MBIR Reflectance Spectrometry for Deep Trench Structure with ANN and Levenberg-Marquardt Combined Algorithm

Chuanwei Zhang, Shiyuan Liu *
State Key Laboratory of Digital Manufacturing Equipment and Technology
Huazhong University of Science and Technology
Wuhan, China

Tielin Shi
Division of Optoelectronic Materials and Micro-Nano Manufacture
Wuhan National Laboratory for Optoelectronics
Wuhan, China

***Abstract*—Model-based infrared (MBIR) reflectance spectrometry has been introduced for characterization of the depth and profile of deep trench structures in dynamic random access memory (DRAM). Modeling the complex trench structure as a multilayer optical film stack with effective medium approximation (EMA) allows the determination of both trench depth and width from Fourier-transfer infrared (FTIR) reflectance spectrum. In this paper an algorithm combining artificial neural networks (ANN) and Levenberg-Marquardt (LM) is proposed to extract the geometric parameters from the measured reflectance data. An initial estimate of the geometric parameters is obtained by the ANN, and then it is used as an input for the LM algorithm which converges to a final solution with a few iterations. The combined algorithm has been implemented on our own experimental platform, and it has been demonstrated to achieve very high accurate results as well as fast enough computation ability.**

Keywords-deep trench, model-based infrared reflectance spectrometry, artificial neural networks, Levenberg-Marquardt

I. INTRODUCTION

Fourier-transfer infrared (FTIR) reflectance spectrometry has been widely used in the semiconductor, thin film magnetic head industries to measure film thickness for decades [1, 2]. Further FTIR reflectance spectroscopy method has been developed as alternative metrology tool for characterizing layer systems with trench structures on a semiconductor wafer [3, 4]. In this paper, we propose a Model-based infrared (MBIR) metrology for high-aspect ratio deep trench with artificial neural networks (ANN) and Levenberg-Marquardt (LM) combined algorithm. The technique is non-destructive and fast which makes it an ideal metrology for process control in dynamic random access memory (DRAM) fabrication. The absolute reflectance spectrum is measured based on the use of a bare crystalline silicon reference wafer [6]. Figure 1 shows a diagram of the optical system of MBIR reflectance spectrometry, which is used in this work. Geometric parameters, including trench depth and width, are calculated by minimizing the differences between measured spectrum and model-generated reflectance spectrum. The LM algorithm is used to minimize the mean square error (MSE) by smoothly interpolating between the gradient and inverse Hessian methods. The MSE is a measure of the quality of the match between measured and model calculated reflectance data.

The wavelength of the incidence beam of the optical system in Figure 1 falls in 2 to 20 micron. As advanced DRAM utilizes 90 nm and below node technology, the complex deep trenches can be treated as submicron periodic structure, and can be represented by multilayer thin films stack with a combination of homogeneous layers on the silicon substrate using effective medium approximation (EMA) approach [7]. Modeling the effective optical properties of each effective layer allows the determination of both trench depth and width from reflectance data. ANN is used to obtain a good estimate of trench depth and width, the estimate then becomes the starting point of the LM regression algorithm which does a few iterations to reach the final solution. Measurement of geometric parameters of deep trenches is normally performed with structure specific programs, so that taper trenches, bottle trenches and recessed trenches are modeled with different programs.

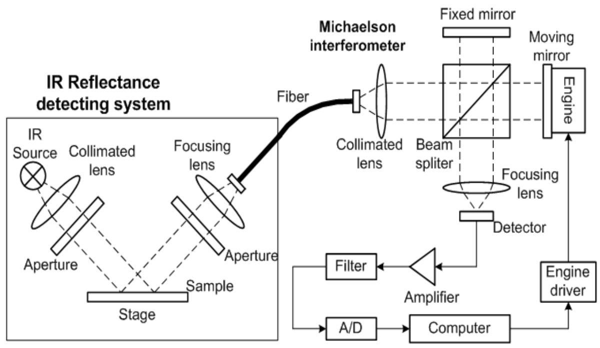

Figure 1. Diagram of the MBIR reflectance spectrometry system

This project was funded by Hi-Tech Research and Development Program of China (Grant No. 2006AA04Z325), National Natural Science Foundation of China (Grant No. 50775090) and Program for New Century Excellent Talents in University of China (Grant No. NCET-06-0639).
*Contact author: Shiyuan Liu; phone: +86-27-87792409; fax: +86-27-87792413; email: shyliu@mail.hust.edu.cn.

II. MODELING

The MBIR reflectance spectrum metrology method is in simplified modeling of complex periodic structures with submicron pitch. At wavelengths greater than the pitch of a structure, light propagates through the structure as if it were a homogeneous medium with an effective refractive index which can be calculated from the geometry of the structure and the refractive indices of its component materials by using EMA. In the infrared region, the optical properties of effective homogeneous medium can be approximated using various EMA models, e.g., Maxwell-Garnett model, depending on the geometry of the trench structure. As for DRAM utilises 90 nm and below node technology, the deep trench structure can be represented as a layered system consisting of a combination of homogeneous layers and graded layers (i.e. layers with varying optical constants) on the Si substrate. Therefore the problem of modeling the optical response of a complex etched deep trench structures can be reduced to the simpler problem of modeling a multilayer film stack. Figure 2 shows a taper trench structure and its corresponding optical film stack model.

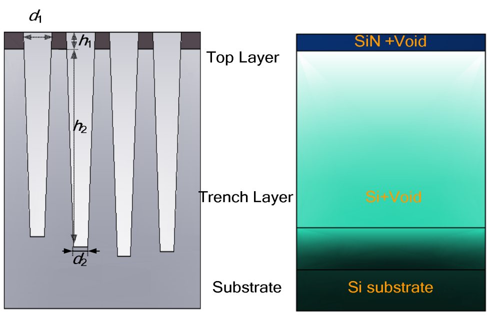

Figure 2. Scheme of a taper trench structure and its optical film stack model

Then the theoretical reflectance spectrum of the complex trench structure is represented by the calculated reflectance spectrum of its optical film stack model, and the reflectance spectrum of film stack can be accurately simulated using Fresnel's reflection equations [5].

III. PARAMETER EXTRACTION ALGORITHM

Due to the high nonlinear relationship between the geometry parameters and the reflectivity of a trench structure, the extraction of the trench depth and width is a cumbersome inverse problem. Statistical methods such as principal component analysis, discriminant analysis, or partial least-square calibration, as well as neural network, and nonlinear regression approaches can be proposed. ANN and the LM algorithm are combined to provide a fast extraction method with high accuracy. The extracting steps are presented in Figure 3 and will be described in detail in the following.

ANN has been shown to provide good approximating functions for nonlinear models with high computational speed, even with large problems due to their highly parallel structure and powerful representational capacity. While there are a variety of different artificial neural network architectures in use, the one used here is the multilayer perceptron (MLP) [8]. Typically, this type of network consists of three or more layers. Figure 4 shows an example of an MLP type ANN, which has 4 input neurons, 5 neurons in the hidden layer, and 3 output neurons. The back-propagation learning algorithm is employed for training the network.

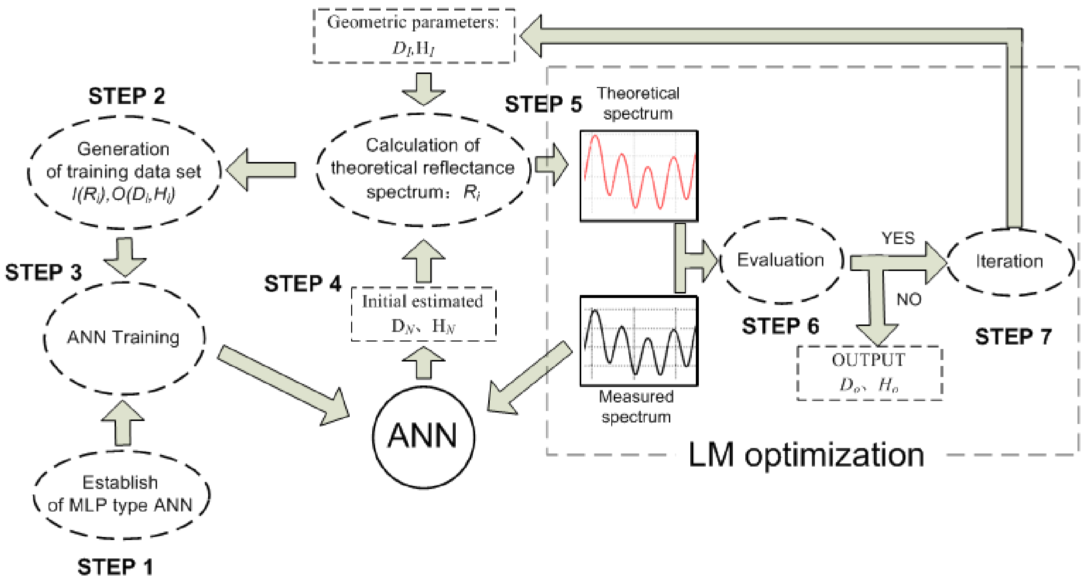

Figure 3. Flow of geometric parameter extraction

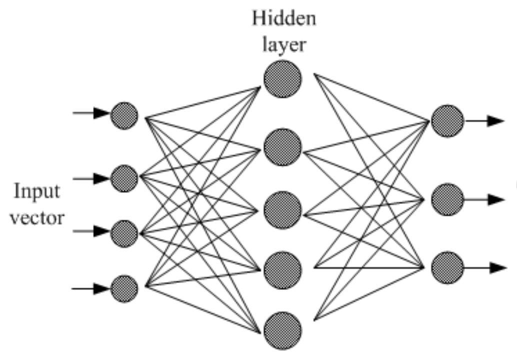

Figure 4. Architecture of MLP type ANN

In order to apply the MLP type ANN to the extraction of geometric parameters from measured reflectance data, we will use the modeling method and Fresnel's reflection equations described in section 2 to generate the training data set. The reflectance data $R(\lambda)$ represents as input, the trench width vector D and depth vector H as output. The training process starts by creating N data sets by applying different input $[D_i\ H_i]$ to the Fresnel's reflection equations, and getting $R_i(\lambda)$, for $i=1,\ldots,N$.

Training the ANN by $R_i(\lambda)$ as input and $[D_i\ H_i]$ as desired output. After several hours or days training, the neural network is ready to find initial trench depth and width with an acceptable accuracy based on the training data.

The measured reflectance data are processed first by the ANN which provides an initial output with a small percentage of error depending on the training program. The initial output become the starting estimate of the LM algorithm, which performs a few iterations and further get the accurate solution. In this way, the advantages of both ANN and LM algorithms are obtained by combining them.

To improve the accuracy and speed of the neural network training, several skills have been developed. First is the choosing of input reflectance data. In our previous research [5], each of the geometric parameters affects the spectrum features respectively, so we choose the reflectivity by wavelength with the equal step. As in the wavenumber range, the reflectance data serial becomes sparser as the wavenumber increase. In this way, the spectrum features are represented by the selected reflectance data comprehensively while avoid too much input for training, thus the training speed and the extracting accuracy can be increased simultaneously. Secondly, a few percent of noise is added to the input training data to represent the noise signal in measured spectrum. Finally, the number of neurons in hidden layer may be set with experimental experience.

IV. EXPERIMENTS AND DISCUSSION

For simplicity, a MLP type ANN with three layers has been created for the taper trench structure, and the corresponding number of neurons in input layer is 37 and in output layer is 4, the appropriate number in hidden layer ranges from 25 to 50 with experiential formula. The geometric parameters in training data set range as following: the top layer ranges from 100 nm to 300 nm, the trench depth ranges from 3µm to 7µm, the void fraction of trenches, which equal to trench width divided by trench period, in each layer ranges from 0.5 to 0.8. The wavelength of the input reflectance data ranges from 2µm to 20 um with equal step of 0.5µm. The training was performed on a 2.66 GHz Celeron computer and may take up about several hours for the taper trench structure.

In the performance of this measurement, the measured reflectance data serial is scaled to 37 point at the corresponding wavenumber. The chosen data serial is presented to the ANN, and then the LM algorithm does several iterations using the output of the ANN.

In 200 times of independent extraction with randomly generated reflectance data, the trained ANN can provide geometric parameters within a few milliseconds, and the LM algorithm converges within ten iterations in less than 3 seconds for a preset MSE with the same computer for training. We have compared the calculation speed of ANN and LM combined algorithm with other global optimization algorithm, such as Adaptive Simulated Annealing (ASA). The ASA algorithm costs more than 1 minute for the same extracting problem in this section with the same computation environment. The time-consuming rises exponentially as the complexity of trench structure increases with ASA, but not happens with ANN and LM combined algorithm.

Figure 5 and Figure 6 show the actual geometric parameters versus the final output of ANN and LM combined algorithm for depth and void fraction of trench layer, respectively.

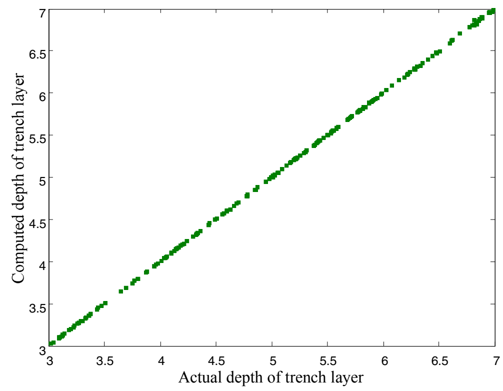

Figure 5. Actual versus computed depth of trench layer

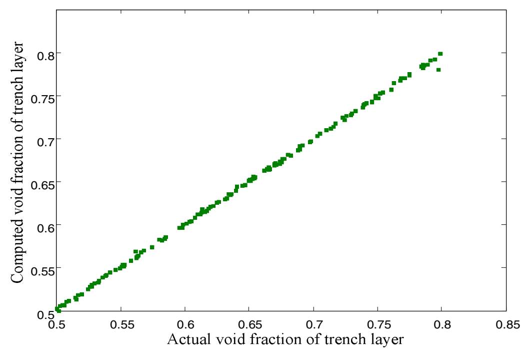

Figure 6. Actual versus computed void fraction of trench layer

Since the LM algorithm requires a starting point near the solution of in order to converge, one more test of the combined algorithm has been performed to determine whether the ANN output is a good start point and convergence with high accuracy is possible. The measurement processes is tested with another 200 times of independent extraction. Figure 7 and Figure 8 show the measurement error distribution of depth and void fraction of the top layer, respectively.

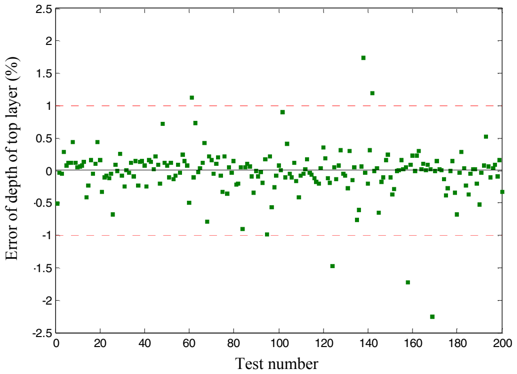

Figure 7. Error distribution of depth of top layer

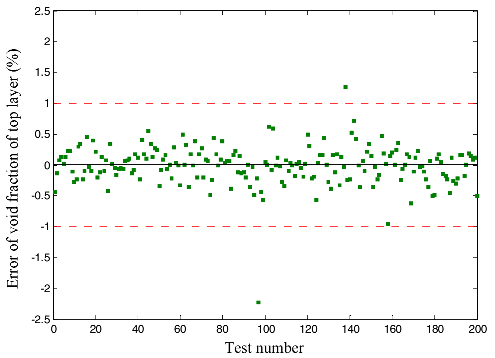

Figure 8. Error distribution of void fraction of top layer

From the error distribution of void fraction of top layer, we can conclude that 99% of tested void fraction converges in ±1% and 97% of tested depth converges in ±1% with ANN output and ten times of iterations by LM algorithm. However, other tested results that distributed out of ±1% can be converged with more of several iterations.

Figure 9 shows the experimental reflectance spectrum, the calculated spectrum with ANN output and final LM output. The geometric parameters of this taper trench are as following: the void fraction of top layer is 0.65, the depth of top layer is 0.16 um, the bottom void fraction of trench layer is 0.6, and the depth of trench layer is 6.7 µm.

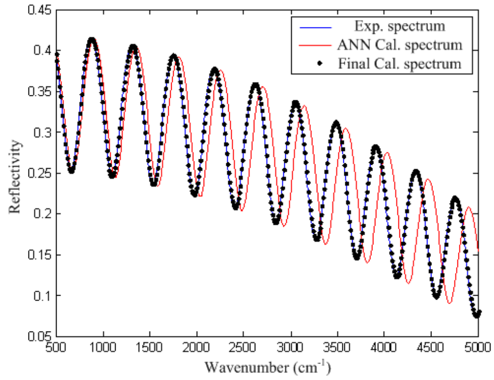

Figure 9. Experimental reflectance spectrum and calculated reflectance spectrum of output parameters.

V. CONCLUSIONS

In this paper, we have focused on the ANN and LM combined algorithms and its application to solve the inverse problem in MBIR reflectance spectrometry. The ANN training may be one of the key processes in this metrology method. As in the application of in-line monitoring of deep trench fabrication, the range of training data set can be decrease to the extension around the expected etching depth or width, and the training of a neural network for a new trench structure can be finished in a few hours with high accuracy. With this fast parameter extracting algorithm, the MBIR reflectance spectrometry offers an ideal approach for the measurement of within-wafer uniformity and wafer-to-wafer process variations, thus it provides more complete data for process optimization and control for deep trench fabrication in DRAM.

REFERENCES

[1] P. Y. Guittet, U. Mantz, P. Weidner, "Infrared spectroscopic ellipsometry in semiconductor manufacturing", Proceedings of SPIE, 5375(2): pp 771-778, 2004

[2] V. Hopfe, D. W. Sheel, C. I. M. A. Spee, R. Tell, P. Martin, A. Beil, et all, "In-situ monitoring for CVD processes", Thin Solid Films, 442(1-2): pp 60-65, 2003.

[3] T. Kessel, H. K. Wickramasinghe, "Measure-ment of trench depth by infrared interferometry", Optics Letters, 24(23): pp 1702-1704, 1999.

[4] S. Charpenay, J. Xu, J. Haigis, P. A. Rosenthal, P. R. Solomon, J. M. Bustillo, "Real-time etch-depth measurements of MEMS devices", Journal of Microelectromechanical Systems, 11(2): pp 111-117, 2002.

[5] C. W. Zhang, S. Y. Liu, T. L. Shi, H. Y. Gu, "Modeling and Simulation of Infrared Reflectance Spectra of Deep Trench Structures of DRAM", Proceedings of 3rd IEEE International Conference on Nano/Micro Engineered and Molecular Systems, pp 227-230, 2008.

[6] S. Y. Liu, H. W. Shen, C. W. Zhang, H. Y. Gu, "Model-Based FTIR reflectometry measurement system for deep trench structures of DRAM", Spectroscopy and Spectral Analysis, in press.

[7] S. Y. Liu, H. Y. Gu, C. W. Zhang, H. W. Shen, "A fast algorithm for reflectivity calculation of micro/nano deep trench structures by corrected effective medium approximation", Acta Physics Sinica, 57(9): pp 5996-6001, 2008

[8] J. E. Dayhoff, Neural network Architectures: An introduction, Van Nostrand Reihold, New York, 1990

[9] D. E. Rumelhart, G. E. Hinton, and R. J. Williams, Parallel Distributed Processing, MIT Press, Cambridge, MA, 1987.