

Modeling the Contact Formation for High-Performance Silicon Solar Cells Using Polynomial Neural Networks

SungJoon Lee⁴⁾, Ju Hyun Park¹⁾, Jae-Woong Youn²⁾, Jun Rim Choi³⁾, and Seung-Soo Han⁴⁾

¹⁾ Yeungnam University, Department of Electrical Engineering
Dae-Dong, Kyongsan, Gyeongbuk 712-749, South Korea
Jessie@ynu.ac.kr

²⁾ Daegu University, School of Automotive, Industrial and Mechanical Engineering
Jillyang, Gyeongsan, Gyeongbuk 712-714, South Korea
jwyoun@daegu.ac.kr

³⁾ Kyungpook National University, School of Electrical Engineering and Computer Science
Daegu, Kyungpook 702-701, South Korea
jrchoi@ee.knu.ac.kr

⁴⁾ Myongji University, Department of Information Engineering, & NPT Center
Nam-Dong, Yongin, Kyunggi, 449-728, South Korea
shan@mju.ac.kr

Abstract - Since the neural network was introduced, significant progress has been made on data handling and learning algorithms. Currently, the most popular learning algorithm in neural network training is feed forward error back-propagation (FFEBP) algorithm. Aside from the success of the FFEBP algorithm, a polynomial neural networks (PNN) learning has been proposed as a new learning method. The PNN learning is a self-organizing process designed to determine an appropriate set of Ivakhnenko polynomials that allow the activation of many neurons to achieve a desired state of activation that mimics a given set of sampled patterns. These neurons are interconnected in such a way that the knowledge is stored in Ivakhnenko coefficients. In this paper, the PNN model has been developed using the contact formation for high-performance silicon solar cells experimental data. To characterize contact formation process using PNN, co-firing was processed under varying conditions were analyzed using central composite design (CCD) with three center points. Parameters varied in these experiments included zone 1, zone 2, zone 3 temperatures and belt speed of the furnace. It was shown that the output of the PNN model follows the real experimental measurement data very well.

1. Introduction

A In the age of industry, the process engineer must often rely on his/her own experience or on books containing recommended operating parameters for given conditions to operate the highly complex equipments. In order to facilitate more reliable results, robust process modeling methodologies are highly desirable. Accurate process models can enable prediction of process variations over a wide range of input conditions. Efficient and tighter process model often offers a competitive edge in today's complex and competitive semiconductor manufacturing.

The neural network based models have recently been shown by several researchers to exhibit superior performance in both accuracy and prediction capability [1-4]. The basic components of a neural network are processing elements (neurons) and weights (connections). The adjustable weights correspond to biological synapses. The weighted inputs to a neuron are accumulated and then passed through an activation function which determines the neuron's response. How to adjust these weights, called learning or training, is the most important in neural network modeling. Since the neural network was introduced, significant process has been made on learning algorithms. Currently, the most popular learning algorithm in neural network training is feedforward error back-propagation (FFEBP) algorithm. Aside from the success of the FFEBP algorithm, polynomial neural network (PNN) learning has been proposed as a new learning method. The PNN learning is a self-organizing process designed to determine an appropriate set of Ivakhnenko polynomials that allow the activation of many neurons to achieve a desired state of activation that mimics a given set of sampled patterns. These neurons are interconnected in such a way that the knowledge is stored in Ivakhnenko coefficients [5-7]. The activation level of a node is determined by a nonlinear activation function with optimal complexity called a Ivakhnenko polynomial [5].

In this paper, the PNN model has been developed using the contact formation for silicon solar cells, which has great impacts on solar cell efficiency. The contact properties of silicon solar cells are determined by the mixture of belt-furnace zone temperatures and belt speed. To characterize the contact formation process, co-firing of a screen-printed Ag grid on the front and Al on the back surface field is implemented. A statistically designed experiment is conducted to make a PNN model and the crucial relationships between input factors and solar cell efficiency is analyzed. Parameters varied in these experiments included zone 1

temperature, zone 2 temperature, zone 3 temperature, and belt speed of the furnace.

2. Experiments

To fabricate n+-p-p+ SC silicon solar cells, p-type, 1.5~2.0 Ω -cm, square textured float zone (FZ) wafers were employed. Saw damage removal by potassium hydroxide (KOH) etching was performed for 3 minutes at 85°C followed by a cleaning step. Before the emitter diffusion process with phosphoric acid on the surface, in order to acquire a hydrophilic feature, sulfuric acid (H₂SO₄) was oxidized uniformly. Phosphoric acid was then deposited on the front surface of the wafers by spin coating. The coated wafers were fully annealed in a ceramic roller hearth furnace with no metal contamination and eight heating zones, and this was followed by parasitic junction removal through edge isolation. After emitter formation by diffusion, phosphosilicate glass (PSG) was etched from the surface in a dilute HF solution. The next step was depositing a SiN_x single layer antireflection coating (ARC) by low-frequency (50 KHz) plasma-enhanced chemical vapor deposition (PECVD) to alleviate reflection losses and to enhance surface and bulk passivation. Ag and Al paste were then screen-printed on the front and back surface, respectively. Lastly co-firing was conducted in an IR beltline furnace with three dissimilar temperature zones to accomplish photo generation in a light-absorbing surface and separation of electrons and holes.

2.1 Statistical Experimental Design

The typical experimental method of collecting large quantities of data while holding each factor constant until all possibilities have been tested is an approach that becomes impossible as the number of factors increases. In addition, the role of each step in determining output response is generally not clear. Statistical experimental design techniques can be used to examine all possible combinations of a set of factors within a process at once and observe the data collectively. These techniques are highly efficient, and the structured approach for characterization using a relatively small number of experiments significantly improve process performance and makes the process more robust [8-9].

During the co-firing process, a set of experimental data was acquired from 2⁴ full factorial designs with 3 center points, 8 axial points, and 5 random points to characterize process variations with four controllable input factors, consisting of the three different zone temperatures and belt speed (all of which have two levels). Random samples were fabricated for the purpose of verification.

3. Polynomial Neural Network Process Modeling

The PNN is a network transformation of $R^n \rightarrow R$, as shown in Figure 1. The PNN learning is a self-organizing process designed to determine an appropriate set of Ivakhnenko polynomials that allow the activation of many

neurons to achieve a desired state of activation that mimics a given set of sampled patterns [5]. These neurons are interconnected in such a way that the knowledge is stored in Ivakhnenko coefficients. The activation level of a node is determined by a nonlinear activation function with optimal complexity called a Ivakhnenko polynomial. This function usually has a form such as;

$$y = A + \sum_{i=1}^m B_i x_i + \sum_{i=1}^n \sum_{j=1}^n C_{ij} x_i x_j + \dots \quad (1)$$

where x_i , x_j and x_k are nodal input variables, and y is the output of an individual neuron. A , B_i , and C_{ij} are the coefficients of the Ivakhnenko polynomial. This activation function endows the PNN the ability to generalize with an added degree of freedom not available in statistical regression techniques.

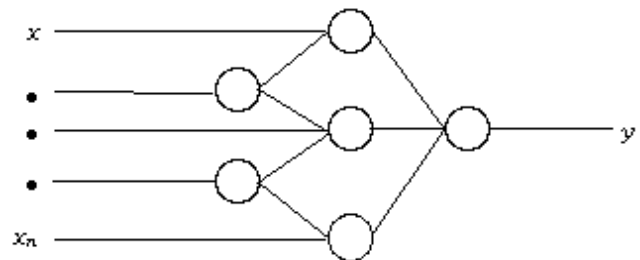


Figure 1. The basic PNN configuration

The PNN utilizes the Group Method of Data Handling (GMDH) for data management. GMDH was first introduced by the Russian cyberneticist Ivakhnenko [5], and has been used to synthesize the building blocks of modeling methodology [7]. In GMDH, the data sample is divided into training set and validation set. The PNN methodology is implemented on the random input-output sets of measured training and validation data obtained from the experiments. An input matrix, consisted of measured (first layer) or calculated (second layer and more) input data, is presented to the each layer, and the output at each node is calculated by combining the inputs of each layer as pairs (or singles or triples) and filtering this, using the least square method. At each layer, new generations of complex equations are constructed which evolves from simple form. Survival of the fittest principle (appropriate thresholds) determines the equations that can be passed to the next layer.

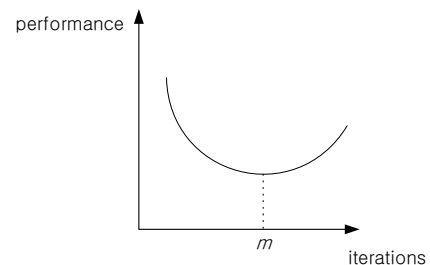


Figure 2. Stopping Criterion

The calculated output vector is then compared to the measured output data vector, and the mean squared difference

between these two vectors determines the error of this model. The number of layers is increased until the newer model begins to have poorer performance than their predecessors. This provides the self-organizing feature of the algorithm, leading to models of optimal complexity.

From experimental work, it has been verified that the curve of the performance vs. iteration has the general shape shown in Figure 2. The stopping criterion was defined to stop the synthesis iteration process after m iterations (generations).

4. PNN Modeling and Results

A PNN structure may be effectively employed to model the input-output behavior of the contact formation experiment. Output of the model represents efficiency of the solar cell. The number of inputs of the model was set to four; one controllable parameter per one input node. The Predicted Squared Error (PSE), an estimate of the Mean Squared Error (MSE) of unseen data, is used as the performance metric. Initially, PNN model was obtained using a set of input pairs and default structures. Since this rough model includes all the polynomial type regression functions of input variables generated on the PNN structure, they were refined by varying the number of hidden nodes (neurons) and layers by analyzing all the PSE s at each layer, and select the polynomial coefficients to minimize the error. In evaluating learning (training) error, 24 experimental data were used to build the models. The prediction error of this model was determined using eight other experimental data which were not used during training process.

To search for the PNN architecture and coefficients of polynomial that minimized both the training error and prediction error, the following PSE was defined as a performance index:

$$PSE = MSE + KP \quad (2)$$

where MSE is the training mean squared error and KP is the complexity penalty (overfit penalty). The KP is defined by:

$$KP = PF \times \frac{2K}{N} \times S_p^2 \quad (3)$$

where K , N , and S_p^2 are determined by the data used to synthesize the network and PF is the penalty factor which is set to 1 in this model. N is the number of training data, S_p^2 is a prior estimate of the true error variance, and K denotes the total number of coefficients. The penalty factor allows the designer to accommodate the computational complexity in the calculation of the error term.

The PSE takes into account the complexity of the belt furnace system, and it attempts to reduce the predicted squared error. Initially, the MSE had a significant effect, but as the model increases in the size of training data, KP becomes more important. A minimum value of PSE will always exist, because MSE decreases with each additional trial but always remains nonnegative, whereas KP linearly increases as the number of trials increases. Therefore, PSE is minimized in the point of compromise of both KP and MSE . The smallest values of PSE s are used to determine the PNN architecture and coefficient set that simultaneously minimize both training and prediction errors. Hence, the presence of

both MSE and KP ensures that PSE favors simple models with low error.

In performing this analysis, it has been assumed that the optimal polynomials fitted by linear regression equations were sufficient to capture the dependence of PNN performance on the optimal coefficients. The fitted final polynomials were subsequently used to generate a PNN that optimized the training and prediction errors.

Figures 3-5 show the synthesized optimal PNN models for the efficiency. The optimal model was determined to find input nodes from the satisfied node, after iteratively calculating the PSE until the PSE was smaller than the previous value. The equation shown Figure 3 represents the first "Triple" in the network structure (shown in thick black square). The x_1 , x_2 , x_3 in the equation represent the first input, the second input, and the third input respectively. In Figure 4, the calculation of second "Triple" in the network structure is shown. The x_1 in this "Triple" is an output of the first "Triple", which is calculated by Zone 1, Zone 2, and belt speed. In this network structure, belt speed is used for both first and second "Triple" calculations. Figure 5 shows the calculation for efficiency and related statistics.

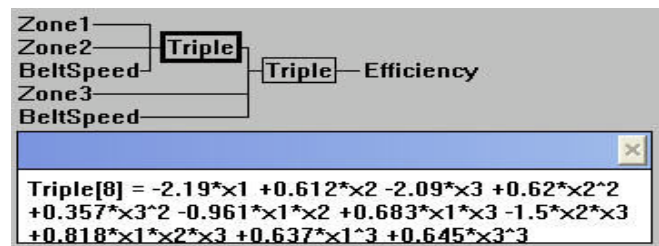


Figure 3. Synthesized PNN and calculation of first Triple

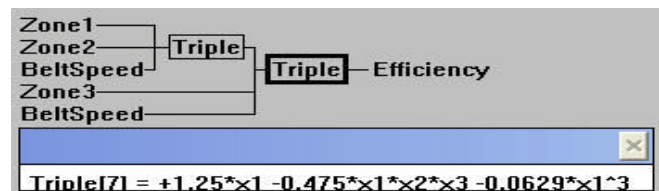


Figure 4. Synthesized PNN and calculation of second Triple

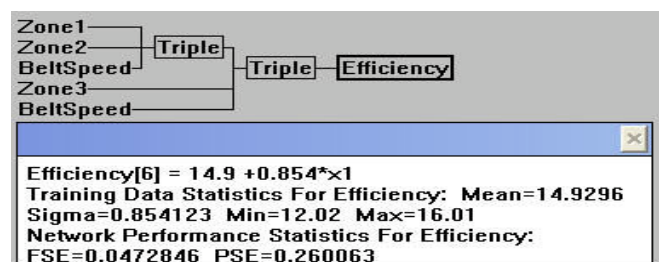


Figure 5. Synthesized PNN and calculation/data for efficiency

After NN process models were established, response surfaces were generated to illustrate the relationships between the input parameters and the responses. Any two of the four process parameters were simultaneously varied, while the remaining parameters were fixed at their mid-range values.

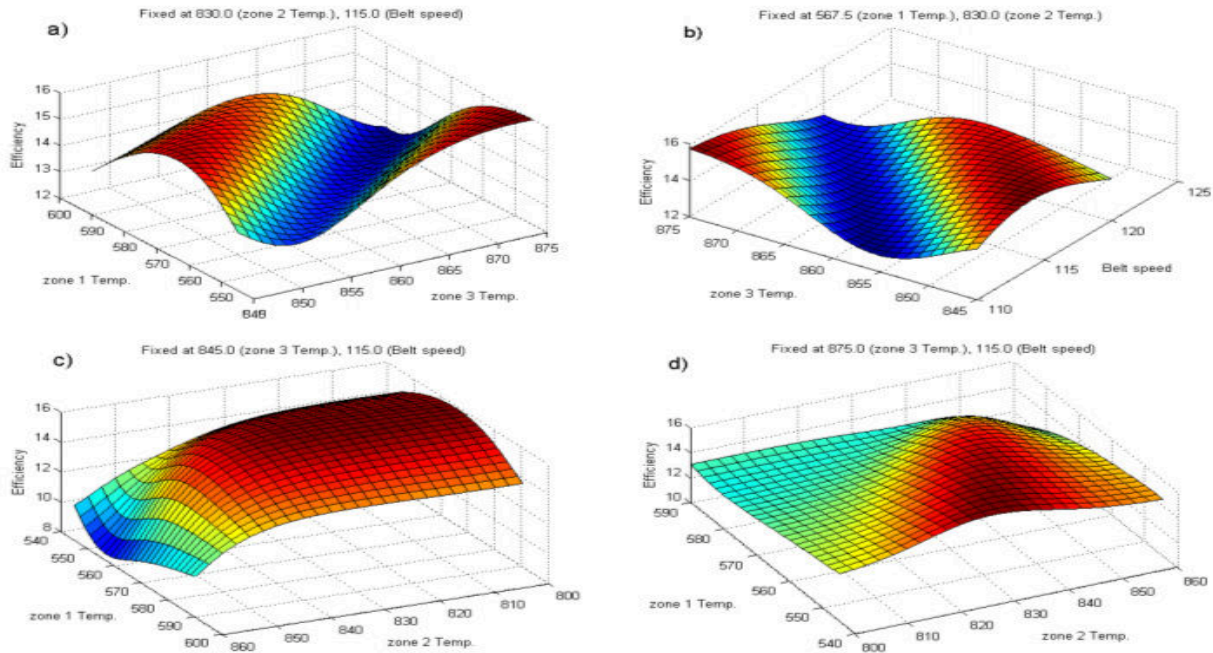


Figure 6. Response surface plots for efficiency

For each model, a temperature variation was observed in zone 3 which has a predominant effect on cell efficiency. The plots in Figure 6 a) and b) indicate that an increase or decrease in zone 3 temperature results in higher cell efficiency. In addition, high efficiency was observed at belt speeds at the approximate middle range. To highlight the effect of zone 3 temperature on cell efficiency, the temperature in zone 3 and belt speed were fixed at 845°C, 870°C at 115 rpm, respectively. The response surface plots at the fixed values are depicted in Figure 6 c) and d).

5. Conclusions

A PNN modeling technique using GMDH method was investigated in this paper. In contrast to the conventional regression technique, PNN has several distinct advantages: a smaller number of data set is required, less computational time, and the final structure of the PNN does not need to be specified. Although, high-order regression often leads to a severely ill-conditioned system equations, the PNN avoids this by constantly eliminating variables and variable interactions at each layer, and helps to reduce linear dependencies. Therefore, complex systems can be modeled without specific knowledge of the system or massive amounts of data. This optimal network synthesis capability was shown in this paper using contact formation experimental data. This PNN model was used in analyzing the impact of each input conditions on the solar cell efficiency. This model also can be used in synthesizing the recipes for the films with special characteristics.

Acknowledgments

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