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Modeling and Simulation of Infrared Reflectance Spectra of Deep Trench Structures of DRAM

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***Abstract*—This paper proposes a nondestructive technique for measuring deep trench structures of DRAM using infrared reflectance spectrometry. By processing layered-film optical model equivalents of various trench array structures with effective medium theory, the reflectance spectra of optical models are accurately simulated with Fresnel's reflection equations, and the relationships between modeled spectra and trench geometric parameters are analyzed. It is fully expected that this technique will be simple to implement and will provide a useful practical tool for the in-line measurement and process control on product wafers.**

Keywords- deep trench; DRAM; effective medium theory; infrared reflectance spectrum; modeling; simulation

I. INTRODUCTION

Deep-trench with high-aspect ratio is widely used in microelectronic and microelectromechanical system (MEMS) devices, e.g., advanced dynamic random access memory (DRAM) devices adopting bottle-shaped trenches can reach an aspect ratio of 50:1 [1, 2]. 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. One important method is atomic force microscopy (AFM), which represents the preferred industrial solution. AFM is a mature monitoring tool for the production of feature sizes down to approximately 90 nm and below [3]. 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 [4], 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 90 nm node and even 65 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 [5-7], this paper proposes a nondestructive method of infrared reflectance spectrometry with simultaneous determining of multiple trench parameters of DRAM. The modeling and simulation of the method are described in detail.

II. MODELING OF DEEP TRENCH

The principle of the measurement utilizes the interference signal caused by infrared radiation that reflected from the top surface of deep trench structure, or thin film material, as well as from the bottom of the trenches. The probing light spectral range must fall within the region of silicon transparency, which in this case for infrared light. As shows in Fig.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.

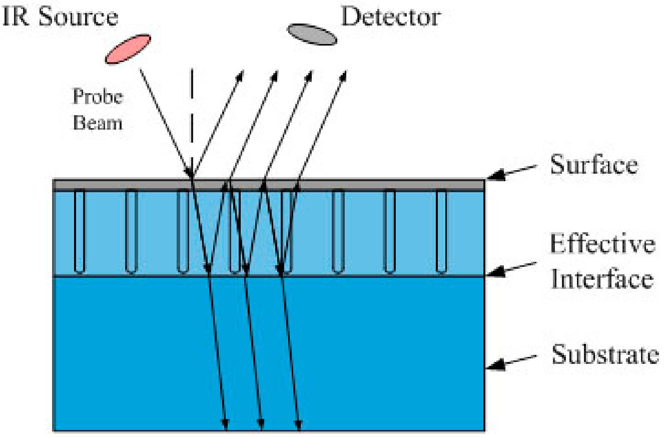

Fig.1. Illustration of infrared reflection spectrometry configuration

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) [8]. In the infrared region, the optical properties can be approximated using various EMA models, e.g., Maxwell-Garnett model, depending on the geometry of the trench structure. As DRAM utilizes 90 nm and below node technology, the deep trench structure can be represented as a layered system consisting of a combination

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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 a simpler problem of modeling a multilayer stack. Figure 2 shows three typical DRAM structures and their corresponding optical film stack models.

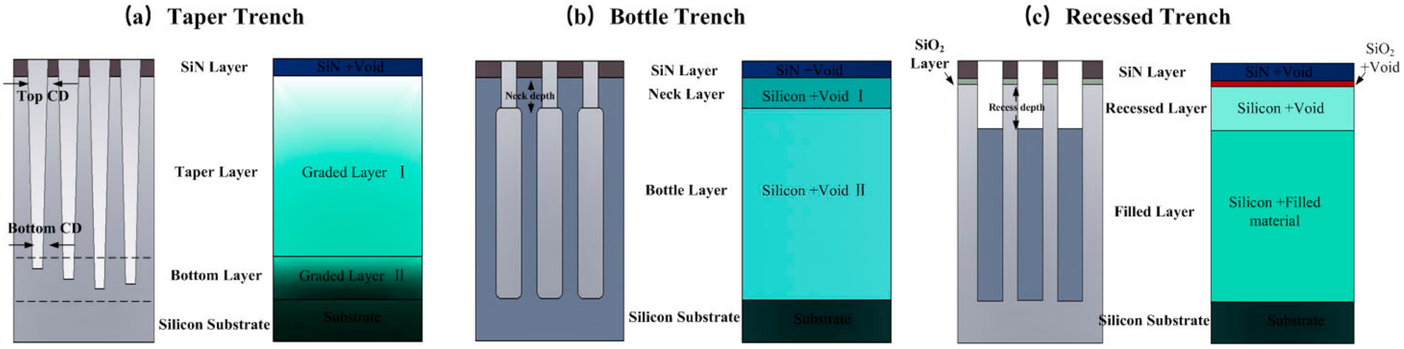

Fig.2. Typical DRAM structures (left) and their corresponding multiple film stack models (right) of a) multi-layered taper trench, b) multi-layered bottle trench, and c) multi-layered recessed trench. Geometric parameters are modeled as layer thickness and void density.

As mentioned above, the optical constants of a homogeneous layer, which represents the deep trench, can be determined with EMA approach. The DRAM deep trench can be considered to be a sub-wavelength periodic structure, and the effective refractive index of the structure is determined by Equations (1-3) for both TE and TM directions.

$$n_{\mathrm{eff}} = \sqrt{\varepsilon_{\mathrm{eff}}} \tag{1}$$

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

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

The effective refractive index n_{eff} depends on the geometric parameters of the deep trench (top CD or bottom CD), which are represented here by void density 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 $\varepsilon_{0,\mathrm{TE}}$ and $\varepsilon_{0,\mathrm{TM}}$ are given by Equations (4) and (5), respectively.

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

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

Equations (2) and (3) are the second order EMA approach, more accurate result can be obtained with higher order equations [9].

The reflectance spectrum of the effective multi-layer stack optical model can be accurately simulated by Fresnel's reflection equations and theory of thin film calculation [8, 10]. For a multi-layer thin film stack, the characteristic matrix is expressed in Equation (5) and (6).

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{j=1}^{K} \begin{bmatrix} \cos\delta_j & \frac{i}{n_j}\sin\delta_j \\ in_j \sin\delta_j & \cos\delta_j \end{bmatrix} \right\} \begin{bmatrix} 1 \\ n_j \end{bmatrix} \tag{5}$$

$$\delta_j = \frac{2\pi}{\lambda} n_j d_j \cos\theta \tag{6}$$

where θ is the incidence angle, n_g is the refractive index of the substrate, n_j and d_j is the refractive index and geometric thickness of jth layer, respectively.

The reflectivity of the effective multi-layer stack optical model can be calculated by Equations (7-9).

$$Y = \frac{C}{B} \tag{7}$$

$$r = \frac{n_0 - Y}{n_0 + Y} \tag{8}$$

$$R = r \cdot r^{*} \tag{9}$$

where Y is the admittance and r is the reflection coefficient.

III. SIMULATION AND ANALYSIS

Comparison of reflectance spectrum calculated by rigorous coupled-wave analysis (RCWA) [11] and EMA was carried out before perfoming simulation of the deep trench structures. Based on the comparison, we use model simulation for preliminary investigation of the relationship between reflectance spectrum characteristic and trench geometric parameters with EMA.

RCWA is an accurate method for the calculation of reflectivity for high aspect 3-D microstructures, but it takes a few minutes for a single reflectance spectrum evaluation. EMA is very attractive for its capability of modeling a complex structure to be a film stack and the simulated calculation can be finished in about 100 milliseconds. As the trench period is about 0.12~0.2 μm, and it is much shorter than the wavelength of the infrared light we used, the simulated spectra between RCWA and EMA get perfect agreement as shown in Fig.3.

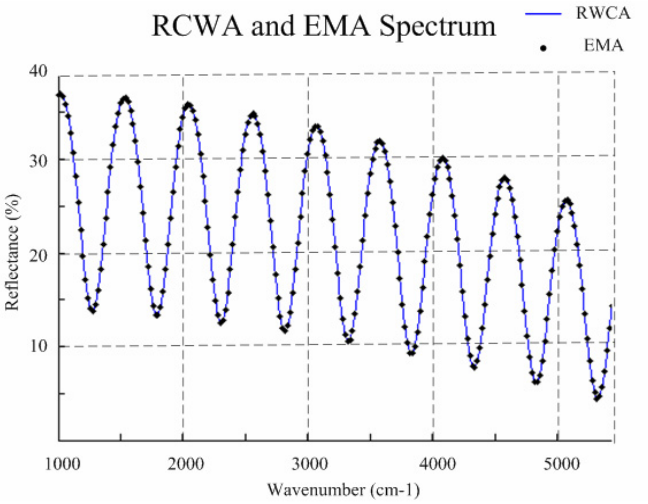

Fig.3. Simulated spectra calculated with RCWA and EMA

Figure 4 to Figure 7 depict the influence of parameters variation on the spectra. All of the simulations are based upon the taper deep-trench along with its optical model shown in Fig.2 (a). Figure 3 shows the simulated reflectance spectrum with trench depth varying from 5 μm to 7 μm; as the trench depth increases, the oscillation pattern period decreases apparently.

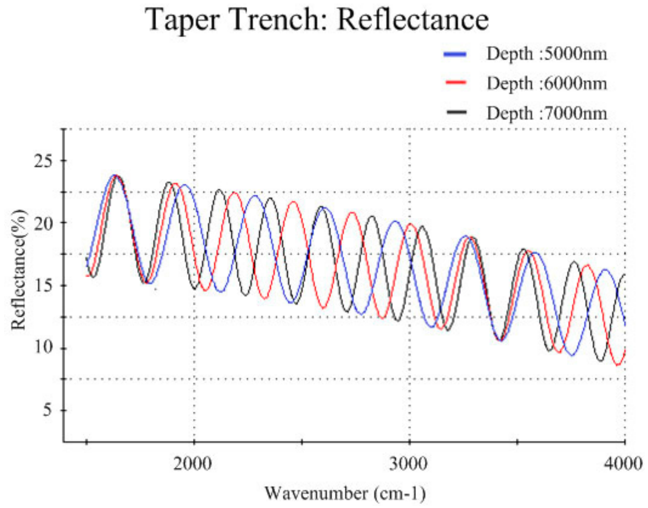

Fig.4. Simulated spectra with different trench depth for a multi-layered taper trench structure

Figure 5 shows the simulated spectra for cap layer with void density from 15% to 25%, i.e., a variation of the top CD. It demonstrates that the top CD has a strong effect on the overall reflectance. As the top CD increases, the optical contrast between air and the cap layer decreases, thus the overall reflectance decreases. Aslo from the simulated spectra we can find that the Top CD has a slight effect on the oscillation period of the reflectance spectrum. As the void density increases, the oscillation period increases proportionally.

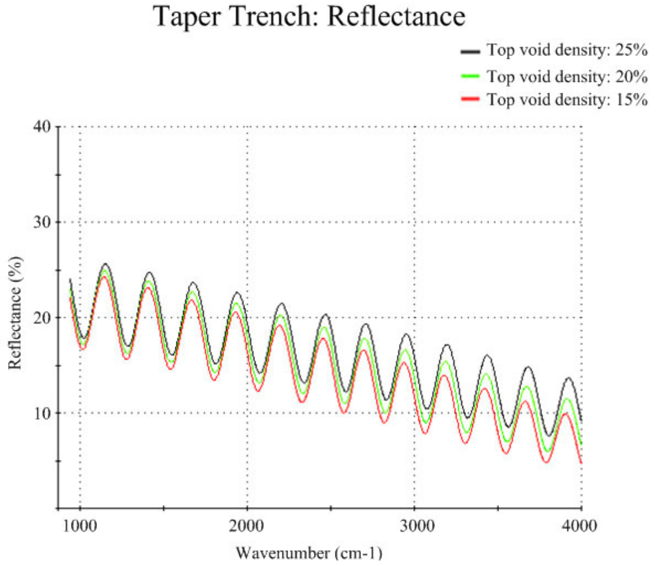

Fig.5. Simulated spectra with different top CD for a multi-layered taper trench structure

Figure 6 illustrates the simulated spectra for bottom layer fraction from 15% to 25%, i.e., a variation of the bottom bottom CD. Similar to the relationship between top CD and overall reflectance, the bottom CD affects the modulation depth of the reflectance spectrum with direct portions.

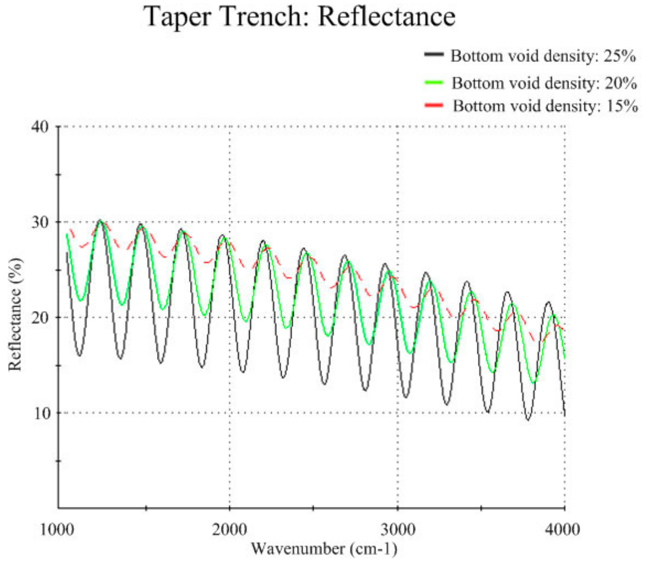

Fig.6. Simulated spectra with different bottom CD for a multi-layered taper trench structure

In an ideal optical model, the trench bottom is supposed to be flat. However, there are gradual narrowing and depth variation at the bottom in real structures. Figure 7 shows the contrast of spectra with and without a graded layer, i.e., a layer with gradually changing optical constants. As shown in the spectra, the interference modulation decays apparently when the graded layer is taken into account.

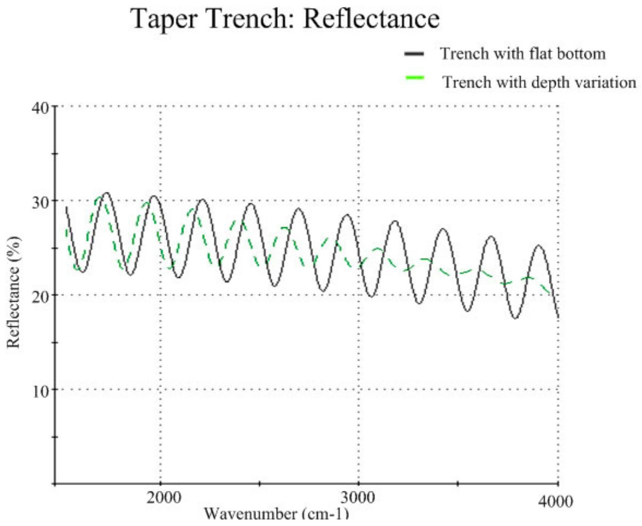

Fig.7. Simulated spectra with trench to trench depth variation for a multi-layered taper trench structure

Other typical trench structures in DRAM, e.g., bottle trench and recessed trench, are modeled similar to taper trench with more complicate multi-layer models in Fig.2 (b) and Fig.2 (c). These kinds of structures generate more than one modulate period which represent related layer depths. Figure 8 illustrates a simulated spectrum of bottle trench structure in Fig.2 (b). The spectrum contains two periodic components, a long period that relates to neck layer thickness and a short period that relates to bottle layer thickness.

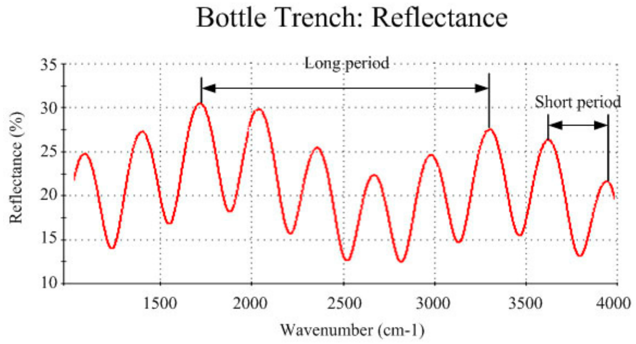

Fig.8. Simulated infrared reflection spectrum for a bottle-trench structure

IV. CONCLUSIONS

The simulation above reveals the relationship between the spectra characteristics and the trench parameters, thus we can conclude that:

(1) The interference modulate period relates to the trench depth and void density, and is mainly effected by each layer depth; the fringe period is inverse proportional to the total trench depth and directly proportional to the void density of each layer.

(2) The overall reflectivity relates to the void density of cap layer, and is inversely proportional to the top CD.

(3) The modulate amplitude of spectrum relates to the void density of the trench layer, and the amplitude is directly proportional to the bottom CD.

(4) The decaying of spectrum modulation relates to the trench depth variation from trench to trench, and the decayed rate is directly proportional to the depth diversity.

(5) The periodic components represent different trench layer depth, and the longer periodic component represents the deeper trench layer.

According to the relationships between reflectance spectrum characteristics and trench geometry dimensions concluded above, the measuring parameters can be easily extracted from measured reflectance spectrum with various spectrum analysis methods, e.g., Fourier transform methods, the frequency is directly proportional to the depth and the amplitude of each frequency related to the void density of corresponding layers.

The investigation in this paper demonstrates that the infrared reflection spectrometry provides a hopeful nondestructive metrology technique for advanced DRAM structures with the potential of measuring multiple parameters and replacing the traditional time-consuming and expensive metrology methods. It is also fully expected to be applied in the measurement of other 3-D submicron pitch devices.

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