemisorptions stage begins corresponding to the oxygen adsorption without any clustering of the oxygen atoms and deformation of oxide. Then at room temperature is followed by nucleation and growth of the amorphous oxide. Finally, the aluminum surface atoms are oxidized and the surface is saturated in oxygen like aluminum. At very low oxygen pressure (2×10^{-6} *Pa*), the values of chemisorptions range obtained for the i-AlCuFe$(Al_{70}Cu_{20}Fe_{10})$ surface are similar to the values for pure aluminum (1 0 0), (1 1 0), and (1 1 1) faces. Fig. 1 shows the oxygen atomic concentration as a function of depth profile of i-AlCuFe layer measured in situ oxidation at various temperature under (5×10^{-5} *Pa*) and after exposure of 7200 L.

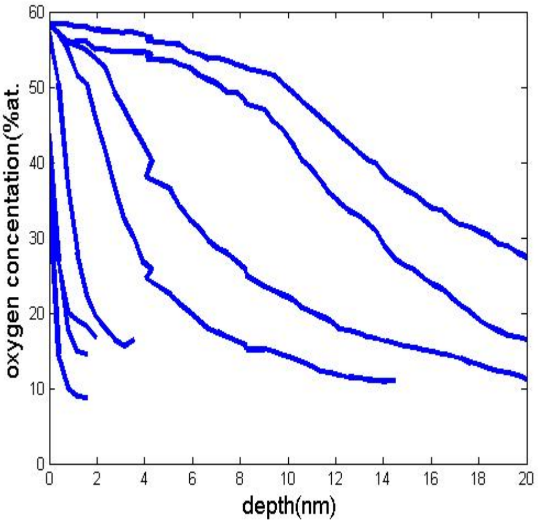

Fig. 1. Oxygen atomic concentration as a function of depth in i-AlCuFe measures after in situ oxidation at various temperature under (5×10^{-5} *Pa*) and after exposure of 7200 L.

3. Neural Network Modeling

Artificial neural networks were originally inspired as being model of human nervous system. Useful information and theories about ANN's can be found in [9]. The important point of the artificial neural net model is the ability to generalize from given training data to unseen data, and they learn from experience rather than by programming.

The data for the input and output of the model must be available. The input-output data enables the neural network to do their abilities such as training, testing and optimization in order to get the minimum error between the real output and the estimated output which resulted from neural net. Learning of a neural net is the process of adjusting the weights and biases by using training data until to obtain the minimum error between the actual and desired outputs. This method of learning which is used in this study is called supervised learning.

The basic model of a single artificial neuron consists of a weighted summer and an activation or transfer function as shown in Fig. 2. Where $x_1 ..... x_i$ are the inputs, $W_{j1} .....\ W_{ji}$ are the weights, B_j is a bias, F_j is the activation function, and Y_j is the output [11].

The weighted sum S_j is therefore

$$S_j(t) = \sum_{i=1}^{N} W_{ji}\, x_i(t) + B_j \tag{1}$$

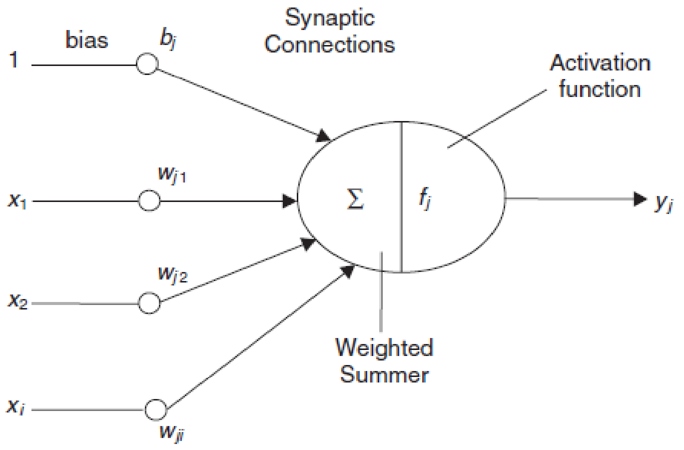

Fig. 2. Basic Model of a Single Artificial Neuron.

The neural net structure consists of inputs feed ward through a hidden layer to the output. The hidden layer contains processing units called nodes or neurons as shown in Fig. 3. Each neuron is described by a nonlinear sigmoid function. The interconnections between input, hidden layer, and the output are associated with a multiplicative parameter called weight. The feed ward neural nets that are considered consists one hidden layer. An artificial neural net mathematical model that represents the stricture shown in Fig. 3 is written as

$$Y = f(U) = W_o * \tanh(W_i * U + B_i) + B_o \tag{2}$$

where Y is the column vector which contains the q outputs, U is the column vector that contains the P inputs of the process, W_0 is the matrix of size $q \times n$ that contains the weight of the neural net model from the hidden layer to the output where, n is the number of the neurons in the hidden layer, W_i is the matrix of size $n \times p$ that contains the weight of the neural net model from the inputs to the hidden layer, B_i is the column vector of size n that contains the biases from the inputs to the hidden layer and B_0 is the column vector of size q that contains the biases from the hidden layer to the outputs. The weights and biases of the ANN are determined by the training the historical input –output data. The available data is divided into two parts: the first part is used to train the net, and the second is used to test the performance net. The number of hidden neurons n is play rule of the performance of the neural net over the training and testing sets of data. The number of nodes is selected such that the best result of the training and test region are obtained.

4. Inverse Controller

The basic idea from the inverse control is the optimization. This means how to obtain the input data from the given output such that the minimum error is obtained. This technique is based on back propagation algorithm. The back propagation algorithm is a supervised learning method for training artificial neural nets. It uses gradient-descent optimization method (delta rule).In this paper we deal with the process whose data are available.

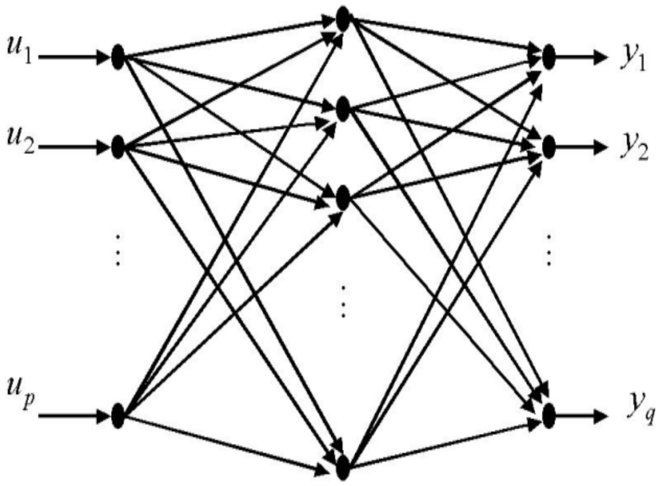

Fig. 3. Neural Net Structure.

Firstly, we modeled the process with artificial neural net based on feed forward techniques by training the data until to obtain the acceptable performance. Then we apply optimization techniques to get the input data, when we drive its output results. The output result will compared with the target values until to get acceptable error. This process is shown in the Fig. 4. The desired values are passed to the inverse controller. The output from the inverse controller is U which is the input of the process. This is done such that the output Y from the neural net is as close as possible to the real output Y_r. The controller operation is characterized by minimizing a positive function. This function is measure the difference between the model output and its desired values. If there is a set of inputs at which the function is equal to zero, which is the minimum value then this is an optimum input. Generally the output is not equal to its target at the initial inputs. The inverse control algorithm is explained in [9].The form of the function which is used for optimization method is

$$J = \sum_{i=1}^{q} (d_i - y_i)^2 \tag{3}$$

where y_i is the ith output of the net, d_i is the desired value of the ith output. Note that the J function is non-negative and is equal zero if and only if all q outputs are equal their desired values.

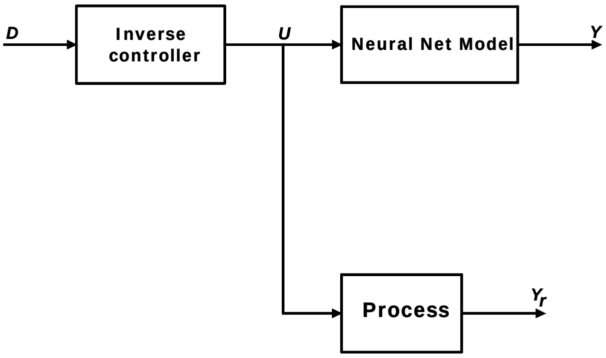

Fig. 4. Inverse Controller.

Since the outputs are functions of the process inputs through the neural net model representation in equation (1). Now, in order to derive the outputs as close as possible to their target we need to minimize the function J. Thus an optimization technique is applied to this case to obtain the best results.

5. Application

In this paper, the data used is consists of the surface oxidation, thin film layer thickness of AlCuFe quasicrystals, and the temperature. Such that the input parameter is the temperature and percentages of oxygen concentration while the output is the depth layer (nm) of the surface oxidation. The input - output data used which is obtained from previous study is represented in Fig. 1. The data used contains 200 patterns, each pattern includes two inputs, and corresponding one output. The input one represents the temperature, while the other input is the percentage of oxygen concentration. The range of temperature used is between (500-700) degree Celsius, whereas the range of oxygen concentration is between (0-60) %.

The number of data is divided into two set, training set and testing set. The number of patterns used for the training the neural net model is one hundred and sixty are used to train an artificial neural net, while forty patterns are used to test the net performance. This training and testing the model was done based on the Matlab software. We try different number of hidden neurons to get the best result.

The accuracy of the results depends on number of hidden neurons. The number of hidden neuron which chosen to generate the model is seven which is acceptable least square errors over the training and testing set. The real and predicted ANN values for training and testing are shown in Fig. 5 - 7 respectively .The performance of the neural reach up to 0.105974 as shown in Fig.7.

In order to increase the performance of the neural, we normalized the input-output data. Fig. 8 and 9 shows the training and testing of the normalized neural net, which shows high level of performance. The performance reaches up to 0.0523479 as shown in Fig.10. So we generate the output results from normalized model. The output normalized results are regenerated to get the equivalent values of un normalized output data. Now, we regenerate the ANN model again by using the modified data which is regenerated from normalized neural model. Fig. 11 and 12 are the real and predicted ANN values for training and testing of the modified neural net model. The performance of modified neural net model is reached up to 0.000211491 as shown in Fig.13, which accurate before normalization.

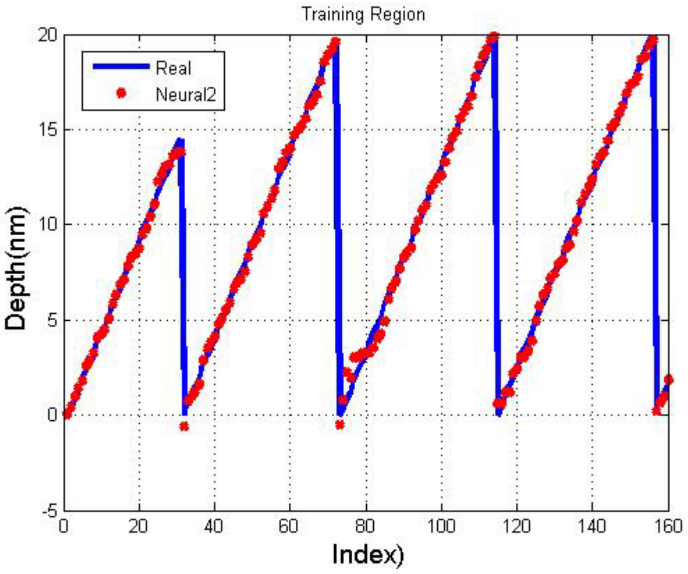

Fig. 5. Neural Net Training Results.

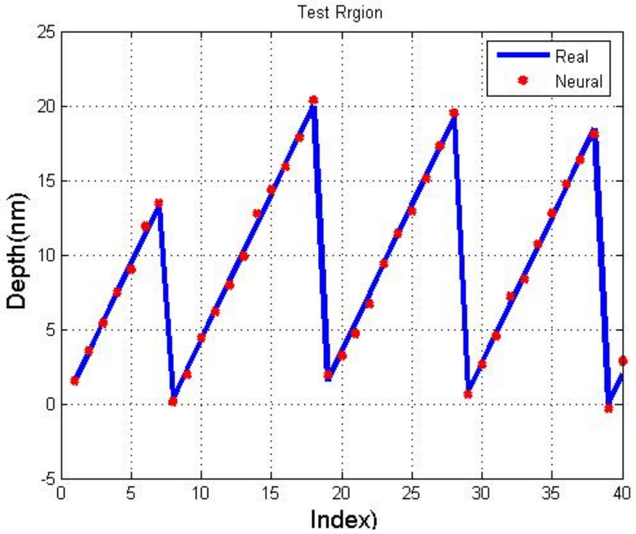

Fig. 6. Neural Net Testing Results.

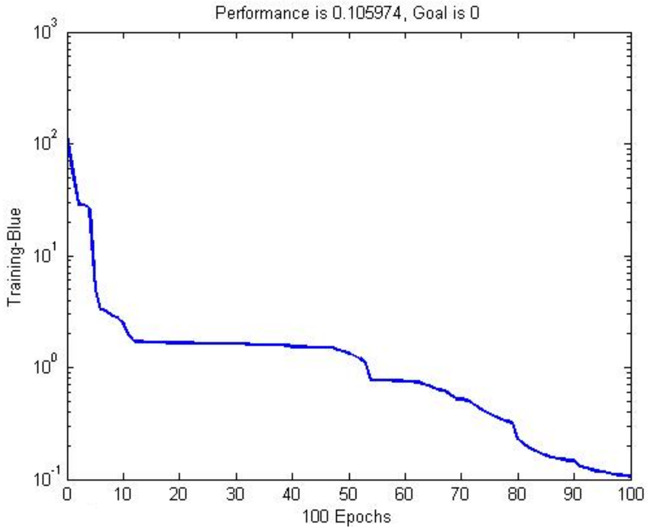

Fig. 7. Performance of Neural Net Before Normalizing Data (Raw Data).

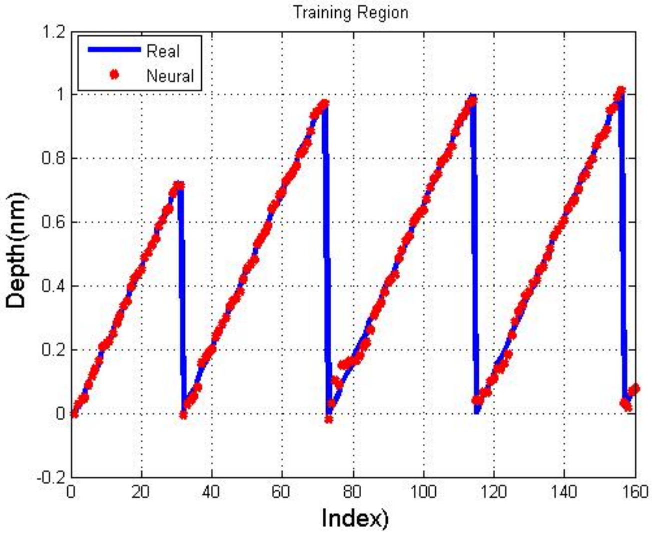

Fig. 8. Neural Net Training Results Normalized.

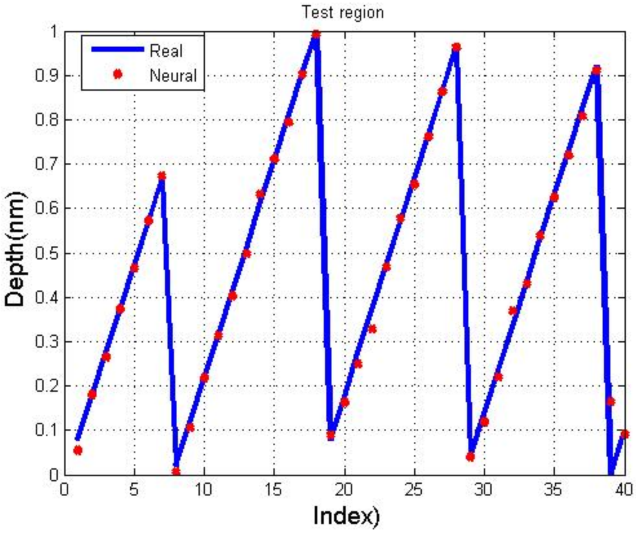

Fig. 9. Neural Net Testing Results Normalized.

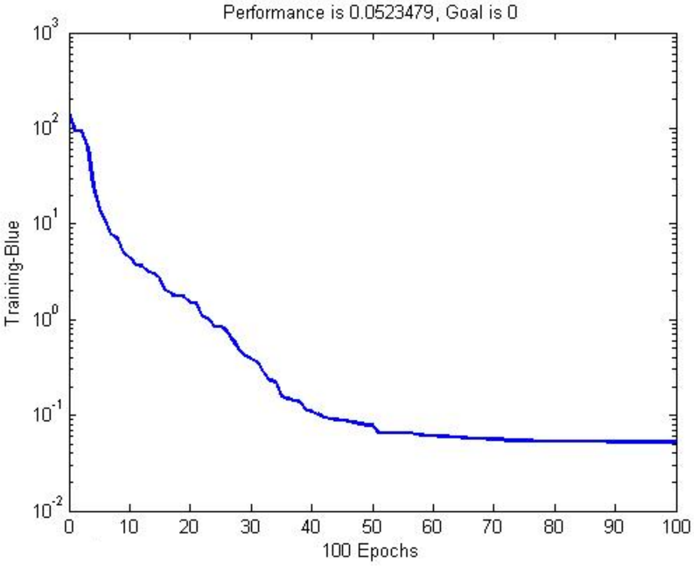

Fig. 10. Performance of Normalized Neural Net.

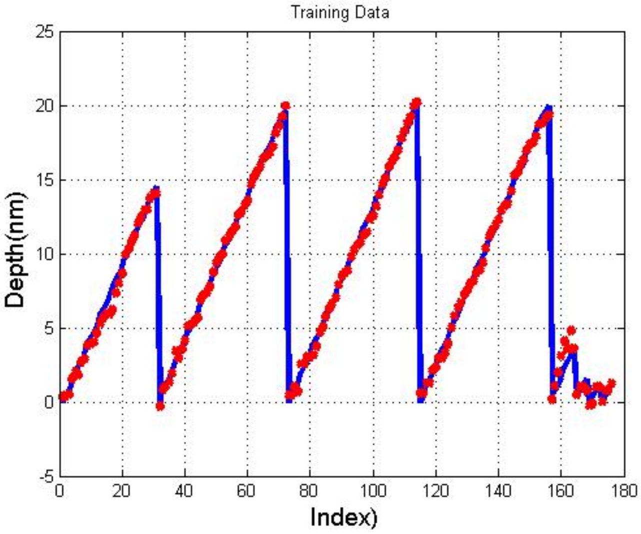

Fig. 11. Modified Neural Net Training.

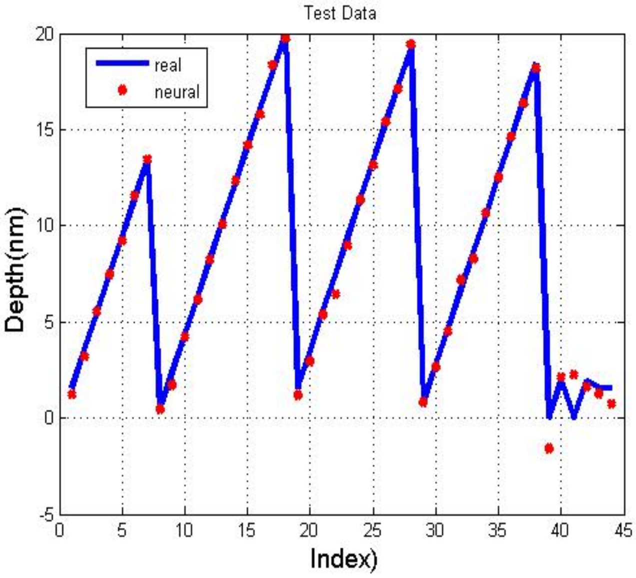

Fig. 12. Modified Neural Net Testing.

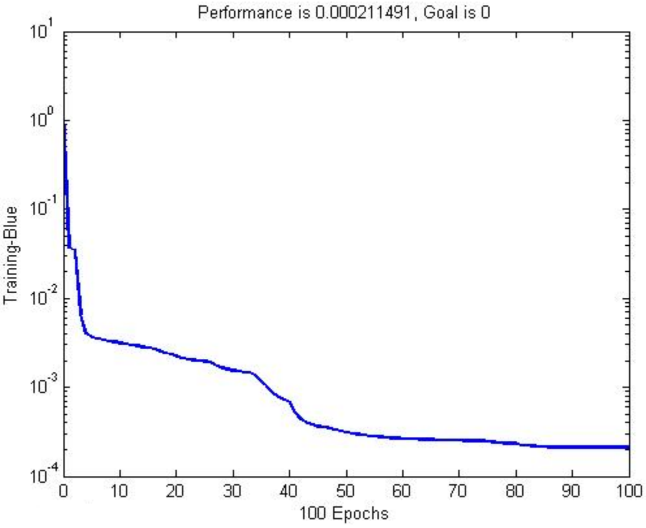

Fig. 13. Performance of Modified Neural Net.

The controller goals in this process is to predicted the temperature needed and the percentage of oxygen concentration that will satisfied the desired value which is the depth of layer(nm) of surface oxidation. Such that the minimization error between the neural result and the target values is acceptable.

For example, for the depth layer of surface oxidation is 16 nm, the inverse controller calculates the temperature and the percentage of oxygen concentration are 631.9683 degree Celsius and 30.8618 % respectively with the corresponding neural output is 15.9488 (depth layer), which are very close to the one obtained from the original data. The input data obtained from optimization is compared with the original input at the depth layer 16 nm. This is plotted versus the counter to get the minimum error, which is equal to 0.3203 % which is acceptable quality results as shown in the Fig. 14.

Table 1 shows the corresponding adjusted weight and bias of the neural net model from the input to the hidden neurons and from the hidden neurons to the output. This data can be used in the equation number (1).

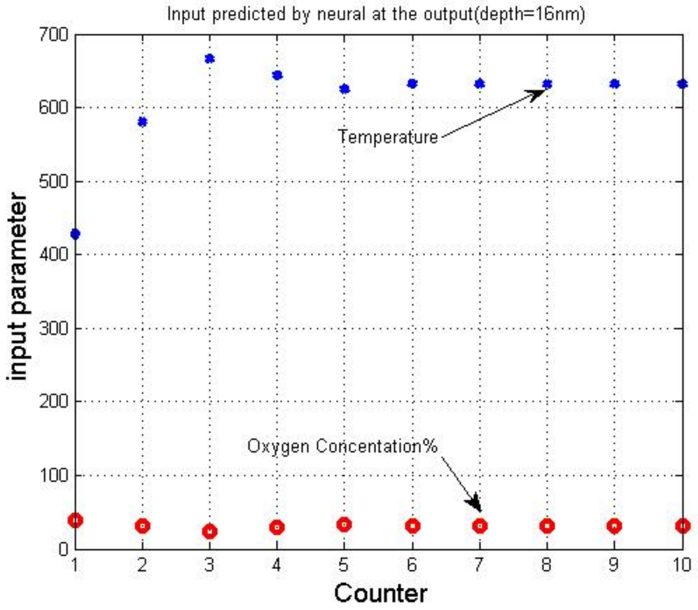

Fig. 14. Predicted Values of Inputs Compared to the Original Inputs.

Table 1. Weights and Bias of the Neural Net Model.

Bias	**Weight of the data**		
	Input (2)	**Input (1)**	**Output**
-18.153	18.0558	-0.98064	-18.153
-0.9895	21.12078	3.729177	-0.9895
-11.6309	8.741881	4.721126	-11.6309
2.2483	11.58599	-14.4403	2.2483
-9.5082	-0.52025	16.11603	-9.5082
16.0813	-11.3754	-7.12925	16.0813
14.3383	-6.2166	-25.5039	14.3383
0.0415	-4.73596	13.99471	0.0415
-10.3766	7.398972	8.691315	-10.3766
7.9679	-4.27194	-6.75831	7.9679
3.3212	2.530468	-19.9143	3.3212
3.9444	-6.1627	7.158905	3.9444
-1.0197	13.04239	-12.1503	-1.0197
3.835	-12.0154	-8.52052	3.835
-8.9043	7.250241	5.768504	-8.9043
4.7373	2.092383	-7.10938	4.7373
7.1655	-11.4701	0.235358	7.1655
10.1169	6.303763	-9.71357	10.1169
12.0104	-17.5355	8.741537	12.0104

6. Conclusions

The neural net model is developed based on the historical data that is generated manually. This data is related to the manufacturing process of i-AlCuFe quasicrystals used in MEMS. The data consists of two inputs and one output. The input data are the temperature and the percentage of oxygen concentration. While the output is the thickness of layer of the oxidation. The training and testing model is built for the un normalized data (original data) based on the feed forward. The normalization of the data is used to increase the equality of the performance. Then regenerated the normalized data to get the un normalized data in order and apply the training and testing model again. This model after modification is used for the inverse control in order to the best optimization for the result. The inverse control predicts the input data which is the temperature and the percentage of oxygen concentration by passing the output which is the minimum thickness of layer.

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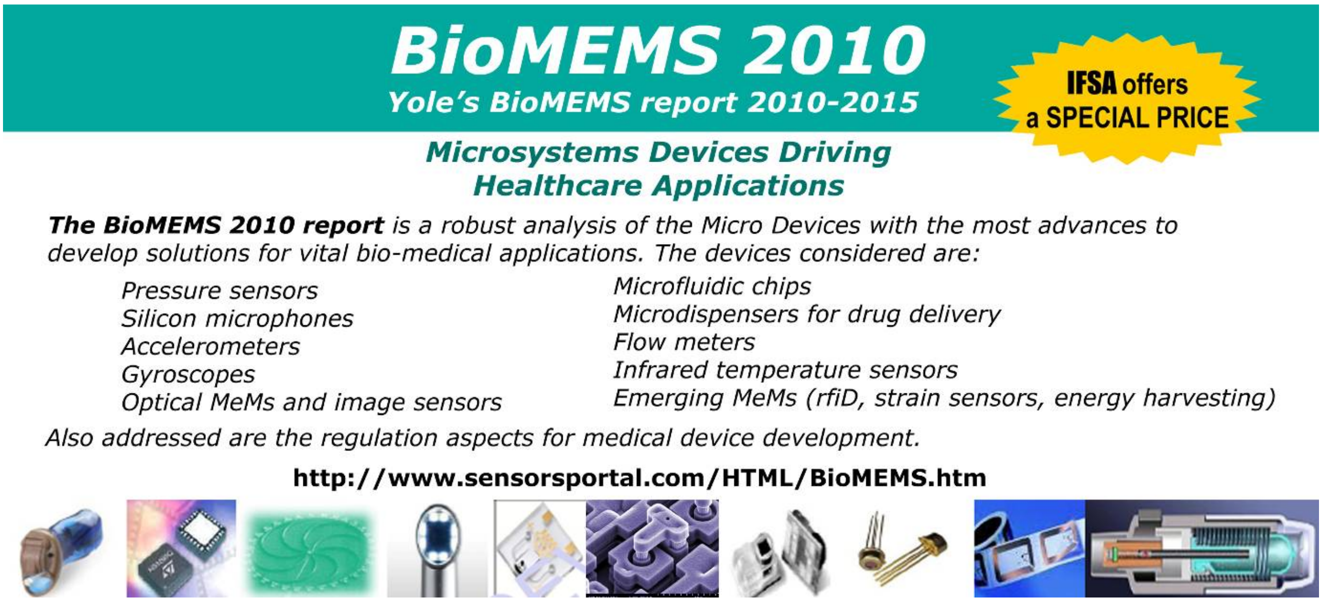

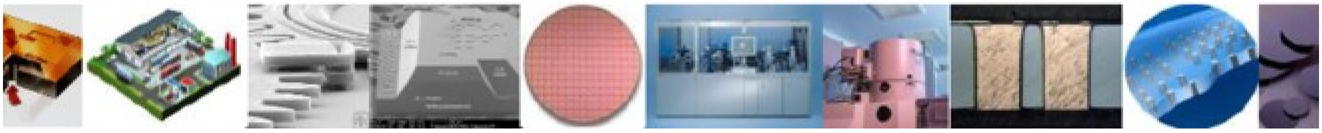

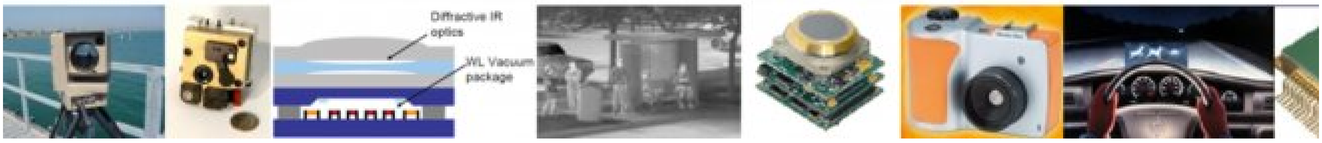
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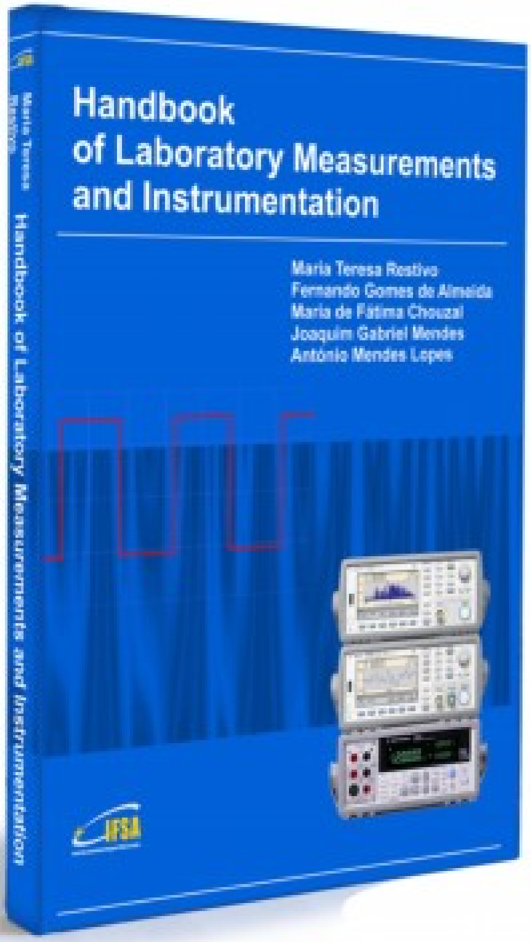
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