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# Neural Network Modeling of PECVD SiN Films and Its Optimization Using Genetic Algorithms

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**Abstract**

Silicon nitride films grown by plasma-enhanced chemical vapor deposition (PECVD) are useful for a variety of applications, including anti-reflecting coatings in solar cells, passivation layers, dielectric layers in metal/insulator structures, and diffusion masks. PECVD systems are controlled by many operating variables, including RF power, pressure, gas flow rate, reactant composition, and substrate temperature. The wide variety of processing conditions, as well as the complex nature of particle dynamics within a plasma, makes tailoring SiN film properties very challenging, since it is difficult to determine the exact relationship between desired film properties and controllable deposition conditions. In this study, SiN PECVD modeling using optimized neural networks has been investigated. The deposition of SiN was characterized via a central composite experimental design, and data from this experiment was used to train and optimize feed-forward neural networks using the back-propagation algorithm. From these neural process models, the effect of deposition conditions on film properties has been studied. A recipe synthesis (optimization) procedure was then performed using the optimized neural network models to generate the necessary deposition conditions to obtain several novel film qualities including high charge density and long lifetime. This optimization procedure utilized genetic algorithms, hybrid combinations of genetic algorithm and Powell's algorithm, and hybrid combinations of genetic algorithm and simplex algorithm. Recipes predicted by these techniques were verified by experiment, and the performance of each optimization method are compared. It was found that the hybrid combinations of genetic algorithm and simplex algorithm generated recipes produced films of superior quality.

**Key Words** : Optimized neural network modeling, Genetic algorithm, Hybrid algorithm, Optimization

## I. Introduction

Silicon nitride films grown by plasma-enhanced chemical vapor deposition (PECVD) are useful for a variety of applications, including anti-reflection coatings in solar cells, passivation layers, dielectric layers in metal/insulator structures, and diffusion masks. Recent studies have indicated that the use of silicon nitride films grown by PECVD as antireflection coatings in polysilicon solar cells can be beneficial in improving cell efficiency [1-3]. In addition to serving as antireflection coatings, these films also enhance cell performance by passivating the device surface by introducing significant amounts of atomic hydrogen, which is produced during the PECVD process [1-2]. Thus, PECVD not only provides the obvious advantage of low deposition temperature, but the SiN film can also be used to avoid defect formation, diffusion, and degradation of the surface metal layer. Furthermore, the PECVD process possesses a number of other qualities which are attractive from a manufacturing standpoint, including high throughput, very good uniformity and thickness control, and excellent reproducibility [3].

The nitride film properties are determined by the nature and composition of the plasma, which are in turn controlled by the deposition variables. As a consequence of the complex nature the plasma, however, it is very difficult to quantify from first principles the exact relationship between input factors (such as substrate temperature, pressure, RF power, and gas flows) and critical output parameters (such as reflective index, effective lifetime, and positive charges). Although empirical models for plasma-based and other semiconductor processes have been developed using statistical response surface methods [4], process models derived from neural networks have recently been shown to offer advantages in both learning accuracy and generalization capability.

Himmel and May reported 40-70% improvement in experimental error, as well as nearly a 40% improvement in generalization by neural nets over statistical models in plasma etching [5]. Similarly, Mocella et. al. [6] and Huang et. al. [7] each also found that neural nets consistently produced models exhibiting better fit than several variations of response surface models in the plasma etch application. Bose and Lord demonstrated that neural networks provided appreciably better generalization than regression based methods for chemical vapor deposition modeling [8]. Furthermore, both Himmel and Mocella found that building these neural process models requires fewer training experiments [5-6], and Huang et. al. showed that it is possible to develop satifactory models from even fewer experimental data than there are

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coefficients in the neural network [7].

This paper seeks to build upon this body of work, and use neural networks to develop obtain accurate and useful manufacturing models for the PECVD of silicon nitride films. In order to characterize films deposition under varying conditions, we have performed a central composite circumscribed experimental design. The central composite design employed consisted of a 26-1 fractional factorial augmented by 12 axial points and three center points [9]. Data from these 47 experiments was used to develop neural process models describing the following deposition responses and film qualities: deposition rate, reflective index, uniformity, effective carrier lifetime, and hydrogen content. Feed-forward neural networks were trained using the error back-propagation (BP) algorithm.

The development of optimal neural process model is complicated by the fact that back-propagation neural networks contain several adjustable parameters whose optimal values are initially unknown. These include structural parameters (such as the number of hidden layer neurons) as well as BP learning parameters (i.e. - learning rate, momentum, and training tolerance) [10]. In this paper, neural process models for PECVD were first developed using a default parameter set. The effect of these factors on network performance was also subsequently investigated via a fractional factorial experiment. The results were analyzed using commercial statistical software package, RS/Discover [11], and parameter sets which minimized the training and prediction error of the $Si_3N_4$ PECVD models were determined [12]. Examination of the resulting process models indicates that there exists a significant positive correlation between hydrogen concentration and effective lifetime. The models developed also show that pressure and RF power have less impact on the quality of the nitride film than temperature and ammonia and silane flow rate.

## II. Experimental Procedure

The silicon nitride films investigated were deposited using ammonia ($NH_3$), silane ($SiH_4$), and nitrogen as feed gases. The deposition conditions were varied in a central composite circumscribed design [9] array over the ranges shown in Table 1. Three-inch, float zone p-type silicon wafers, with a (100) orientation and a resistivity of 2.0 Ω-cm, were used as the substrates. The wafers were thoroughly cleaned using the following process:

| | |
|---|---|
| DI water rinse | 3 min. |
| $H_2SO_4$:$H_2O_2$ = 4:1 | 4 min. |
| DI water rinse | 3 min. |
| $HNO_3$:HF = 20:1 | 3 min. |
| DI water rinse | 3 min. |
| HCl:$H_2O_2$ = 5:2 (100 ℃) | 20 min. |
| DI water rinse | 3 min. |
| HF:H2O2 = 1:100 | 5 min. |
| DI water rinse | 10 min. |

Table 1. Ranges of deposition parameters

| Parameter | Range |
|---|---|
| Substrate Temperature | 200 - 400 ℃ |
| Pressure | 0.6 - 1.2 Torr |
| RF Power | 20 - 40 watt |
| $NH_3$ Flow | 1 - 1.4 sccm |
| $SiH_4$ Flow | 180 - 260 sccm |
| $N_2$ Flow | 0 - 1000 sccm |

After cleaning, the wafers were blow dry using nitrogen gas. Each three inch wafer was then cut into four pieces and subjected to PECVD silicon nitride deposition. During the deposition, SiH4 was diluted to 2% in nitrogen. Following the deposition of approximately 0.05 $\mu$m of silicon nitride, the samples to be used for effective lifetime and positive charge concentration measurements underwent annealing at 350 ℃ for 20 minutes.

To facilitate the measurement of positive charge concentration, capacitors were made on these samples. The thickness and refractive index of the films were measured by ellipsometry by a helium-neon laser having a wavelength of 6328Å. The positive charge concentration was obtained using C-V measurements. The effective lifetime was measured using a laser photoconductive decay (PCD) tester. In this technique, laser light falls on the silicon samples under test and generates electron-hole pairs. The duration of the pulse is short compared with the expected lifetime of the charge carriers. These holes and electrons increase the sample conductivity. The additional charge carriers produced by the incident light recombine once the light is removed. Those excess carriers do not recombine instantaneously, but decay in concentration according to:

$$N(t) = N_0 \exp\left(\frac{-t}{\tau_{eff}}\right)$$

where N(t) is carrier concentration at the time t, N0 is the initial carrier concentration, and $\tau_{eff}$ is effective lifetime. The starting bulk lifetime prior to annealing was measured as 1.2 ms using this technique. A central composite circumscribed experimental design was used to characterize film deposition. This design employed consisted of 26-1 fractional factorial augmented by 12 axial points and three center points. Based on data obtained from these 47 experimental trials, three-layer neural network models were trained using error back-propagation algorithm.

## III. Neural Process Modeling

As mentioned above, the highly complex particle interactions within a plasma have limited the success of PECVD modeling from a fundamental physical standpoint. Recently, however, neural networks have emerged as an attractive alternative to physically-based models and statistical methods [5-8]. Neural networks possess the capability of learning arbitrary nonlinear mappings between noisy sets of input and output patterns. Neural network learning is a "self-organizing" process designed to determine an appropriate set of connection strengths which facilitate the activation of many simple parallel processing units to achieve a desired state that mimics a given set of sampled patterns. In other words, these rudimentary processors (called "neurons") are inter-connected in such a way that knowledge is stored in the weight of the connections between them. The activation level of a neuron is determined by a sigmoidal "activation function" such as:

$$y=\frac{1}{1+e^{-x}}$$

where x is the weighted sum of neural inputs and y is the output of an individual neuron. This nonlinear activation function enables neural networks to generalize with an degree of freedom not available in statistical regression techniques [5]. Feed-forward neural networks used for semiconductor process modeling are trained via error back-propagation, a supervised learning method [13]. In this algorithm, the network begins with a random set of weights. An input vector is presented to the network, and the output is calculated by summing the weighted input connections of each layer and filtering this sum with the sigmoidal activation function. The calculated output is then compared to the measured output data, and the squared difference between these two vectors determines system error. This error is then minimized using the gradient descent approach in which weights are adjusted in such a way as to minimize the overall system error.

### 3.1 Network Structure and Learning

Individual neurons in a BP neural network receive, process, and transmit information regarding the relationships between input and output pairs. The input layer of neurons corresponds to the six adjustable input parameters which are varied in the PECVD experiment. The output layer corresponds to the deposition variables to be modeled. The network also incorporates one hidden layer of neurons which assist the network in learning the nonlinear mapping between the input and output layers. Conceptually, the hidden layer neurons can be viewed as representing fundamental, yet not directly controllable plasma properties such as electron temperature or reactive species concentration.

In the BP training algorithm, model performance is influenced by both the number of hidden layers and the number of neurons in each layer. It has been previously shown that an BP network containing a single hidden layer can encode any arbitrarily complex input-output relationship [14]. Therefore, in order to determine the optimal network structure for PECVD modeling, the number of layers has been fixed to three, and only the number of neurons in the hidden layer has been varied. A large number of hidden neurons is required to model complex relationships, but too many can result in an over-trained network and render it incapable of generalizing input/output relationships that differ from the training samples.

The performance of BP networks in process modeling also depend on parameters such as learning rate, momentum, and training tolerance [10]. The learning rate ($\eta$) determines the speed of convergence by regulating the step size. However, the network may settle too far from the actual minimum value of the error surface if h gets too large. On the other hand, smaller rates can ensure the stability of the network by diminishing the gradient of noise in the weights, but results in longer training time. The momentum term in the weight adjustment expression is designed to prevent the training algorithm from settling in local minima, and also increases the speed of convergence. This additional term, computed adding a fraction of the previous weight change, tends to keep the weight changes going in the same direction. Another important parameter is network training tolerance. This parameter specifies an acceptable tolerance for the accuracy of the neural outputs. A smaller training tolerance usually increases learning accuracy, but can result in less generalization capability as well as longer training time. Conversely, a larger tolerance enhances convergence speed at the expense of accuracy in learning. A procedure for choosing the learning rate, momentum, and training tolerance is outlined below.

### 3.2 Network Optimization

Since there were six controllable input parameters and three measured output characteristics in this Si3N4 PECVD experiment, the number of neurons in the input and output layers were set to six and three, respectively. In optimizing the neural process models, four parameters were considered: number of hidden neurons, learning rate, momentum, and training tolerance. Initially, neural PECVD models were obtained using a set of default network structure and set of learning parameters. These rough models were then refined by varying the values of the four critical parameters according to a 24-1 fractional factorial design and analyzing the results using RS/Discover [11]. The experimental ranges of each

parameter and their default values are summarized in Table 2.

Table 2. Ranges of neural network papameters

| Parameters | Range | Default Value |
|---|---|---|
| No. Hidden Neuron | 6 - 10 | 8 |
| Learning Rate | 0.05 - 0.5 | 0.275 |
| Momentum | 0 - 0.4 | 0.2 |
| Training Tolerance | 0.01 - 0.13 | 0.07 |

In varying the above factors, two important characteristics of neural process models have been investigated: network learning ability and prediction capability. These performance metrics are quantified in terms of their root-mean-squared (RMS) error ($\sigma$ 2), given by:

$$\sigma^2 = \frac{1}{n-1}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2$$

where n is the number of trials, yi is the measured value of each response, and $\hat{y}_i$ is the corresponding neural process model prediction. In evaluating learning (or training) error, n ranges over the number of trials used to build the model. As for prediction error on the other hand, n represents some number of test trials apart from the original training set. The prediction error in this experiment was determined by using the trained networks to predict the nitride film properties for ten of the original 47 experimental runs selected at random.

To search for parameter values which minimized both training error and prediction error, the following performance index (PI) was implemented for each of the seven PECVD output responses:

$$PI = K_1\sigma_t^2 + K_2\sigma_p^2$$

where $\sigma_t$ is the network training error, $\sigma_p$ is the prediction error. The constants $K_1$ and $K_2$ are weights representing the relative importance of each performance measure. Since the prediction error is typically the more important quality characteristic, the values chosen for these constants were $K_1$ = 1, and $K_2$ = 10. Optimization of the neural process models was then performed using Nelder-Mead simplex search algorithm [15] to minimize the performance index itself. This objective is to determine a network architecture and parameter set which simultaneously minimizes both training and prediction error based their relative importance [12]. The resulting optimal values for the BP training parameters, training error, and prediction error for each of the five PECVD process models is shown in Table 3.

Table 3. Optimized network parameters and network error

| PECVD Response | Hidden Neuron | Learning Rate | Moment-um | Toler-ance | Trainin g Error | Predictio n Error |
|---|---|---|---|---|---|---|
| Effective Lifetime ($\mu$s) | 6 | 0.05 | 0 | 0.01 | 10.54 | 16.09 |
| Positive Charge (1012/cm 2) | 10 | 0.05 | 0 | 0.13 | 0.372 | 0.556 |
| Reflectiv e Index | 6 | 0.07 | 0 | 0.13 | 0.074 | 0.096 |

## IV. Modeling Results and Discussion

The motivation for choosing effective lifetime, positive charge, and refractive index as response variables to characterize is as follows. Effective lifetime is one of the most important measures of solar cell performance because cell efficiency greatly depends on the lifetime. Long effective lifetime results in high efficiency [16-17]. Positive charge concentration in silicon nitride film impacts the effective lifetime of a conventional solar cell, and is of critical importance for metal- insulator-semiconductor (MIS) inversion solar cells [18]. High positive charge concentration not only improves the surface passivation of a solar cell (which leads to longer effective lifetime), but also results in stronger inversion and low sheet resistance in MIS inversion cells. Finally, the refractive index of a Si3N4 film is also an important measure of solar cell performance. In order to achieve high efficiency solar cells, the refractive index has to be so chosen that the total reflection on the front surface is minimized [3]. The refractive index of the PECVD Si3N4 films deposited under different conditions can vary from 1.54 to 2.96.

A discussion of the changes in these three critical nitride film properties as a function of substrate temperature, RF power, pressure, and gas flow is therefore warranted. Feeding various combinations of process conditions into the trained neural network allows relationships between input and outputs parameters to be visualized using three dimensional graphics. The various relationships extracted from the neural process models of PECVD silicon nitride are described in detail below.

### 4.1 Temperature and Pressure Effects

Figure 1 shows the effect of pressure and temperature on the refractive index of the PECVD nitride films. It is clear that both substrate temperature and plasma pressure have a significant impact. Increasing substrate temperature and chamber pressure results in a higher refractive index. This occurs partly due to the fact that a higher temperature increases the desorption of radicals on the

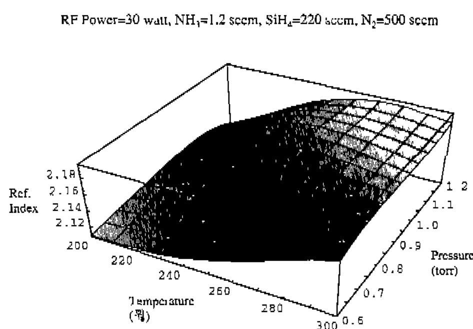


Fig. 1. Refractive index vs. temperature and pressure

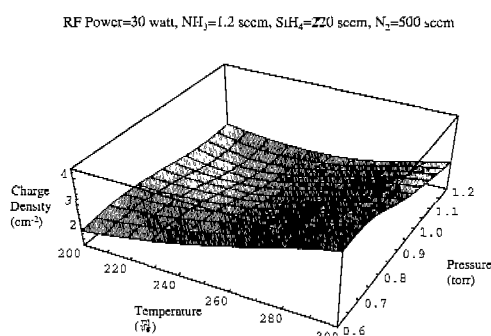


Fig. 2. Effective lifetime vs. temperature and pressure

surface and promotes the rearrangement of the species on the surface of the substrate. Therefore, a high substrate temperature allows the formation of a denser film which in turn results in a higher refractive index. The chamber pressure determines the mean free path of electrons colliding with the gas molecules. Higher pressure results in a shorter mean free path and lowers the electron temperature. Therefore, the reaction proceeds incompletely and more excess silicon is incorporated in the film, which results in higher refractive index.

Figure 2 shows the effective carrier lifetime of the samples as a function of temperature and pressure. It can be seen that increasing the substrate temperature increases the lifetime, while pressure has less of an effect. Effective lifetime is a measure of the quality of the bulk and surface passivation. For a given bulk lifetime, high effective lifetime means better passivation. For the samples processed at lower temperatures, the bulk lifetime is not affected.

The effect of temperature and pressure on the positive charge concentration in the silicon nitride film is shown in Figure 3, which exhibits similar trends as effective lifetime. Positive charge stems from dangling Si+ or NH+ bonds in the film, the presence of which can be reduced by increased atomic hydrogen. It is known that an increase in deposition temperature results in less bonded hydrogen [19], which therefore increases the positive charge density. It has also been predicted that the amount of positive charge in silicon nitride film is closely related to the surface quality - higher concentration yields better surface passivation and therefore, longer lifetime [20]. For the first time, these models show a correlation between effective lifetime of a sample and positive charge concentration in the silicon nitride film. This correlation is further supported by Figures 4 and 5 which show the effect of temperature and RF power on effective lifetime and positive charge concentration (see below).

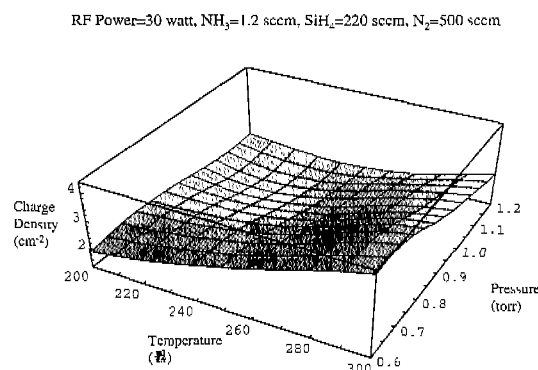


Fig. 3. Positive charge density vs. temperature and pressure

### 4.2 Effect of Temperature and RF Power

Figure 4 shows the effect of substrate temperature and RF power on the effective lifetime. It can be seen that the effective lifetime increases with temperature, but varies only slightly with RF power. It is known that higher substrate temperature results in higher quality silicon nitride films, therefore leading to better passivation. This explains why high deposition temperatures have been widely used for silicon nitride coatings in solar cells.

RF power determines the level of ion bombardment. Higher RF power increases the amount of bombardment by more energetic ions. This causes a greater number of collisions as the ions are accelerated through the plasma sheath. Increased levels of ion bombardment also aid the removal of reaction by-products from the substrate surface. With increasing power, therefore, films that are denser and more structurally and chemically homogeneous are deposited, which results in better passivation. However, increasing ion bombardment too much can damage the silicon surface, which leads to reduction of the lifetime. Overall, though, the RF power has less effect on the lifetime than temperature. Figure 5 shows positive charge concentration in the silicon nitride film as a

function substrate temperature and RF power. A comparison of Figures 4 and 5 once again shows a correlation between the amount of positive charge and the effective lifetime.

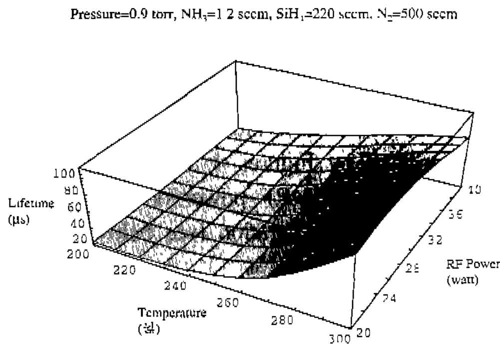


Fig. 4. Effective lifetime vs. temperature and RF power

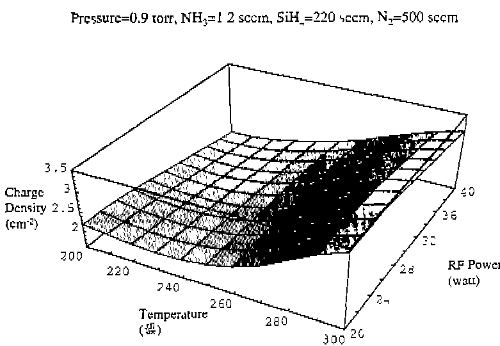


Fig. 5. Positive charge density vs. temperature and RF power

### 4.3 Effects of Ammonia and Silane

It is well known that the ratio of ammonia to silane strongly affects the refractive index of silicon nitride films deposited by the plasma enhanced chemical vapor deposition technique [21]. By using the neural network models of the PEVCD process, the relationship between ammonia and silane and their combined effect on refractive index may be observed (Figure 6). Compared to ammonia, silane has a greater effect on the refractive index of the film in the experimental range of gas flow investigated. For an ammonia flow rate below 1.2 sccm, the refractive index increases rapidly with the increase of silane and then saturates, while for an ammonia flow rate above 1.2, the refractive index increases with silane flow without exhibiting saturation.

Figure 7 shows the effect of ammonia and silane on the effective lifetime. A strong interaction is observed. Increases in either ammonia or silane flow increases the

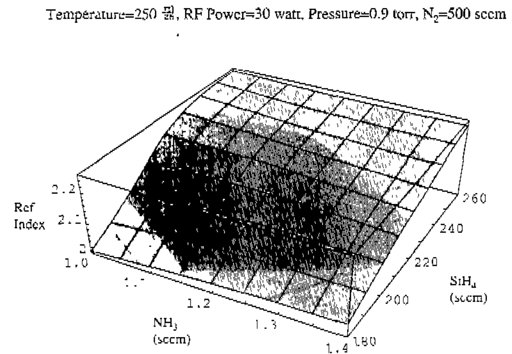


Fig. 6. Refractive index vs. ammonia and silane flow rate

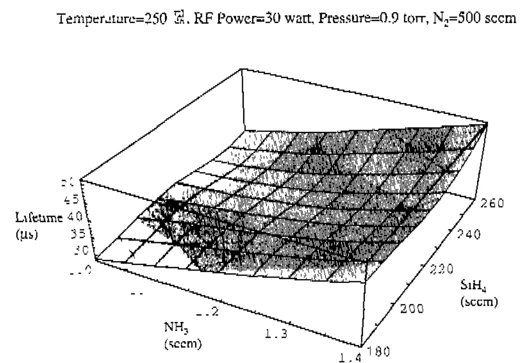


Fig. 7. Effective lifetime vs. ammonia and silane flow rate

effective lifetime of the samples. The improvement of the lifetime can also be explained by surface passivation. During the PECVD process, silane and ammonia are dissociated into radicals and atomic hydrogen. Atomic hydrogen passivates the dangling bonds on the surface of silicon substrate, and therefore, improves the effective lifetime.

## V. Recipe Synthesis (Optimization)

Recipe synthesis procedures using genetic algorithms were successfully applied to PECVD silicon dioxide models, thereby providing motivation for their use in silicon nitride growth. In the silicon nitride application, genetic algorithms, hybrid combinations of genetic algorithms and Powell's, and of genetic algorithms and the simplex algorithm are used as recipe synthesis procedures. The desired output characteristic of the PECVD SiN film to be produced are reflected by the following fitness function (F):

$$F = \frac{1}{1 + \sum_{\gamma} |K_{\gamma}(y_d - y)|}$$

where r is the number of process responses, Kr are the weights of process responses, yd are the desired process responses, and y are the process outputs dictated by the current choice of input parameters. Maximization of F continued until a final solution was selected after 500 GA generations. In the other methods, the optimization stopped when F was within a predefined tolerance. For genetic algorithms, the probabilities of crossover and mutation were set to 0.6 and 0.01, respectively. A population size of 100 was used in each generation. Each of the six process input parameters were coded as 40-bit string, resulting in a total chromosome length of 240 bits. The values of reflection coefficient($\alpha$), contraction coefficient ($\beta$), and expansion coefficient ($\gamma$) were set to 1, 0.5, 2, respectively for the simplex algorithm. In both hybrid methods, the genetic algorithms stopped at 30 generations and handed over the resulting solution as the initial point of the simplex algorithm or Powell algorithm.

In this recipe synthesis procedure, the optimal deposition recipes for the high charge density and long lifetime were determined. To achieve these goals, the neural network process models were trained for one response, and then the three previously mentioned recipe synthesis procedures were applied to determine the required deposition conditions. Tables 4-5 show the recipes synthesized using each of these three methods, along with simulation results predicted by the neural process model using these recipes as inputs and actual measured values of the responses for the grown film.

If we compare the results with typical values of charge density (typically less than 3.5×1012/cm2) and lifetime (typically less than 120 $\mu$s), we can see that the film deposited with optimized recipes have improved properties. For the charge density recipes, all the three methods generated recipes with high temperature, medium pressure and medium power. These followed the trend shown in Figures 3 and 5. In Figures 2 and 4, longer effective lifetime goes longer with higher temperature, low pressure, and medium RF power. The generated recipes for longer lifetime also follow these trends. Figure 7 shows that higher ammonia flow rate and higher silane flow rate lead to longer lifetime, but the generated recipes show lower ammonia flow rate and medium silane flow rate produce longer effective lifetime. The reason for this is that the effects of temperature, RF power, and pressure are more significant than those of the gas flow rates. For both charge density and effective lifetime optimization, the films deposited with GA-generated recipes have higher charge density and longer lifetime than the films deposited with the other two hybrid methods.

Table 4. Synthesized recipes for high charge density (1012/cm2) and experimental data

| Method | Temp. | Power | Pressure | NH3 | SiH4 | N2 | Simulation Results | Experimental Results |
|---|---|---|---|---|---|---|---|---|
| GA | 298 | 32 | 0.82 | 1.40 | 237.87 | 492.12 | 5.29 | 5.11 |
| GA & Simplex | 299 | 31 | 0.82 | 1.40 | 236.86 | 518.35 | 5.30 | 5.04 |
| GA & Powell | 288 | 34 | 0.80 | 1.39 | 240.12 | 507.99 | 5.24 | 5.04 |

Table 5. Synthesized recipes for long lifetime ($\mu$s) and experimental data

| Method | Temp. | Power | Pressure | NH3 | SiH4 | N2 | Simulation Results | Experimental Results |
|---|---|---|---|---|---|---|---|---|
| GA | 300 | 40 | 0.60 | 1.01 | 208.43 | 5.83 | 170.06 | 160 |
| GA & Simplex | 300 | 40 | 0.60 | 1.08 | 202.18 | 5.15 | 168.53 | 156 |
| GA & Powell | 299 | 40 | 0.61 | 1.06 | 213.70 | 16.24 | 167.35 | 154 |

## VI. Conclusions

The properties of PECVD silicon nitride films have been modeled using optimized back-propagation neural networks. The PECVD process was characterized by varying six controllable parameters in a central composite experimental design. BP neural networks were trained, and later optimized, to predict three key PECVD output responses. The optimized networks were then used to visualize the effects on each output of input parameters using three dimensional graphics. These models were also used to determine the optimal process conditions necessary to grow films which result in higher charge density and longer lifetime. The synthesized recipes were verified via actual experiments, and the results show the film deposited with optimized recipes have higher charge density and longer lifetime than the film deposited with typical recipes.

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