Evaluation of the fitting efficiencies of general effective medium equation and its modification

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The general effective medium equation (GEM) [1] and its modified form (mGEM) [2] have been widely fitted to effective dielectric constants of diphase composite dielectrics [3, 4]. GEM has the form:

$$\frac{V_l\left(\varepsilon_l^{1/t}-\varepsilon_m^{1/t}\right)}{\varepsilon_l^{1/t}+A\varepsilon_m^{1/t}}+\frac{V_h\left(\varepsilon_h^{1/t}-\varepsilon_m^{1/t}\right)}{\varepsilon_h^{1/t}+A\varepsilon_m^{1/t}}=0 \qquad (1)$$

where ε_h and ε_l are the relative dielectric constants of the high-dielectric phase and low-dielectric phase, respectively, V_h and V_l the volume fractions of the high-dielectric phase and low-dielectric phase ($V_h + V_l = 1$), ε_m the effective dielectric constant of the composite. t is an exponent parameter in GEM; and the other parameter A can be written as

$$A=\frac{1-V_c}{V_c} \qquad (2)$$

where V_c is the critical volume fraction of the high-dielectric constant phase. mGEM can be written as

$$\frac{V_l\left(\varepsilon_l^{1/s}-\varepsilon_m^{1/s}\right)}{\varepsilon_l^{1/s}+A\varepsilon_m^{1/s}}+\frac{V_h\left(\varepsilon_h^{1/t}-\varepsilon_m^{1/t}\right)}{\varepsilon_h^{1/t}+A\varepsilon_m^{1/t}}=0 \qquad (3)$$

An additional exponent parameter s is introduced here.

When fitting experimental data to predictive equations, the quantity of

$$\chi=\left[\frac{1}{n-p}\sum_{i=1}^{n}\left(\frac{\varepsilon_m-\varepsilon_{equ}}{0.01\varepsilon_m}\right)^2\right]^{\frac{1}{2}} \qquad (4)$$

is always minimized by varying the fittable parameters in the predictive equation. Here ε_{equ} is the effective dielectric constant calculated by the predictive equation using appropriate variable parameters, n is the number of data points and p is the number of variable parameters in that equation [1].

Wu and McLachlan suggested that the fitting efficiencies of GEM and mGEM were nearly the same over the whole range of volume fractions [5]. We also observed the phenomenon that, when fitted to the same data set, GEM and mGEM had very close χ values, which means similar fitting efficiencies [4]. At each data point, however, are the fitting efficiencies of GEM and mGEM nearly the same as well?

As χ can only reflect fitting efficiency in whole range of volume fraction, after the parameters of a predictive equation have been calculated, the quantity:

$$\alpha=\left(\frac{\varepsilon_m-\varepsilon_{equ}}{\varepsilon_m}\right)^2 \qquad (5)$$

is abstracted from χ for each volume fraction to evaluate the fitting efficiency of that equation at each data point. The distribution pattern of α, if it exists, so can be deduced.

We simulated effective dielectric constants of diphase composite dielectrics (ε_m) by Monte Carlo-finite element method on 2D square lattice for $C = \varepsilon_h : \varepsilon_l = 200$, 500 and 700 [4]. Then, for each C value, we calculated a group of parameters for GEM or mGEM. Using the quantity $\alpha_{GEM} = (\frac{\varepsilon_m-\varepsilon_{GEM}}{\varepsilon_m})^2$, we first evaluate

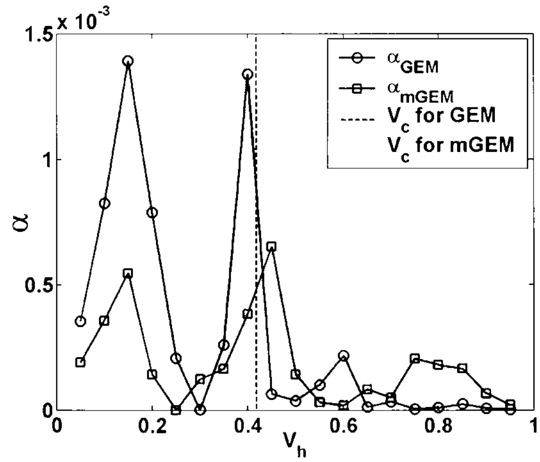

Figure 1 When $C = 200$, α_{GEM} vs. V_h and α_{mGEM} vs. V_h.

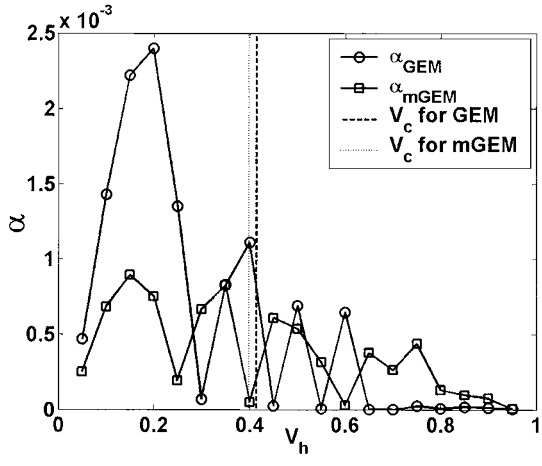

Figure 2 When $C = 500$, α_{GEM} vs. V_h and α_{mGEM} vs. V_h.

TABLE I Averages and standard deviations of α for GEM and mGEM

	GEM		mGEM	
	$V_h < V_c$	$V_h > V_c$	$V_h < V_c$	$V_h > V_c$
$\bar{\alpha}$				
$C = 700$	1.318×10^{-3}	1.053×10^{-4}	5.397×10^{-4}	2.593×10^{-4}
$C = 500$	1.253×10^{-3}	2.126×10^{-4}	5.737×10^{-4}	2.887×10^{-4}
$C = 200$	5.476×10^{-4}	1.552×10^{-4}	2.272×10^{-4}	1.668×10^{-4}
STD of α				
$C = 700$	8.245×10^{-4}		3.722×10^{-4}	
$C = 500$	7.770×10^{-4}		2.920×10^{-4}	
$C = 200$	4.492×10^{-4}		2.920×10^{-4}	

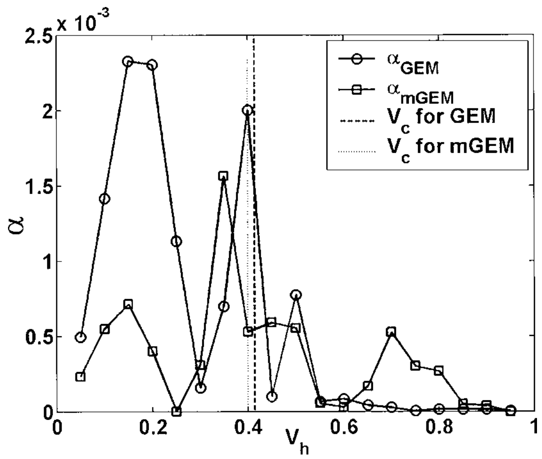

Figure 3 When $C = 700$, α_{GEM} vs. V_h and α_{mGEM} vs. V_h.

the fitting efficiency of GEM at each data point. In Figs 1–3, we plot α_{GEM} vs. V_h for each C value. The critical volume fraction V_c for GEM is also shown in each figure. It is evident that, for each value, most of the α_{GEM} computed when $V_h < V_c$ are much greater than α_{GEM} computed when $V_h > V_c$ and that when $V_h > 0.6$ α_{GEM} are especially small.

Thereafter, the fitting efficiency of mGEM at each data point was also examined by $\alpha_{mGEM} = (\frac{\varepsilon_m - \varepsilon_{mGEM}}{\varepsilon_m})^2$. The plots of α_{mGEM} vs. V_h are also shown in Figs 1–3 for each C value with V_c for mGEM marked as well. We can observe that for mGEM the discrepancies between α_{mGEM} calculated when $V_h < V_c$ and $V_h > V_c$ are not as large as those for GEM.

In Table I, we present the average values of α_{GEM}, $\langle\alpha_{GEM}\rangle$, calculated when $V_h < V_c$ and $V_h > V_c$, and the standard deviation (STD) of α_{GEM} for each C value the corresponding values for mGEM are also shown.

From this table we conclude that:

1. The fitting efficiency of GEM when $V_h > V_c$ is much better that when $V_h < V_c$.
2. For mGEM, the fitting efficiency discrepancy with volume fraction is not so large as that of GEM.
3. Fluctuation of mGEM's fitting efficiency at each data point is much smaller than that of GEM, which is reflected by their STD values.

Therefore, if a predictive equation has to be chosen from GEM or mGEM to give the effective dielectric constants of diphase composite dielectrics, some suggestions are:

1. When volume fraction of the high-dielectric phase is very high, for example V_h is larger than 0.6 here, it is strongly advisable to use GEM to predictive effective dielectric constant.
2. When V_h is so low as smaller than V_c, mGEM will be a better choice for predictive equation.
3. When V_h is neither low nor high, mGEM should be used, for it will not give such large α values as GEM does at mid-range values of V_h.
4. If only one predictive equation is to be chosen from GEM or mGEM for the whole range of V_h, mGEM may be the preferable choice; for its α values have comparatively smaller fluctuation.

References

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