

Metrology of deep trench structures in DRAM using FTIR reflectance spectrum

Chuanwei ZHANG^a, Shiyuan LIU^{*,a}, Tielin SHI^b

^a State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan, China.

^b Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan, China.

ABSTRACT

The demand for advanced DRAM technologies with smaller ground rules lead to new challenges for online metrology of high aspect-ratio deep trench structure. In addition to common metrology methods like ellipsometry, scanning electron microscopy (SEM), and atomic force microscopy (AFM), the use of further measurement techniques are needed for advanced node technology. This paper proposes a technique for metrology of critical dimension (CD) of deep trenches formed as capacitors in advanced dynamic random access memory (DRAM) using Fourier-transform infrared (FTIR) reflectance spectrometry. This technique is based on a fast but accurate modeling of the complex periodic deep trench structure, which is represented as a multilayer thin film stack with a combination of homogeneous layers on the silicon substrate using effective medium approximation approach. The metrology problem is solved by an artificial neural network (ANN) and Levenberg-Marquardt (LM) combined algorithm to find the values of the modeling parameters which should produce a best fit to the given measured spectrum. This technique is validated by simulation of extracting geometry parameter of actual DRAM trench structures, and demonstrated to be an adequate approach for the determination of the structure parameters.

Keywords: deep trench, DRAM, FTIR reflectance spectrum, metrology

1. INTRODUCTION

The manufacturing of advanced deep trench DRAM devices presents a number of important metrology challenges related to the high-aspect-ratio deep trench capacitor structure formed on silicon substrate. Bottle-shaped trench with an aspect-ratio in the order of 50:1 is widely adopted in the 90 nm node technique^[1]. As deep-trench devices have been packed more tightly, the top critical dimension (CD), bottom CD and depth-dependent features must now be monitored to ensure process control. Many conventional methods exist for the occasional, periodic or quasi-continuous monitoring of the parameters mentioned above. AFM is a mature monitoring tool for the production of feature sizes down to approximately 90 nm and below^[2]. However, it yields only incomplete information about trenches, e.g., only a total etching depth and an etching depth profile. Other major barriers to AFM monitoring are the slow throughput, the limited scanned depth and the accuracy degradation associated with probe tip wear and spike noise caused by unwanted oscillation on the steep slopes of high-aspect-ratio patterns. Scan electron microscopy (SEM) is a dominating metrology technology in current industry process control^[3], yet it is destructive, expensive and time consuming as the sample needs to be cross-sectional cut and prepared.

As deep trench technology transits to 65 nm node and even 45 nm node, metrology challenges are introduced for traditional approaches, and optical metrology methods are highly desired because they provide rapid measurements on product wafers, enabling routine monitoring and advanced process control. Based on Fourier transform infrared reflectance (FTIR) spectroscopy which has been traditionally used in semiconductor manufacturing for monitoring chemical composition of boro phospho silicate glass (BPSG) and other films and measuring the thickness of epitaxial layers^[4,5], this paper proposes a nondestructive method of infrared reflectance spectrometry with simultaneous determining of multiple trench parameters of DRAM. This technique is based on a fast but accurate modeling of the

* Contact author: shyliu@mail.hust.edu.cn; phone: +86 27 87792409; fax: +86 27 87792413.

complex periodic deep trench structures. At wavelengths greater than the pitch of a periodic structure, light propagates through it as if it were homogeneous medium layers. As DRAM utilizes 90 nm and below node technology, the deep trench structure can be represented as a multilayer thin film stack with a combination of homogeneous layers on the silicon substrate using effective medium approximation approach. This modeling uses the geometric parameters and the optical properties of the trench structure as inputs, and calculates the corresponding theoretical spectrum as output by Fresnel's reflection equations. Then the metrology problem can be considered to find the values of the modeling parameters which should produce a best fit to the given measured spectrum. This is performed by an artificial neural network and Levenberg-Marquardt combined algorithm. The validity of this metrology technique was investigated by simulation of extracting geometry parameter of taper trenches structure of 90 nm node with an aspect-ratio of more than 50:1. The measured spectrum was simulated with rigorous coupled-wave analysis method. The simulation results show that the technique is simple to implement while the measurement error falls in 0.1% and the standard deviation falls in 6.03×10^{-6} . The technique is demonstrated to be an adequate approach for the determination of the structure parameters from the infrared reflectance spectrum, and it is expected to provide a useful practical tool for the in-line measurement and process control on product wafers.

2. MATHEMATICAL EQUATIONS

2.1 General description of the measurement scheme

The principle of the measurement utilizes the interference signal caused by infrared radiation that reflected from the top surface of deep trench structure as well as from the bottom of the trenches. The probing light spectra range falls within the region of silicon transparency, which in this case for infrared light. As shows in Figure 1, the infrared radiation interacts with the etched trenches and homogeneous layers, e.g., cap layers of silicon dioxide or silicon nitride. The light reflects at trench surfaces and layer interfaces, and yield interference pattern that contains trench geometry information.

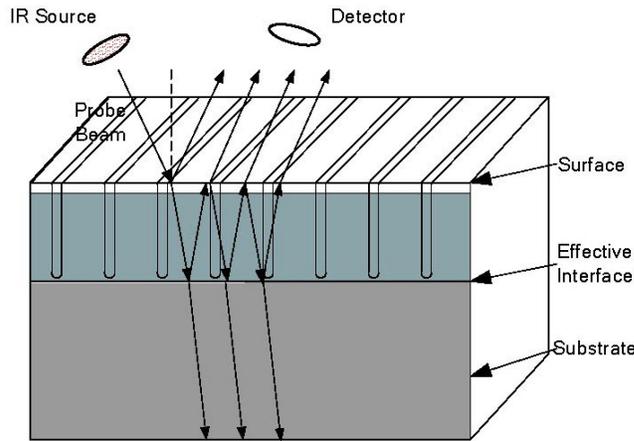


Fig.1. Scheme of measurement of FTIR spectrum

The infrared metrology proposed in this paper 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 an effective medium approximation (EMA) [6-10]. 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 utilizes 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 stack. Figure 2 shows the recessed DRAM structure and its corresponding optical film stack model.

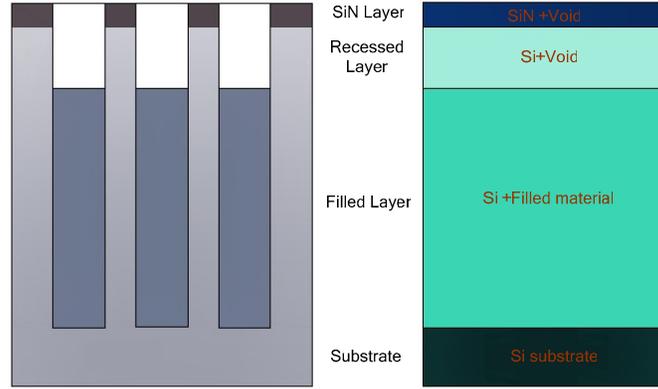


Fig.2. Scheme of recessed trench structure and its corresponding optical film stack model

FTIR reflectance spectrometry method consists of following steps: the first step is the numerical calculation of theoretical reflectance spectrum of trench structure, which is simplified by calculating the reflectance of its corresponding optical film stack model. Then the reflectivity of actual structure is measured experimentally. The third step is the extraction of geometry parameters of measured structure with comparison of measured spectrum and theoretically calculated spectrum. The theoretical spectrum with the best math to the measured spectrum is found, and we can conclude that that the parameters (trench width and depth) of analyzed structure coincide with parameters corresponding to theoretical spectrum with the best match. The detail process for theoretical spectrum calculation and parameter extraction will be described in the subsection 2.2 and 2.3, respectively.

2.2 Calculation of reflectance spectrum

As mentioned above, the optical property of a homogeneous layer in Figure 2(b), which represents the corresponding trench layer in Figure 2(a), can be determined with EMA approach. For deep trenches on DRAM can be considered to be a sub-wavelength periodic structure, and the effective refractive index of the homogeneous layers are described by Eqs. (1-3) for both TE and TM directions.

$$n_{\text{eff}} = \sqrt{\varepsilon_{\text{eff}}} \quad (1)$$

$$\varepsilon_{\text{eff,TE}} = \varepsilon_{0,\text{TE}} + \frac{\pi^2}{3} f^2 (1-f)^2 (\varepsilon_1 - \varepsilon_2)^2 \left(\frac{\Lambda}{\lambda}\right)^2 \quad (2)$$

$$\varepsilon_{\text{eff,TM}} = \varepsilon_{0,\text{TM}} + \frac{\pi^2}{3} f^2 (1-f)^2 \left(\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2}\right)^2 \varepsilon_{0,\text{TM}}^3 \varepsilon_{0,\text{TE}} \left(\frac{\Lambda}{\lambda}\right)^2 \quad (3)$$

The effective refractive index n depends on geometric parameters (top CD or bottom CD), which were represented here by void fraction f , which is the ratio of top CD (or bottom CD) and the grating period Λ , and along with incident wavelength λ where ε_1 and ε_2 are relative dielectric constants of constituent materials. The zeroth-order effective dielectric constants $\varepsilon_{0,\text{TE}}$ and $\varepsilon_{0,\text{TM}}$ are given by Eqs. (4) and (5).

$$\varepsilon_{0,\text{TE}} = f\varepsilon_1 + (1-f)\varepsilon_2 \quad (4)$$

$$\varepsilon_{0,\text{TM}} = \frac{\varepsilon_1 \varepsilon_2}{f\varepsilon_2 + (1-f)\varepsilon_1} \quad (5)$$

Eqs. (2) and (3) are second order effective approximation approach, and more accurate result can be calculated with higher order equations.

The reflectance spectrum of effective multi-layer stack optical model can be accurately simulated by Fresnel's reflection equations and theory of optical propagation matrix of thin films^[11]. For a multi-layer thin film stack, the optical characteristic matrix is expressed in Eqs. (6) and (7).

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{j=1}^K \begin{bmatrix} \cos \delta_j & \frac{i}{n_j} \sin \delta_j \\ in_j \sin \delta_j & \cos \delta_j \end{bmatrix} \right\} \begin{bmatrix} 1 \\ n_j \end{bmatrix} \quad (6)$$

$$\delta_j = \frac{2\pi}{\lambda} n_j d_j \cos \theta \quad (7)$$

where θ is the incidence angle, n_j and d_j is the refractive index and geometric thickness of j th layer, respectively. The reflectivity of the effective multi-layer stack optical model can be calculated by Eqs. (8-10).

$$Y = \frac{C}{B} \quad (8)$$

$$r = \frac{n_0 - Y}{n_0 + Y} \quad (9)$$

$$R = r \cdot r^* \quad (10)$$

where Y is admittance, r is the reflection coefficient and R is the reflectivity.

2.3 Extraction of geometric parameters

Due to the highly nonlinear relationship between the geometry parameters and the reflectivity of the trench structure, the extraction of CD and trench depth is a cumbersome inverse problem, and 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. In this paper, artificial neural network and the Levenberg-Marquardt algorithm are combined to determine the geometric parameters from measured reflectance spectrum. A neural network is a set of simple, highly interconnected processing elements imitating the activity of the brain, which are capable of learning information presented to them. In this paper artificial neural network are used to obtain good initial estimates for geometric parameters, these estimates are then used as the starting point for the Levenberg-Marquardt algorithm which converges to the final solution in a few iterations. The extracting steps shown in Figure 3 are as following^[12]:

Step 1: Establishment of ANN. Neural networks are used mainly in areas involving pattern mapping and pattern classification, like visual images and speech recognition and other problems that are too complicated for traditional methods. There are a variety of different artificial neural networks architectures, and in this paper we established a multilayer perceptron (MLP) type of ANN.

Step 2: Generation of training data set for ANN. In order to apply the MLP type of ANN we used the reflectance equations described in subsection 2.2 to generate our training data set. The process starts by creating N data set by applying different input (D_i, H_i) to the reflectance equations and get output R_i . D_i, H_i and R_i represent the trench critical dimension, trench depth and reflectance spectrum, respectively, for $i=1, \dots, N$.

Step 3: Training of ANN. The back-propagation learning algorithm is employed for training the network. This algorithm is a classified as a supervised learning algorithm since it requires a target value for a given set of input parameter, in this work the network is trained with $I(D_i, H_i)$ and $O(R_i)$ for input and output patterns.

Step 4: Calculation with ANN. The measured spectrum is used as the input of trained ANN, and get the initial estimated critical dimension D_N and trench depth H_N .

Step 5: Calculation of theoretical reflectance spectrum. The initial estimated D_N and H_N are used to get a theoretical reflectance spectrum using reflectance equations.

Step 6: Evaluation of the result. The theoretical spectrum is compared with measured spectrum, and an evaluation function is introduced to estimate the difference. If the evaluation function was fulfilled the pre-established criterion, D_N and H_N are considered as the geometric parameter of measured trench structure. If the criterion is not fulfilled, the Levenberg- Marquardt optimization algorithm get a new pair of interactive parameters D_i and H_i , and repeat step 6 until the criterion is fulfilled.

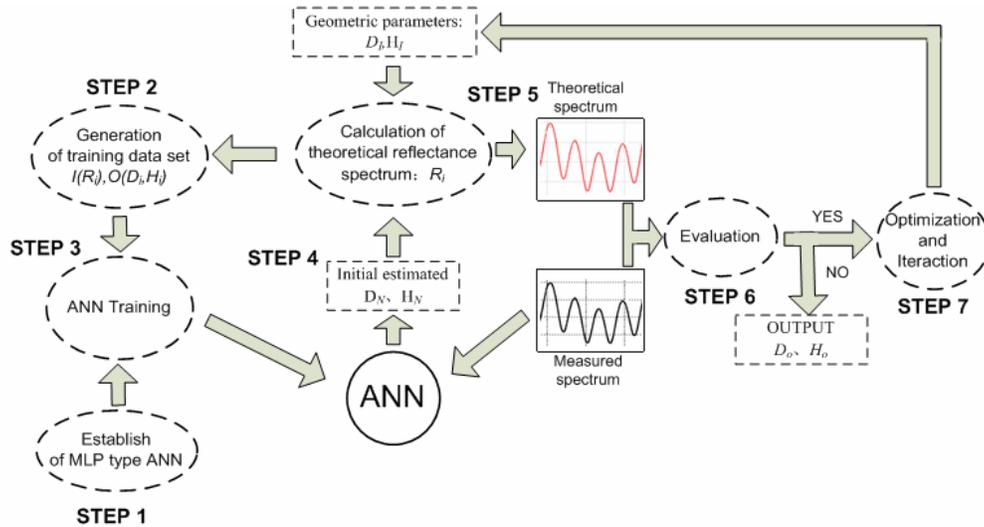


Fig. 3. Flow of geometric parameter extraction with ANN and LM algorithms

3. SIMULATION AND ANALYSIS

The validity of this metrology technique was investigated by simulation of extracting geometry parameter of a taper trenches structure an aspect-ratio of more than 50:1. Parameter for the simulation as following: the simulation based on an taper trench structure show in Figure 4, which is in the middle process for recessed trench fabrication shown in Figure 2. The pitch of deep trench P is 0.18 μm , the void fraction of top layer $f_1=d_1/P$ is 0.73, the trench depth of top layer and trench layer are 0.17 μm and 5.27 μm , respectively. The wavenumber of incidence beam ranges from 500 to 5000 cm^{-1} (wavelength ranges from 2 to 20 μm), and the incidence angle is 45° . The measured spectrum was simulated with rigorous coupled-wave analysis (RCWA), which is an accurate method for the calculation of reflectivity of trench structure, but it's time-consuming^[13]. Some random noise signal is added to the RCWA simulated spectrum in order to represent the measured noise signal.

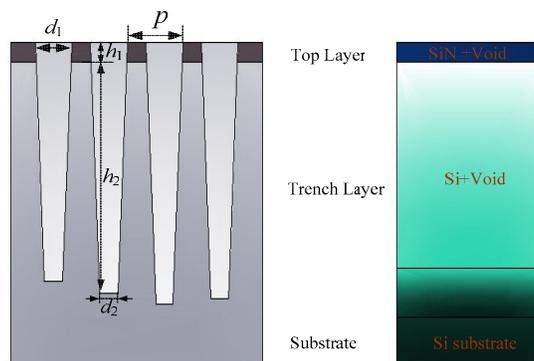


Fig.4. Scheme of taper trench structure and its effective multilayer stack

The extraction results in Figure 5 shows 71 times of independent simulation. The standard deviation of void fraction of top layer, void fraction of trench layer, depth of top layer, depth of trench layer are 2.33×10^{-6} , 1.85×10^{-6} , 6.03×10^{-6} , 3.32×10^{-6} , respectively, and the extraction error falls in 0.1%. All the extraction processes are finished in 3 seconds, which is adequate for the online metrology in the deep trench fabrication.

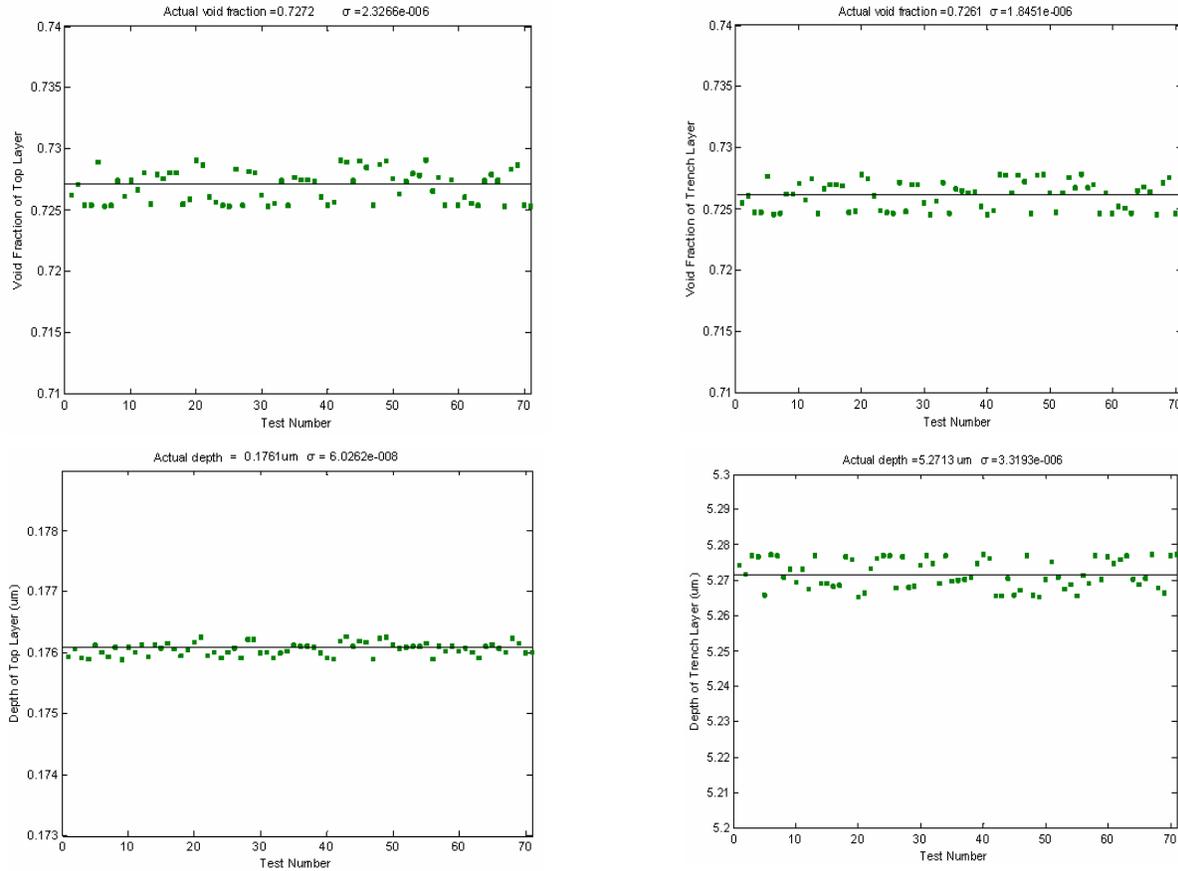


Fig.5. Extraction results of simulation for taper trench structure

The comparison of actual spectrum, which is simulated with RCWA method, and theoretical spectrums, which are simulated with EMA by the extraction results of ANN and LM algorithms, is shown in Figure 6. It is demonstrated that the ANN algorithm gets more accurate results than the LM algorithm.

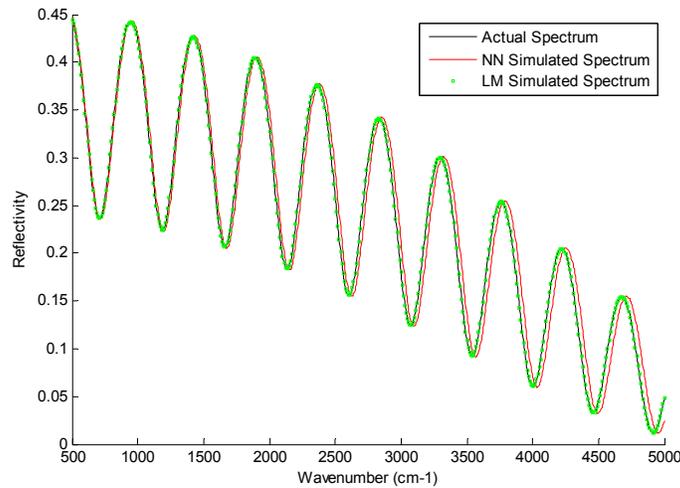


Fig.6. Comparison of actual spectrum and theoretical spectrum

4. CONCLUSION

A method for measuring deep trench structures of DRAM based on FTIR is described in detail. The measured reflectance spectrum of trench structure is simulated with RCWA method, and the trench parameter is extracted from the RCWA simulated spectrum with ANN and LM combined algorithm. The validity of the modeling and parameter extracting algorithm are investigated by the extraction of profile parameters of the taper trench structure. For its high accuracy and fast extraction ability, the FTIR reflectance spectrometry is demonstrated to be adequate for the monitoring of deep trench fabrication on DRAM, and it can offer 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 on DRAM. For the simplicity of the modeling method of sub-wavelength periodic structure, this method can also be developed and applied to the measurement of deep trenches on power devices such as MOSFETs.

AKNOWLEDGEMENT

The authors wish to acknowledge the financial support from 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).

REFERENCES

- [1] Rudolph, U., Weikmann, E., Kinne, A., Henke, A., VanHolt, P., Wege, S., Khan, A., Pamarthy, S., Schaftlein, F., and Lill, T., "Extending the capabilities of DRAM high aspect ratio trench etching", Proceedings of 2004 IEEE/SEMI Advanced Semiconductor Manufacturing Conference and Workshop, 89-92 (2004).
- [2] Watanabe, M., Baba, S., Nakata, T., Kurenuma, T., Kuroda, H., and Hiroki, T., "An advanced AFM sensor for high-aspect ratio pattern profile in-line measurement", Proceedings of SPIE, 61522A (2006).
- [3] Srivastava, R., Yelehanka, P., Kek, H. A., Ng, S. L., Srinivasan, V., and Peltinov, R., "A novel approach to characterize trench depth and profile using the 3D tilt capability of a critical dimension-scanning electron microscope at 65nm technology node", Proceedings of SPIE, 61524I (2006).
- [4] Mazzola, M. S., Sunkari, S. G., Mazzola, J. P., and Das, H., "Improved resolution of epitaxial thin film doping using FTIR reflectance spectroscopy", Materials Science Forum 483, 397-400 (2005).

- [5] Kibe, M., Sakai, T., Ohiwa, T., Mikami, T., Tsumura, A., and Kanazashi, Y., "In-situ damascene trench RIE depth monitor using infrared interferometric spectrometry", Proceedings of 2003 IEEE International Symposium on Semiconductor Manufacturing, 362-365 (2003).
- [6] Born, M. and Wolf, E., [Principles of Optics], Seventh Edition, Cambridge University Press (1999).
- [7] Vidal, F. G., Pitarke, J. M., and Pendry, J. B., "Effective medium theory of the optical properties of aligned carbon nanotubes", Phys. Rev. Lett. 78, 4289-4292 (1997).
- [8] You, C. Y., Shin, S. C., and Kim, S. Y., "Modified effective medium theory for magneto-optical spectra of magnetic materials", Phys. Rev. B 55, 5953-5958 (1997).
- [9] Kikuta, H., Yoshida, H., and Iwata, K., "Ability and limitation of effective medium theory for subwavelength gratings", Opt. Rev. 2, 92-99 (1995).
- [10] Zhang, C., Yang, B., Wu, X., Lu, T., Zheng, Y., and Su, W., "Calculation of the effective dielectric function of composites with periodic geometry", Physica B 293, 6-32 (2000).
- [11] Pochi, Y., [Optical Waves in Layered Media], New York: Wiley (1988).
- [12] Zhang, C. W., Liu, S. Y., and Shi, T. L., "MBIR reflectance spectrometry for deep trench structure with ANN and Levenberg-Marquardt combined algorithm", Proceeding of 3rd International Conference on Sensing Technology, in press (2008).
- [13] Moharam, M. G., Grann, E. B., and Pommet, D. A., "Formulation for stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings", J. Opt. Soc. Am. A 12, 1068-1076 (1995).
- [14] Zhang, C. W., Liu, S. Y., Shi, T. L., and Gu, H. Y., "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, 227-230 (2008).
- [15] Liu, S. Y., Gu, H. Y., Zhang, C. W., and Shen, H. W., "A fast algorithm for reflectivity calculation of micro/nano deep trench structures by corrected effective medium approximation", Acta Phys. Sin. 57, 5996-6001 (2008).