

# Modeling of 3-D Trench Structures with Corrected Effective Medium Approximation for Model-Based Infrared Reflectometry

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**Abstract**- Model-based infrared reflectometry (MBIR) has been introduced recently for measuring deep trench structures in microelectronics. The success of this technique relies heavily on accurate modeling and fast calculation of the infrared metrology process, which still remains as one challenge. In this paper, we propose a modeling method named corrected effective medium approximation (CEMA) for accurate and fast reflectivity calculation of three-dimensional (3-D) trench structures. The independence of the CEMA on trench depth, azimuth of incidence and the polarization state has been investigated to demonstrate the validity of the CEMA.

## BACKGROUND

The demands on optical metrology of deep trench structures continue to increase as microelectronic devices become more complex and three-dimensional (3-D). Recently, model-based infrared reflectometry (MBIR) has been developed for measuring deep trenches in DRAM and FinFET devices [1]. The success of this technique relies heavily on accurate modeling and fast calculation of the infrared metrology process, which still remains as one challenge. The rigorous coupled wave analysis (RCWA) theory is commonly used for modeling with very high accuracy, but the calculation is quite time-consuming. The effective medium approximation (EMA) theory is an attractive modeling tool as it allows for a complex trench structure to be modeled as a film stack with each layer having an effective optical property. After modeling with EMA, the reflectance spectrum of the trench structure can be rapidly calculated using the Maxwell-Garnett type equations. However, the zero-order EMA method adopted in MBIR for modeling can only achieve acceptable accuracy in the static-limit region with wavelength much larger than the trench pitch. In our previous work [2], we proposed a fast algorithm for reflectivity calculation of high aspect-ratio deep trench structures by an improved modeling method named corrected effective medium approximation (CEMA), which has been demonstrated to be not only fast in calculation but also accurate enough in comparison with the RCWA for both one-dimensional (1-D) and two-dimensional (2-D) trench arrays. In this paper, we further refine the CEMA method for modeling of 3-D trench structures. The independence of the CEMA on trench depth, polarization and azimuth of incidence has been investigated to demonstrate the validity of the CEMA.

## CURRENT RESULTS

Inspired by the simple form of CEMA equation for the 2-D structures [2], we propose a similar CEMA approach for the 3-D trench array as shown in Fig. 1(a). The formula takes the

simple form as follows:

$$n_{\text{eff}} = n_0 + B \left( \frac{1}{\lambda} \right)^2 \quad (1)$$

where  $n_{\text{eff}}$  represents the effective refractive index for the 3-D trench array;  $n_0$  represents the zero-order effective refractive index; and  $B$  represents the correction factor. As different from the 2-D structure, there is no simple analytical solution to the zero-order effective refractive index  $n_0$ . Noticing that  $n_{\text{eff}}$  is independent on the trench depth [3], we therefore propose a fitting based method to determine  $n_0$  and  $B$  by finding an effective optical model of a periodic deep trench structure with effective refractive index, as shown in Fig. 1. We obtain  $n_0$  and  $B$  by simulating the trench structure with RCWA theory and subsequently fitting the result to the reflectance curve of the effective optical model as shown in Fig. 1(b). The reflectance curve calculated by RCWA theory and the best fitted curve calculated by CEMA method are depicted in Fig. 1(c). With some certain values of the filled factor  $f$  between 0.2 to 0.8,  $n_0$  and  $B$  can be calculated with the fitting based method, as shown in Fig. 3 and Fig. 4 respectively. As an attempt to find the relationship between  $n_0$  and  $f$  and the relationship between  $B$  and  $f$ , we adopt the 4th order polynomial to fit the discrete data of  $n_0$  and  $B$ .

To further discuss the accuracy and validity of the proposed CEMA modeling method, we then carried out simulations on the structure in Fig. 1(a). Fig. 4 and Fig. 5 depict the simulation results of the reflectance spectrum in TE polarization and TM polarization states respectively. It is clear that within the full wavenumber range the CEMA method achieves more accurate approximation than the Maxwell-Garnett type EMA in comparison to the RCWA theory. From the simulations shown in Fig. 6 to Fig. 8, it is noted that  $n_0$  and  $B$  are independent on trench depth and azimuth angle. It is also observed that the CEMA method leads to more accurate results in the TE polarization than the TM polarization state with the fill factor  $f$  from 0.3 to 0.8, as shown in Fig. 9.

In summary, from the investigations above we conclude that the CEMA method achieves more accurate results than the Maxwell-Garnett type EMA method for modeling of 3-D trench structures. The simulations also demonstrate that the zero-order effective refractive index  $n_0$  and the correction factor  $B$  are independent on trench depth and azimuth of incidence. It is expected that the proposed CEMA method will be applied to MBIR for 3-D deep trench metrology.

## REFERENCES

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This project was supported by Hi-Tech Research and Development Program of China (2006AA04Z325), National Natural Science Foundation of China (50775090) and Program for New Century Excellent Talents in University of China (NCET-06-0639).

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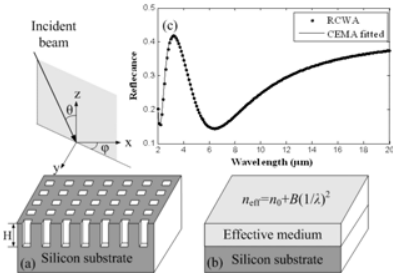


Fig. 1 (a) A 3-D structure, (b) its effective optical model, and (c) the reflectance spectrum that calculated by RCWA theory and its fitted curve by CEMA method.

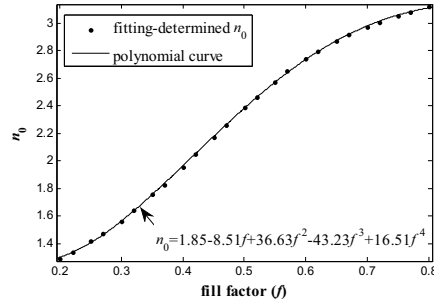


Fig. 2 Plot of fitting determined zero-order refractive index by the 4th order polynomial.

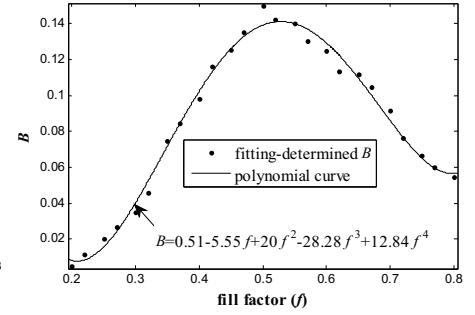


Fig. 3 Plot of fitting determined correction factor by the 4th order polynomial.

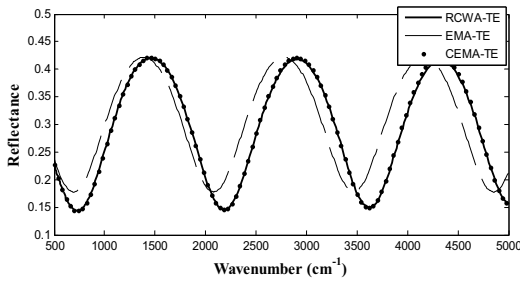


Fig. 4 Simulated reflectance spectra modeled with RCWA, Maxwell-Garnett type EMA and CEMA in TE polarization of the 3-D structure.

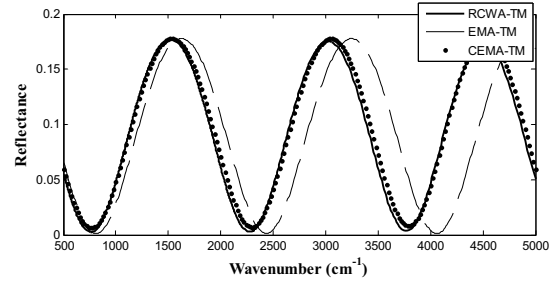


Fig. 5 Simulated reflectance spectra modeled with RCWA, Maxwell-Garnett type EMA and CEMA in TM polarization of the 3-D structure.

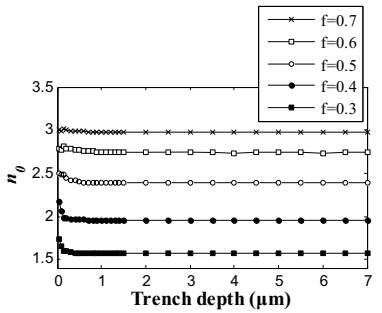


Fig. 6 Influence of trench depth on zero-order refractive index  $n_0$ .

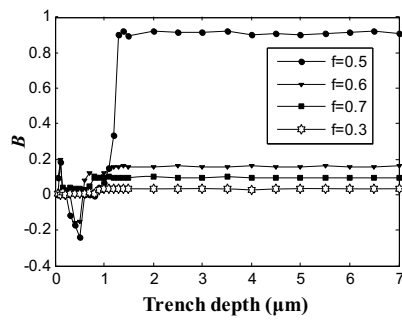


Fig. 7 Influence of trench depth on correction factor  $B$ .

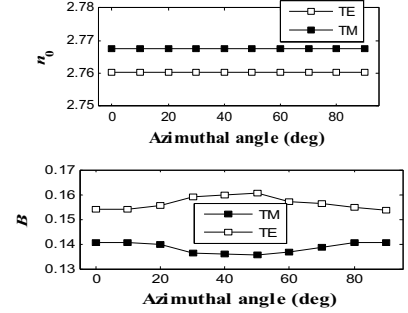


Fig. 8 Influence of azimuthal angle on zero-order refractive index  $n_0$  and correction factor  $B$ .

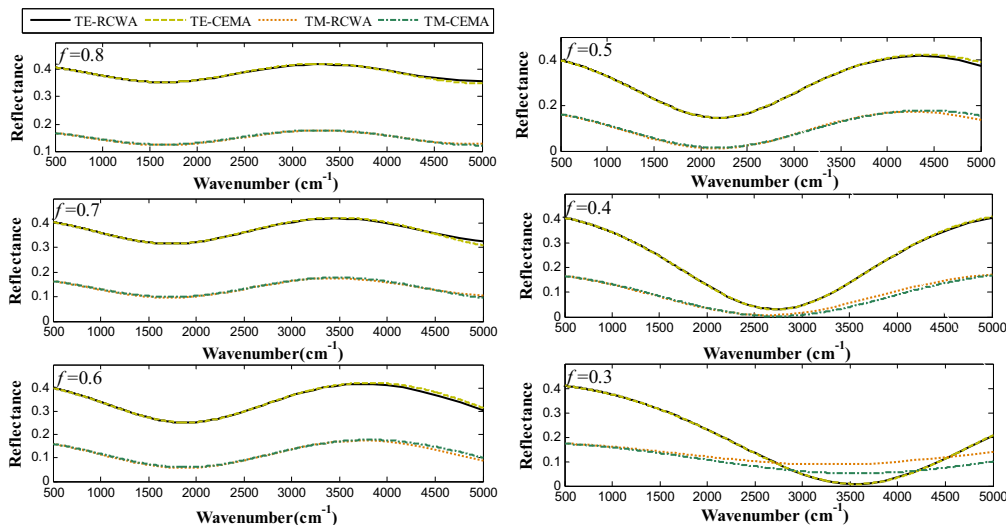


Fig. 9 Simulations of the approximated accuracy in different polarization states