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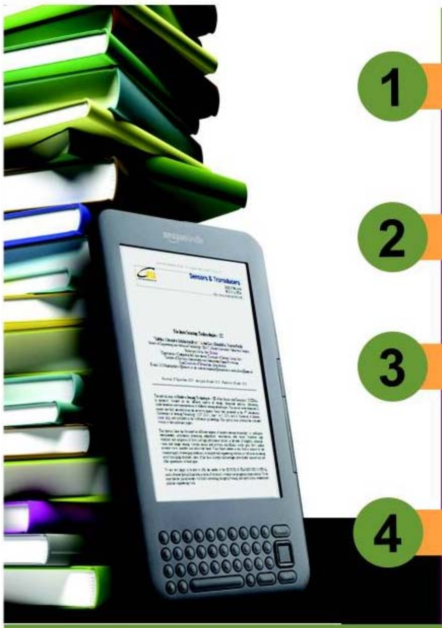


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Neural Net Based Optimization of Wet Thermal Lateral Oxidation Rates

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Abstract: Critical parameters, AlAs mole fraction, temperature of the sample and the carrier gas flow must be controlled to establish a repeatable and uniform oxidation process. Modeling and simulation of these parameters has enabled the compilation of oxidation rate data for AlGaAs which exhibits Arrhenius rate dependence. The output is related to the inputs of the process by an artificial neural net model which is trained with historical input-output data. The data is originally extracted and manipulated from experimental laboratories measurements. The proposed method is tested through computer simulation and the results demonstrate the effectiveness of the code and the algorithm. The objective of this study is the prediction of lateral oxidation rates at variances of temperature and mole fraction for different compositions. This is done through optimization techniques.
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Keywords: Experimental measurements, Neural networks, Optimization, Modeling, MEMS lateral oxidation.

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1. Introduction

In many cases of micro fabrications, oxidation plays vital role to complete a design at an efficient manner. There is a need to calculate the inputs such as sample temperature and mole fraction to a process of lateral oxidation that will drive its output of lateral oxidation rate in a desired way and thus achieve some optimum (desired) goal [1]. In such applications the model could be based on the physical phenomena or available historical and experimental input-output data from previous robust studies. Once the model is developed, optimization techniques can be applied to determine the inputs to the process that will satisfy a certain given criteria.

One of the examples of micro fabrication processes for which modeling and optimization research have been conducted is manufacturable compound oxidation process [2]. Data is available from experimental significant study which discusses vertical –cavity surface –emitting laser (VCSEL) performance that has been realized by employing wet thermal oxidation of selected AlxGa1-x layers in the device structure to form the current apertures and to provide the lateral index guiding for the lasing mode [1, 3]. The data is shown graphically in the Fig. 1. Neural net based optimization will be applied to this data.

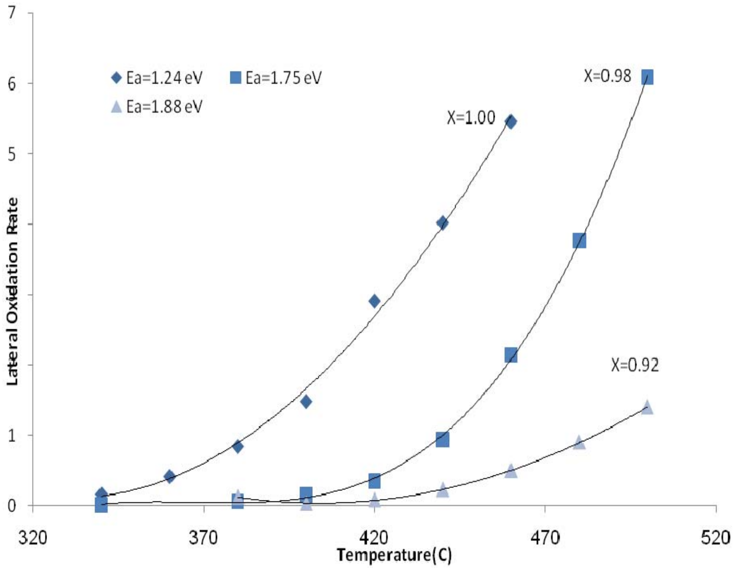

Fig. 1. Lateral oxidation historical data.

This paper considers the inverse control or optimization problem of a two-input one-output process whose historical input-output data is already available. The objective of the controller is to determine the set of inputs that will drive the output of the process to its desired target value. The available process data is used to train an artificial neural net (ANN) model with one hidden layer which gives a good approximation for continuous functions [4]. Control techniques can be applied to an ANN model since it is an input-output mathematical description of a system. To achieve our objective of obtaining the process output at its desired target value we build a positive cost function that measures the difference between the ANN output and its corresponding target value. We then use a modified version of the complex method constrained optimization of [5] to minimize the cost function. The resultant group of inputs will drive the ANN output as close as possible to its target value. An accurate ANN approximation is important and essential in assuring that the controller achieves its objective. The presented minimization algorithm offers the feature that it can be applied to a subset of the inputs which gives the freedom for setting the remaining inputs at values that satisfy other system requirements. ANN’s are practical for nonlinear systems that are complex and difficult to identify based on the physical phenomena such as oxidation processes. System identification with neural networks has been applied to highly nonlinear chemical processes [6] where the availability of an input-output ANN model for a complex process allows the design of a control law for that process. Furthermore, in [7] prediction of surface oxidation process of AlCuFe quasicrystals was carried out using artificial neural networks and optimization techniques.

Research on using ANN's for control can be found in [8]. It was also shown in [9] that the inverse model can be learned by an artificial neural network. Our approach computes the inputs to a process based on the forward (input to output) neural net model. This is done using constrained optimization techniques. An advantage of the method is that it keeps the forward ANN which is obtained from the computationally expensive training and can be re-used for other purposes such as prediction and adaptive control. The developed algorithm is tested on the wet thermal lateral oxidation process. The simulation results demonstrate the effectiveness of the inverse controller or optimization algorithm.

2. Oxidation System Configuration

The wet thermal oxidation system consists of a simple breaker on a hot plate with crude gas flow control, a single zone tube furnace to a constant temperature bubbler bath, a mass flow controller and a tube furnace. The schematic diagram of the system shown in Fig. 2.

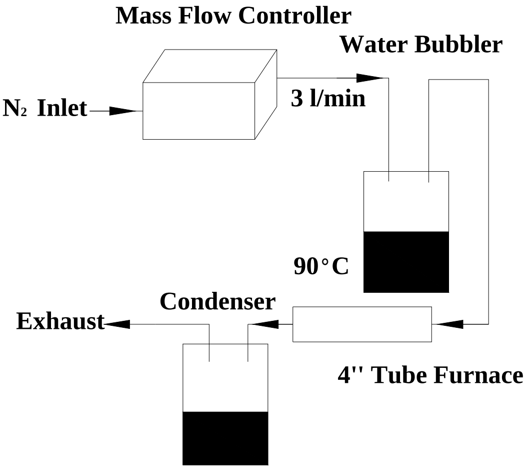

Fig. 2. A schematic diagram of the compound semi conductor oxidation system.

The amount of water vapour that can be transferred into the Nitrogen gas stream is proportional to the water temperature in the bubbler. This effect yields to the change in oxidation rate with a change in the bath temperature. Oxidation rates were obtained in the system by using 850 nm VSCEL (vertical cavity surface emmiting laser) structures grown with a single 1/4 wavelength thick high Al content layer (98 %) near the active region. The samples were grown using EMCORE Gs3200 metal organic vapour phase epitaxy rotating disc reactor which provides extremely good uniformity on a cross 3'' wafer and good accurate oxidation rate [1]. A typical monolithic oxide –confined VCSELs structure produced at Sandia National Laboratories uses an AlAs mole fraction of 92 %, 98 % and 100 % for the buried oxide aperture. Typical oxidation extents for VCSEL range from 10-50 µm. Finally the stability of bubbler temperature, gas flow calibration and good control should be the minimum requirements to insure repeatable and uniform oxidation for VCSEL fabrication.

3. Neural Net Modeling

Artificial neural networks were originally inspired as being models of human nervous system. They have been shown to exhibit many abilities, such as learning, generalization, and abstraction [10]. Useful information and theory about ANN's can be found in [11]. These networks are used as models for processes that have input-output data available. The input-output data allows the neural network to be trained such that the error between the real output and the estimated (neural net) output is minimized. The model is then used for different purposes among which are estimation and control. The neural net structure is shown in Fig. 3.

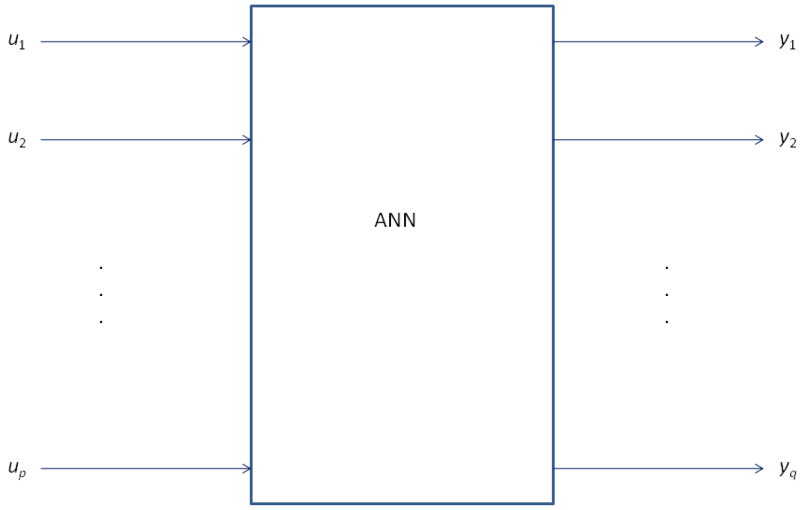

Fig. 3. Neural net structure.

The inputs feed forward through a hidden layer to the outputs. The hidden layer contains processing units called nodes or neurons. Each neuron is described by a nonlinear sigmoid function. The inputs are linked to the hidden layer which is in turn linked to the outputs. Each interconnection is associated with a multiplicative parameter called weight. Note that the feed-forward neural net of Fig. 3 has only one hidden layer and this is the case that we are going to consider. A number of results have been published showing that a feed-forward network with only a single hidden layer can well approximate a continuous function [12]. In practice, most of the physical processes are continuous. However, the results of this paper can easily be extended to include multi layer neural networks. An artificial neural net mathematical model that represents the structure shown in Fig.3 is written as:

$$Y = f(U) = W_o \tanh(W_i U + B_i) + B_o \,, \tag{1}$$

where, Y is a column vector which contains the q outputs of the process, U is a column vector that contains the p inputs of the process, W_o is a matrix of size qxn that contains the weights of the neural net model from the hidden layer to the outputs with n being the number of neurons in the hidden layer, W_i is a matrix of size nxp that contains the weights of the neural net model from the inputs to the hidden layer, B_i (not shown in Fig. 3) is a column vector of size n that contains the biases from the inputs to the hidden layer and B_o (not shown in Fig. 3) is a column vector of size q which contains the biases from the hidden layer to the outputs. Each input u_j, j=1,2,…p has lower and upper bounds, Lb_j and Ub_j, respectively. These bounds are calculated from the available input-output data. Lb_j is the minimum value of the jth input over the given input data whereas Ub_j is the maximum value of the jth input over the same data. If all the inputs lie within their lower and upper bounds then the estimated output by the ANN should lie within the given output data range. The output bounds are dictated by the ANN and the input bounds. The weights and biases of the ANN are determined by training with the historical input-output data. Back propagation is an example of a training algorithm. The available data is divided into two parts: one part is used for training the net whereas the other usually smaller part is used to test the performance of the ANN. The number of hidden neurons n affects the performance of the neural net over the training and test sets of data. More neurons make the fitting of data more accurate over the training region. It is more important to check the generalization performance of the model over the test set of data since it was not used to calculate the parameters of the model. The number of nodes is usually chosen by trying different values and selecting the one that gives best results over both the training and test regions.

4. ANN Based Optimization

The optimization of a process is to find the inputs to that process that will drive its output as close as possible to a given desired value. In order to solve this problem a mathematical model of the process is needed. In this paper we deal with processes whose historical input-output data are available. We model the process with artificial neural networks. Optimization techniques are then used to determine the inputs to the process that will drive its output as close as possible to the given desired goal. Fig. 4 illustrates these ideas. A desired signal *D* is passed to the optimizer. The optimization algorithm determines the input signal *U* to the process such that the output *Y* of the neural net model is as close as possible to the desired signal *D*. In other words, the error *E* represented by the difference between the desired signal and neural net output is minimized. The capability of the algorithm in producing a real output as close as possible to the desired value *D* depends on the accuracy of the neural net model which is measured by the error E_r, namely, the difference between the neural net and real outputs.

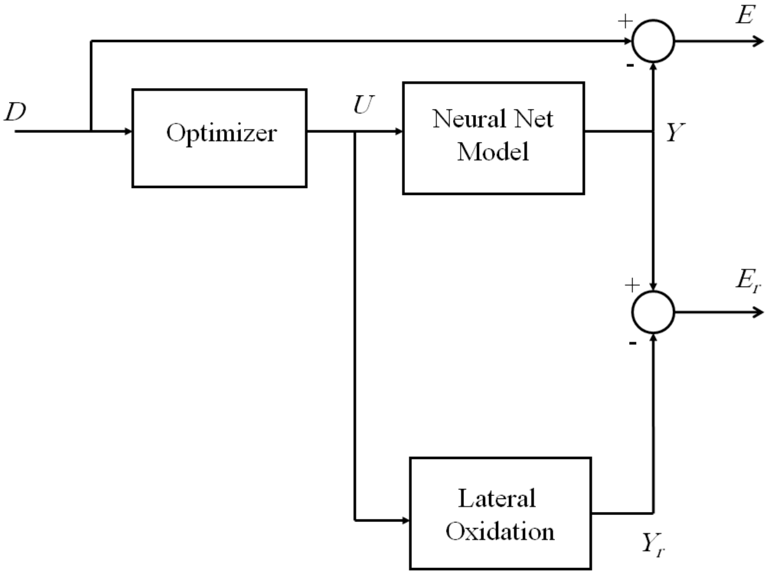

Fig. 4. Optimization algorithm demonstration.

The optimizer operation is characterized by minimizing a positive cost function that measures the differences between the ANN model outputs and their desired values. If there is a set of inputs at which the cost function is equal to zero (minimum) then this is an optimum input. Generally speaking, the output is not equal to its target values at the initial inputs. Thus, the optimizer coordinates the inputs or part of them to achieve the desired output if possible. Optimization over a subset of the inputs is a feature of the developed algorithm that leaves the freedom to the user to determine the remaining inputs such that other essential requirements of the process are met. Given a neural net model of a process in the form given in equation (1), we define the cost function *J* as the weighted sum

$$J = (D - Y)^2 \tag{2}$$

The cost function is expressed explicitly in terms of the model output. However, since the output is a function of the process inputs through the neural net model representation given in equation (1), the cost function is expressed implicitly in terms of the inputs. Note that the cost function J is non-negative and is equal to zero if and only if the output is at its desired value. In order to drive the output as close as possible to its target value we need to minimize J. Optimization techniques are best in tackling such a problem. We are now ready to define our optimization problem: Given a process with p inputs and one output and a neural net model for this process. Assume that pc of the p inputs (pc is less than or equal to p) are allowed to change by the controller. These are called the control inputs. We denote the vector that contains the control inputs by U_c . It is required to minimize the cost function J subject to the following constraints

$$Lb_i \le U_i \le Ub_i \text{ , } i = 1,2,\cdots, p \tag{3}$$

We will use a modified version of the complex method [5] to solve this optimization problem. The complex method was proposed as a better alternative to the simplex direct search-method. The considerations that led to the simplex modification are: 1) the destruction of the regularity of the simplex, 2) many of the points of the regular initial simplex will be infeasible, and 3) the points must be generated sequentially rather than being essentially simultaneously defined using the formula for the regular simplex. It was proposed that the set of M trial points be generated randomly and sequentially. p samples are required to define a point in p dimensions. Each newly generated point is tested for feasibility, and if infeasible it is retracted toward the centroid of the previously generated points until it becomes feasible. The total number to be used, M, should be no less than p_c+1 but can be larger. The optimization algorithm can be summarized as follows:

Given an initial strictly feasible point U^o (set of inputs), reflection parameter α, and termination parameters ε and δ.

1) Generate the initial set of M feasible points. For each point $m = 1,\ldots,M\text{-}1$,
(a) Sample p_c times to determine the point U^m. Note that the inputs that are not allowed to change are left constant at their initial values.
(b) If U^m is infeasible, calculate the centroid U_a of the current set of points and reset.
$U^m = U^m + \frac{1}{2}\left(U_a - U^m\right)$ Repeat until U^m becomes feasible.
(c) If U^m is feasible, continue with (a) until M points are available.
(d) Evaluate $J(U^m)$, for $m = 0,1,\ldots,M\text{-}1$.

2) Carry out the reflection step.
(a) Select the point U^R such that

$$J(U^R) = \max J(U^m) \equiv J_{\max}$$

(b) Calculate the centroid U_a and the new point

$$U^n = U_a + \alpha(U_a - U^R)$$

(c) if U^n is feasible and $J(U^n)$ is greater than or equal to $J_{\max}$, retract half the distance to the centroid U_a. Continue until $J(U^n)$ becomes less than $J_{\max}$.
(d) If U^n is feasible and $J(U^n) < J_{\max}$, go to step 4.
(e) If U^n is infeasible, go to step 3.

3) Adjust for feasibility
(a) Reset violated variable bounds:
If $u_i^n < Lb_i$, set $u_i = Lb_i$.

If $u_i^n > Ub_i$, set $u_i = Ub_i$.

Note that the subscript *i* denoted the i^{th} input. This step will be applied only to the control inputs since the other fixed inputs are set within their constraints initially.

(b) If the resulting U^n is infeasible, retract half the distance to the centroid. Continue until U^n is feasible, then go to step 2 (c).

4) Check for termination.

(a) Calculate

$$\overline{U} = \frac{1}{M}\sum U^m \quad \text{and} \quad \overline{J} = \frac{1}{M}\sum J(U^m)$$

(b) If

$$\sum_m (J(U^m) - \overline{J})^2 \le \varepsilon \qquad \text{or}$$

$$\sum_m \left\| U^m - \overline{U} \right\| \le \delta$$

Terminate. Otherwise, go to step 2(a).

The search is terminated when the pattern of points has shrunk so that the points are sufficiently close together and / or when the differences between the cost function values at the points become small enough. Numerical experiments has been performed with this algorithm [5], and on this empirical basis it is recommended to use $\alpha = 1.3$ and $M = 2p_c$. On the other hand, good results with $M = p_c + 2$. The $\alpha > 1$ compensates for shrinking of the complex caused by halving the distances, while the large number of vertices is intended to prevent the complex from collapsing and flattening out along the constraints. The setting at the value of the bound is intended to avoid unnecessary contraction of the complex. The complex method requires that the feasible region be a convex set. This requirement arises in two places: in the calculation of the centroid and in the retraction of a feasible but unsatisfactory point. For no convex regions the method could fail to converge satisfactorily. In practice, the method is widely used and has successfully solved numerous no convex problems. Thus, the above situation must arise with low probability.

5. Application to Oxidation Process

The proposed neural net based optimizer is applied to chemical process of lateral oxidation which is frequently needed for micro fabrication processes in manufacturing electromechanical systems especially micro- sensors , micro-actuators and different wide range of nozzles [13]. In this kind of process the wet thermal oxidation system consists of a simple beaker on a hot plate with crude gas flow control, a single zone tube furnace of a constant temperature bubbler bath, mass flow gas control and three zone tube furnaces. The bath temperature regulation, and AlAs mole fraction are used here as inputs of the process whereas the rate of lateral oxidation is considered as an output.

The data which is used in this paper consists of 48 patterns. Each pattern includes two inputs and the corresponding output. The first input is the temperature of the process and it ranges from 380 ºC to 500 ºC while the second input is the AlAs mole fraction which ranges from 92 % to100 %. The data is extracted from experimental measurements as mentioned earlier (see Fig. 1). The data is arranged in a suitable way for neural net training and testing, namely, the data is divided into two sets: training set and test set. The number of patterns which used for training the neural is thirty six while twelve patterns are used to test the neural net performance. Simulation was carried out by a code based on Matlab software. Several numbers of hidden neurons are tried to obtain the best results of simulation since the accuracy of simulation depends on the number of hidden neurons. In this study the optimum number of hidden neurons was selected as four which gives acceptable least square error over the training and test sets. Both of the real and predicted artificial neural net values for training and test regions are shown in Figs. 5 and 6, respectively. Fig. 7 demonstrates how the minimum squared error depends on the number of epochs in Matlab during training the neural net. It is worthwhile to mention that normalizing the data enhances the performance of the neural net, but in our case the performance is good enough without the assistance of the normalizing technique.

The neural net based optimizer objective in the lateral oxidation process is to predict the regulating temperature and the percentage of AlAs mole fraction which will match the desired target value of the lateral oxidation rate (µm/min). The optimization algorithm minimizes the error between the neural output and the corresponding target value. For example, for the lateral oxidation rate target value of 6.5 µm/min, the optimization algorithm calculates the temperature and the mole fraction of AlAs as 487.2495 ºC and 99.5801 %, respectively. The corresponding neural output is 6.5012 µm/min which shows excellent accuracy. The input values obtained from optimization are also very close to the real inputs at the lateral rate of oxidation 6.5 µm/min. Fig. 8 shows the two inputs iteration (counter) history as given by the optimization algorithm. Note that the optimizer needed 28 iterations to achieve the optimum inputs.

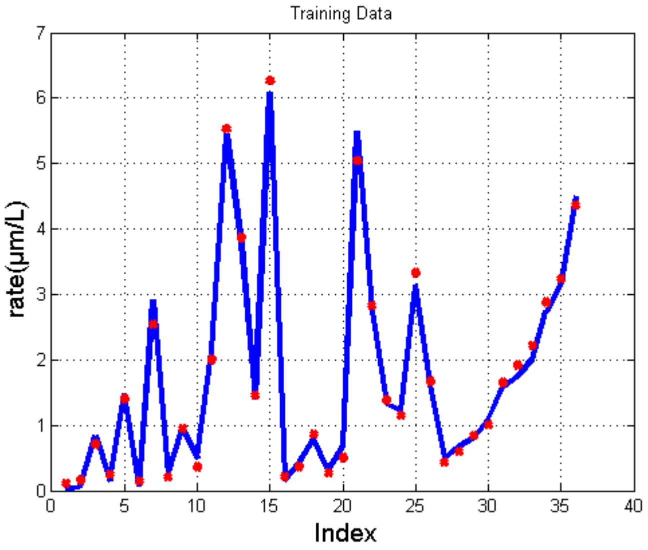

Fig. 5. Nueral net trainning.

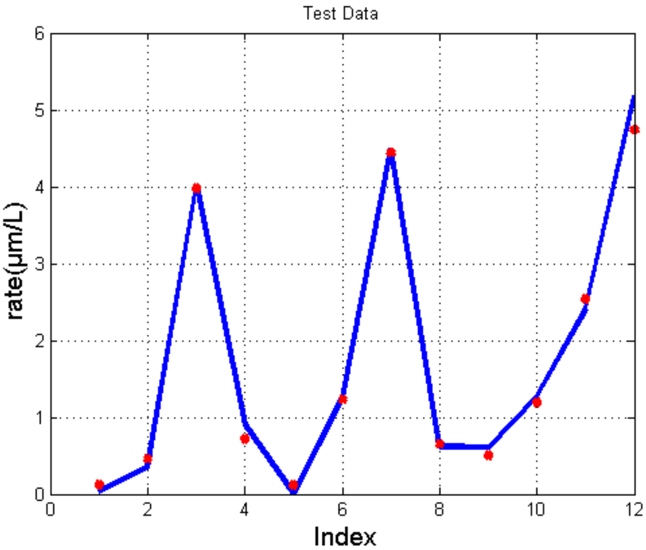

Fig. 6. Neural net testing.

6. Conclusions

Constrained optimization of a two-input, one output process with available historical data was developed. The algorithm combines neural net modeling and a modified version of the complex method constrained optimization to calculate process inputs or part of them that will drive the output at its target value. The developed neural net based optimization technique was tested on the lateral oxidation process for micro electromechanical systems (MEMS). The two inputs are the process temperature and AlAs mole fraction whereas the output is the lateral oxidation rate. The neural net prediction ability is excellent. In addition, the results show that the neural net based optimizer achieves well its objective of obtaining the inputs that will produce a pre-specified desired output. Application of neural networks in the lateral oxidation studies can further be expanded for larger number of oxidation parameters.

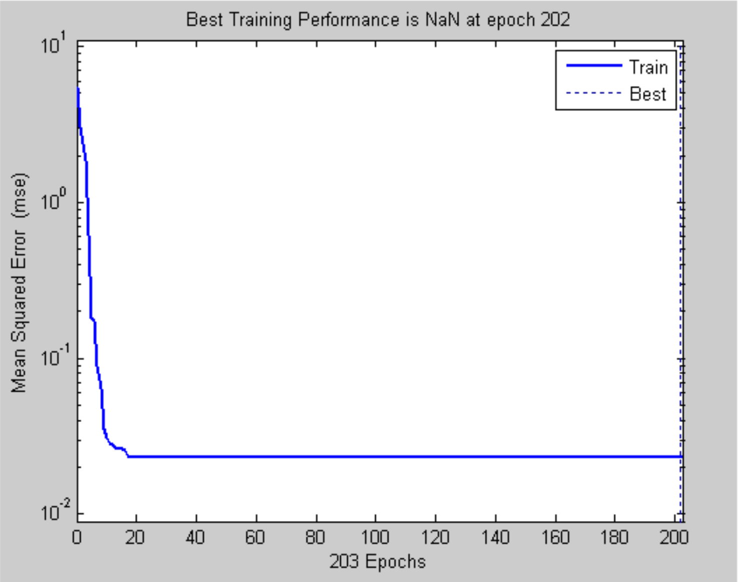

Fig. 7. Best ANN training performance.

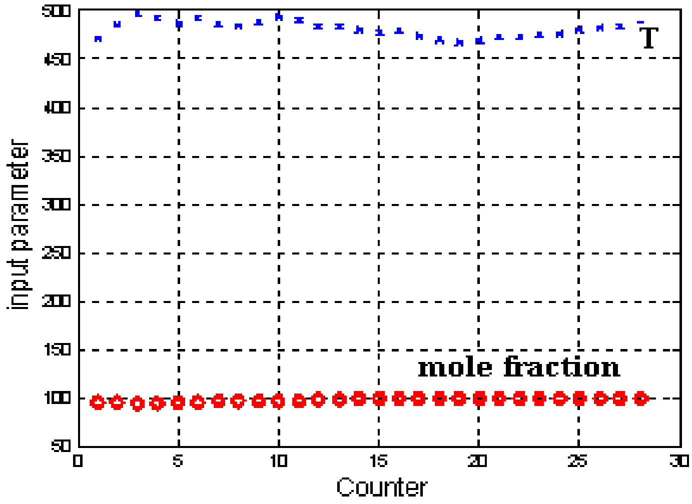

Fig. 8. The optimization algorithm inputs iteration history.

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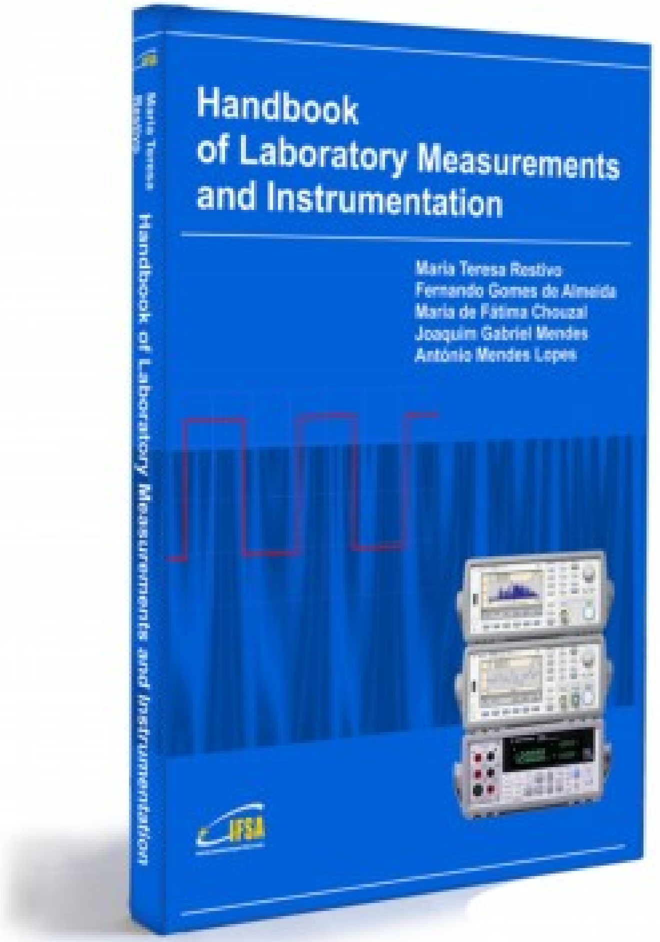
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