Investigation Of Pores Influence on Dielectric Constant Value in Low k Materials Using Monte Carlo Method

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This paper investigates the pores influence on dielectric constant of low-k materials. Cylindrical, hexagonal and cubic pores shapes have been investigated using Monte-Carlo Method. Mixture composed of matrix and cylindrical pores presents the low dielectric constant with minimum of porosity. Moreover, new formula concerning volume scale transformation is proposed for making the usual mixing rules based on two phases more useful to predict the dielectric constant value in mixture composed for different pores shapes. To assess the performance of this new approach, Lichtenecker and Volume Average Theory mixing rules have been used through classical models and applying volume scale transformation. The obtained results show the success of volume scale transformation method. The proposed technique may have the potential in analyzing other properties such as electrical conductivity and thermal conductivity in porous ultra low-k dielectrics.

Keywords: Low k, Pores Shape, Mixing Rules, Monte-Carlo Method.

I. Introduction

Low dielectric constant (low k) materials are the subject of intense investigation and development in order to replace conventional SiO_2 dielectrics for the manufacturing of future-generation microelectronic devices [1-3]. The primary method of lowering the dielectric constant is to make the dielectric film less dense by introducing porosity. Organic silicate glass films or OSGs can reach dielectric constants down to 2.6, but the films become mechanically less robust as the dielectric constant decreases [4]. Material SiOCH seems the most adapted matrix for a potential integration in advanced interconnects [5].The introduction of porosity in SiOCH insulating matrix can be obtained by different techniques for example spin coated layers and porogen approach [6].

If experimental measurements are one of the effective ways to evaluate the value of the dielectric constant, predictions by analytical models represent as well a good mean for the comprehension and the control of dielectric constant value in porous materials. This work studies the pores geometry influence on dielectric constant value. In addition, it is an attempt to make the usual mixing rules, based on two phases, more useful to predict the dielectric constant value in mixture composed of different pores (empties, full pores). Monte-Carlo Method is used for mixing rule simulation.

II. Simulation Models

In mixture of two-phase (matrix with a relative permittivity equal to ε_m and a fraction of pores with ε_i as dielectric constant value) different mixing rules have been proposed to calculate the effective dielectric constant ε_{eff}. We report:

-Maxwell's equation of Volume Averaging Theory (VAT) expressed by equation (1) [7]

$$\varepsilon_{eff}=(1 - P)\varepsilon_m + P\varepsilon_i \qquad (1)$$

where $P = \upsilon/V$

v: pores volume, V: total volume

-Lichtenecker's rule (case of arbitrary inclusions) given by equation (2) [8]

$$\ln\varepsilon_{eff} = P * \ln\varepsilon_i + (1 – P) * \ln\varepsilon \qquad (2)$$

-Looyenga's rule (case of spherical inclusions and random oriented ellipsoids) expressed by equation (3) [8]

$$\varepsilon_{eff} = [\varepsilon^{1/3}{}_m + P * (\varepsilon^{1/3}{}_i + \varepsilon^{1/3}{}_m)]^{1/3} \qquad (3)$$

In the previous expressions, since no particular shape nor orientation is privileged with regard to the direction of the external field, therefore, these expressions were chosen to simulate the dielectric constant versus pores shapes of random mixtures using three different pores shapes: cylindrical, hexagonal and cubic.

So, three mixtures composed of the same matrix but with different kind of pores shapes (cylindrical, hexagonal and cubic). The side of hexagonal and cubic and radius of cylindrical pores as well as the depths

have been considered equals. The number of pores was fixed to N for the three mixtures. The curves obtained by Monte Carlo method, under Matlab Software, are presented in Fig.1 for two case empties pores and full pores.

Fig.1a, Fig.1c and Fig.1e show that Volume Averaging Theory (VAT) presents a linear change of the dielectric constant value versus porosity conversely to Lichtenecker model. For the two models (VAT and Lichtenecker), the permittivity decreases with increasing the empty pores concentration, until reaching 1 at 100 % of empty cylindrical shape pores corresponding to vacuum permittivity. The number of pores was fixed to N for the three mixtures. It is observed that the 100% of cylindrical porosity corresponds to 82% of hexagonal porosity and 31% of cubic porosity. Hence, when the pores are sealed, it is suggested that the use of the cylindrical pores occupy more space with less porosity. Whereas in the case of open pores, the mixture attracts more moisture (water dielectric constant equal to 78.4) leading to the increase of the mixture dielectric constant value (Fig.2a, Fig.2c and Fig.2e) and then suggesting the use of cubic pores in this case.

When the mixture is composed of matrix and two kinds of pores shapes having porosity P_1 and P_2, if the pores shapes are arbitrary, Lichtenecker [9] model may be used for calculating the dielectric constant value. However, if the pores are spherical but mixed with full or empties pores, the dielectric constant value of the mixture using the usual mixing rules based on two phases (Maxwell Garnett, Bruggeman and Looyenga…) can be calculated. To compute the dielectric constant of mixture of three components, model presented in Fig.2 has been used. In this model, the dielectric constant of the mixture was calculated by two steps. Firstly, empties pores were separated from the mixture. The remaining components (matrix and full pores) constituted the primary mixture then the dielectric constant was calculated using the known mixing rules based on two components. Secondly, empty pores will be added to this mixture and the permittivity of the mixture was calculated as in the firstly step. However, this operation is not accomplished without considering pores fraction scale transformation.

For more clarification, the first mixing rule (according to pores shape) is used to compute the dielectric constant of matrix and pores shape with porosity P_1. For example, according to Looyenga mixing rule (equation 3), the term $1\text{-}P_1$ translates the matrix porosity in the presence of inclusions porosity P_1. Nevertheless, the porosity of matrix is equal to $1\text{-}P_1\text{-}P_2$ in the presence of the two inclusions porosity P_1 and P_2 (P_2 means the second porosity inclusions). So, $1\text{-}P_2$ value was changed to 1 for being adequate to usual mixing rule. Hence P_1, in this new scale, is considered equal to P'_1:

$$P'_1 = \frac{P_1}{1 - P_2}$$

Where $P_1 = \frac{v_1}{V}$ $P_2 = \frac{v_2}{V}$

v_1: pores volume (inclusions1) V: total volume v_2: pores volume (inclusions2)

$$\varepsilon = [\varepsilon^{1/3}_m + P'_1 * (\varepsilon^{1/3}_1 + \varepsilon^{1/3}_m)]^{1/3} \quad (4)$$

v_1 in this new scale is transformed to v'_1

$$v'_1 = \frac{v_1}{V - v_2} \quad (5)$$

$$\varepsilon = \left[\varepsilon_m^{\frac{1}{3}} + \left(\frac{v_1}{V - v_2}\right) * \left(\varepsilon_1^{\frac{1}{3}} + \varepsilon_m^{\frac{1}{3}}\right)\right]^{\frac{1}{3}} \quad (6)$$

The second Mixing rule (corresponding to pores shape) computes the dielectric constant ε_{eff} of the resulting dielectric constant ε (calculated by equation 4 or 6), representing the matrix and inclusions porosity P_2. The dielectric constant ε_{eff} of mixture (matrix, inclusions with porosity P_1 and inclusions with porosity P_2) is equal to:

$$\varepsilon_{eff} = \left[\varepsilon^{\frac{1}{3}} + P_2 * \left(\varepsilon_2^{\frac{1}{3}} + \varepsilon^{\frac{1}{3}}\right)\right]^{\frac{1}{3}} \quad (7)$$

$$\varepsilon_{eff} = \left[\varepsilon^{\frac{1}{3}} + \frac{v_2}{V} * \left(\varepsilon_2^{\frac{1}{3}} + \varepsilon^{\frac{1}{3}}\right)\right]^{\frac{1}{3}} \quad (8)$$

For the validation of the volume scale transformation, mixture composed of matrix and cylindrical and cubic pores with respectively P_1 and P_2 as porosity has been considered. The effective dielectric constant value of mixture using Volume Averaging Theory (VAT) (linear model) is expressed by equation (9) [7]

$$\varepsilon_{eff} = (1 - P_1 - P_2)\varepsilon_m + P_1\varepsilon_1 + P_2\varepsilon_2 \quad (9)$$

$$\varepsilon_{eff} = (1 - (v_1 - v_2)/V)\varepsilon_m + (v_1\varepsilon_1 + v_2\varepsilon_2)/V \quad (10)$$

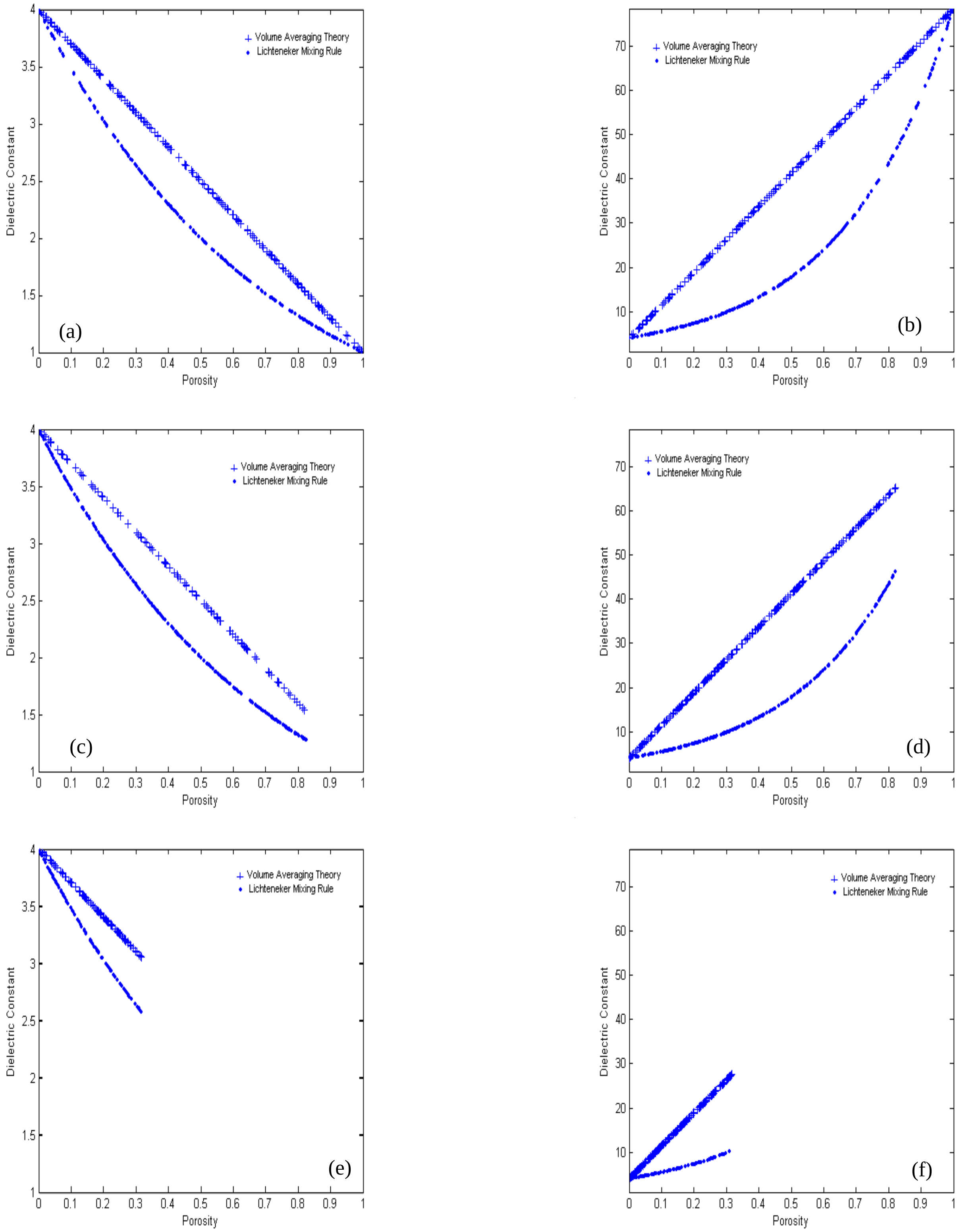

Fig. 1: Dielectric constant variation versus porosity: (a), (b) cylinder pores with empty and full pores respectively; (c), (d) hexagonal pores with empty and full pores respectively; (e), (f) cubic pores with empty and full pores respectively

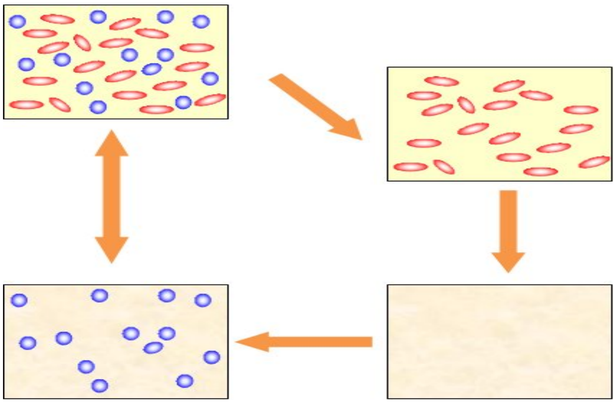

Fig.2 Decomposition process of material components: empties pores, full pores

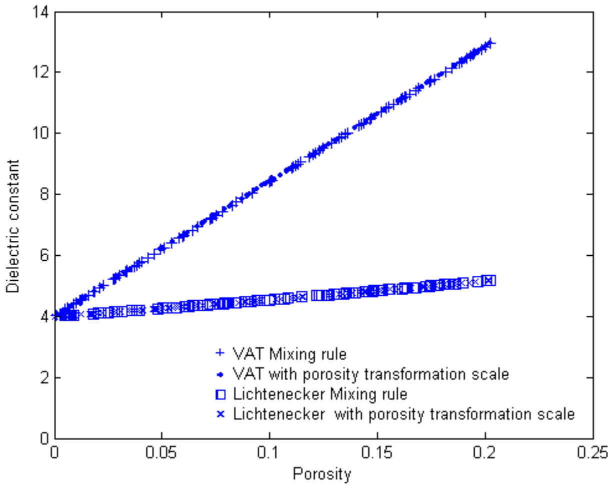

Fig. 3: Dielectric constant variation versus porosity: Matrix ε_s= 4, cylinders and cubes pores with porosity and dielectric constant value ε_1=78.4, P_1=0.15 and ε_1=1, P_1= 0.077 respectively

Applying porosity transformation scale to Volume Averaging Theory (VAT) [10], the effective dielectric constant value of mixture can be calculated by the equations 11 and 12

$$\varepsilon = \left(1-\left(\frac{v_1}{V-v_2}\right)\right)\varepsilon_m + \left(\frac{v_1}{V-v_2}\right)\varepsilon_1 \qquad (11)$$

$$\varepsilon_{eff} = \left(1-\frac{v_2}{V}\right)\varepsilon + \frac{v_2}{V}\varepsilon_2 \qquad (12)$$

The same process has been applied to Lichtenecker mixing rule, formula13, (non linear model) [9].

$$\varepsilon_{eff} = \prod_{k=1}^{k=n} \varepsilon_k^{P_k} \qquad (13)$$

Figure 3 shows simulation results of the effective dielectric constant versus porosity using VAT and Lichtenecker models treated by the two ways described above. The obtained curves are superposed and then, this confirms the success of volume scale transformation method.

In mixture composed of *N* different pores shapes, to determine the effective dielectric constant, it is recommended to use (*N*-1) mixing rules (corresponding to pores shape) with considering volume scale transformation. The volume scale transformation follows the rule:

$$v'_i = \frac{v_i}{V - \sum_{k=i+1}^{n} v_k}$$

So, volume scale transformation is the way to incorporate the N component in the mixing rules based on two phases.

III. Conclusion

This work simulated the dielectric constant versus porosity for different pores shapes. It was found that the cylindrical pores presented the low dielectric constant with minimum porosity. In addition new formula of volume scale transformation has been proposed to make the usual mixing rules, based on two phases, more useful for calculating the effective dielectric constant of mixture composed of different shapes pores. To assess the performance of this new approach, Lichtenecker and VAT mixing rules have been used through two ways: classical models and applying porosity scale transformation. The obtained curves are superposed confirming the success of volume scale transformation method. The proposed technique may have the potential in analyzing other properties such as electrical conductivity and thermal conductivity in porous ultra low-k dielectrics.

IV. References

[1] J. Shen, A. Luo, L.Yao and X. Lin, Materials Science and Engineering C, Elsevier, (2007), Vol. 27, pp. 1145–1148.

[2] V. Jousseaume, G. Rolland, D. Babonneau, J.-P. Simon, Applied Surface Science, (2007), Vol. 254, pp. 473–479.

[3] S. K. Singh, A.A. Kumbhar, R.O. Dusane, Materials Letters, (2006), Vol. 60, pp. 1579–158

[4] K. Maex, M.R. Baklanov, D. Shamiryan, F. Lacopi, S. H. Brongersma and Z.S. Yanovitskaya, Applied Physics, (2003), Vol. 93, pp. 8793–8841.

[5] V. Jousseaume, L. Favennec, A. Zenasni, Surface & Coatings Technology, Elsevier, (2007), Vol. 201, pp. 9248–9251.
[6] V. Jousseaume, G. Rolland, D. Babonneau , J-P. Simon, Applied Surface Science, (2007), Vol. 254, No. 1, pp 473–479
[7] M. M. Braun, L. Pilon, Thin Solid Films, (2006), Vol. 496, pp. 505 - 514.
[8] J. Widjajakusuma , B. Biswal , R. Hilfer , Physica A, (2003), Vol.318 , pp.319-333.
[9] A. Fabbri, T.Fen-Chong, O. Coussy, Cold Regions Science and Technology, (2006), Vol.44 , pp.52-66.
[10] G. J. Boer, I. N. Sokolik, S. T. Martin, Quantitative Spectroscopy &Radiative Transfer, (2007), Vol. 108 , pp.39-53.