Theoretical investigation of the nanoinclusions shape impact on the capacitance of a nanocomposite capacitor

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A first-principles theoretical approach to the effective dielectric permittivity of a nanocomposite which contains nanoinclusions dispersed in a host dielectric enclosed between two parallel metallic electrodes is developed. The inclusions are modelled by spheroids and their response to the external electric field is found using the point dipole approximation and Green’s function approach. As a result, besides the mutual interactions between the induced dipoles, the local field in the nanocomposite contains also a contribution from the dipole field reflected from the capacitor electrodes. It is shown that the nanocomposite dielectric permittivity is determined by an average inclusion polarizability density and its dependence on the aspect ratio and orientations of inclusions is found analytically and investigated. The theoretical predictions derived in the paper are in excellent agreement with the available experimental data and can be used for a proper design of nanocomposite capacitors.

I. INTRODUCTION

The polymer-based nanocomposite capacitors have received recently growing attention due to their low cost, easy fabrication and excellent flexibility. They combine the advantages of high operating voltages, typical for polymers, and large dielectric permittivities of nanosized inclusions, thus providing high power densities. \(^1\)\(^-\)\(^5\)

This approach stems from a common belief that the embedding of ferroelectric ceramic inclusions, which have a huge dielectric permittivity, into the host polymer should significantly increase the effective dielectric permittivity of the polymer-based nanocomposite material. Nevertheless, the permittivity values experimentally obtained for different nanocomposites are much lower than those for volume samples of ferroelectric ceramics, even at large volume fractions of inclusions. \(^6\)\(^-\)\(^14\)

This discrepancy can be partly explained by a decrease of the permittivity of small ceramic particles due to the existence of a surface non-ferroelectric layer. \(^15\)\(^-\)\(^17\) It was noticed, however, that for spherical inclusions with the permittivity much larger than that of the host material, the specific value of their permittivity is actually unimportant. \(^6\)

The observed divergence between the measured dependence of the dielectric permittivity on the volume fraction of ceramic inclusions and the one which follows from the Maxwell Garnett approximation \(^18\)\(^,\)\(^19\) can be attributed to the non-spherical shape of inclusions. This effect is described in terms of the "shape parameter" which is adjusted to fit the experimental data and does not play therefore a predictive role.

The further experimental investigations of the dielectric properties of nanocomposites have revealed a significant role of the aspect ratio and orientations of inclusions. \(^20\)\(^-\)\(^31\) There were also attempts to simulate the observed dependencies by either the Maxwell Garnett approximation \(^20\)\(^,\)\(^22\) or numerically, using finite element models. \(^21\) In the first case, an agreement with the experimental data was achieved by considering either the aspect ratio or the permittivity of inclusions as a fitting parameter which is not necessarily consistent with the measured values, especially for large aspect ratios of inclusions. In the second case, a large discrepancy with the experimental data was ascribed to a possible partial alignment of inclusions due to the compression molding process.

Another aspect, which should be taken into account when designing a nanocomposite capacitor, is a drastic deterioration of the adhesion strength, thermal stress reliability and mechanical properties at high ceramic filler loadings. \(^10\)

This dictates a high demand for approaches which provide large permittivity values of nanocomposites at low volume fractions of inclusions. \(^32\)\(^-\)\(^34\) To achieve this aim, one can take advantage of nanowire (NW) inclusions which have much larger polarizabilities than their spherical counterparts. \(^22\) In light of the above, a theoretical approach, which adequately describes the dielectric properties of nanocomposite capacitors with high-aspect-ratio inclusions and allows their proper design, is of paramount importance.

Recently, we have paid attention that the Maxwell Garnett approximation is not applicable to nanocomposites for the operating frequencies exploited in electrical engineering. \(^35\)

In a proper approach, one should take into account the electromagnetic field emitted by the dipoles, induced in the inclusions by an external field, and reflected back by the capacitor electrodes. The theoretical analysis performed for spherical inclusions has demonstrated a remarkable difference with the classical Maxwell Garnett formula, even in the quasi-static limit. The developed approach was also applied to analyze the breakdown voltage in nanocomposite capacitors and the predicted tendencies have been shown to agree well with the experimental data. \(^36\)

In the present paper, we theoretically investigate the effective dielectric permittivity, \(\varepsilon\), of a nanocomposite which contains ellipsoidal inclusions disposed between parallel metallic electrodes. The capacitance of a parallel-plate capacitor is then determined in terms of \(\varepsilon\) as \(C = \varepsilon A/d\) with \(A\) and \(d\) being the area of the plates and the separation between them, respectively. The inclusions are modelled by arbitrarily oriented either prolate or oblate spheroids. The linear dimensions of inclusions are assumed to be much less than those of
the capacitor and the microscopic electromagnetic field in the nanocomposite is found using the point dipole approximation and Green’s function approach. We analyze the influence of the aspect ratio and orientations of inclusions on the dielectric permittivity of the nanocomposite and its dependence on the volume fraction of inclusions. The theoretical predictions are compared with the experimental data available in the literature.

II. THEORY

A. Model

We consider a parallel-plate capacitor with metallic electrodes of linear dimensions $L_1$ and $L_2$ along the axes $x$ and $y$, respectively, in which the dielectric slab of thickness $d$ contains ellipsoidal inclusions (see Fig. 1a). We assume that the host dielectric and the material of inclusions have the dielectric permittivities $\varepsilon_h$ and $\varepsilon_i$, respectively, and the inclusions are either prolate or oblate spheroids with the semi-axes $a$, $b$ and $c$, the semi-axis $c$ being directed along the axis of rotational symmetry (see Fig. 1b).

An induced dipole moment of an inclusion in the electric field $\mathbf{E}(\mathbf{r})$ is found as

$$\mathbf{p}(\mathbf{r}) = \alpha_\xi \mathbf{E}_\xi(\mathbf{r}) + \alpha_\eta \mathbf{E}_\eta(\mathbf{r}) + \alpha_\zeta \mathbf{E}_\zeta(\mathbf{r}),$$

where $\mathbf{E}_\xi$, $\mathbf{E}_\eta$ and $\mathbf{E}_\zeta$ are the projections of the field onto the semi-axes $a$, $b$ and $c$, respectively, and the polarizability components are given by ($j = \xi, \eta, \zeta$)

$$\alpha_j = \frac{1}{3} \varepsilon_i c \varepsilon_0 \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_h + L_j (\varepsilon_i - \varepsilon_h)}.$$  

with the depolarization factors

$$L_\zeta = L_\eta = \frac{1}{2} (1 - L_\zeta).$$

Here for a prolate spheroid ($c > a$)

$$L_\zeta = \frac{1 - e^2}{2e^3} \left( \ln \frac{1 + e}{1 - e} - 2e \right)$$

with $e = \sqrt{1 - a^2/c^2}$ and for an oblate spheroid ($c < a$)

$$L_\zeta = \frac{1 + e^2}{e^3} (e - \tan^{-1} e)$$

with $e = \sqrt{a^2/c^2 - 1}$. In particular, for a sphere ($a = b = c$) $L_\zeta = L_\eta = L_\xi = 1/3$, whereas for a cylinder with its axis along the $\zeta$ direction ($\zeta \to \infty$) $L_\zeta = L_\eta = 1/2$ and $L_\xi = 0$.

B. Local Field

The microscopic (local) field $\mathbf{E}(\mathbf{r})$ in the nanocomposite interior results from both the electric field $\mathbf{E}_0$ applied between the capacitor plates and the field of the dipoles induced in the inclusions, Eq. (1). This can be written in the form of an integral equation as

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 + \int_{\mathbf{r}'} \mathbf{F}(\mathbf{r}, \mathbf{r}') \mathbf{P}(\mathbf{r}') d\mathbf{r}' ,$$

where

$$\mathbf{P}(\mathbf{r}) = N \langle \mathbf{p}(\mathbf{r}) \rangle$$

is the polarization of inclusions with $N$ being their number density, $\mathbf{F}(\mathbf{r}, \mathbf{r}')$ is the so-called field susceptibility tensor that relates the electric field at the point $\mathbf{r}$ generated by a dipole with the dipole moment itself, located at $\mathbf{r}'$; $V'$ denotes the nanocomposite volume after removal of a small volume around the inclusion under consideration and the angular brackets denote the averaging over the orientations of inclusions. Here, following Maxwell Garnett’s assumption, we treat the inclusions as point dipoles and use the Green’s function formalism to find their field near flat electrodes.

In the problem under consideration, the field $\mathbf{E}_0$ is directed along the $z$ axis and the projection $E_z$ is the quantity of concern. In the absence of any alignment of inclusions with respect to the $x$ and $y$ axes, the only non-zero component of their polarization is $P_z$. One comes therefore to a scalar integral equation

$$E_z(\mathbf{r}) = E_0 + \int_{\mathbf{r}'} F_{zz}(\mathbf{r}, \mathbf{r}') P_z(\mathbf{r}') d\mathbf{r}' .$$

To find the polarization one needs to express the dipole moment of a single inclusion, Eq. (1), in terms of the local field $E_z$ and average it over different orientations of inclusions. The projections of $E_z$ onto the spheroid semi-axes are found as follows

$$E_\xi = E_z \sin \theta \cos \phi,$$

$$E_\eta = E_z \sin \theta \sin \phi,$$

$$E_\zeta = E_z \cos \theta,$$

where $\phi$ and $\theta$ are the azimuthal and polar angles, respectively, of the spherical coordinate system associated with the
The quantity \(\alpha\) is the polarizability of inclusions. The maximum variation of the dielectric permittivity of the nanocomposite which determines the capacitance of the nanocomposite capacitor is found as

\[
p_z = p_z \sin \theta \cos \phi + p_{\eta} \sin \theta \sin \phi + p_{\zeta} \cos \theta = (\alpha_z \sin^2 \theta + \alpha_\eta \cos^2 \theta) E_z. \tag{15}
\]

Now substituting this relation into Eq. (8) one obtains the equation

\[
E_z(r) = E_0 + N\alpha \int_{r'} F_z(z, r') E_z(r') dr'. \tag{16}
\]

We have introduced here the notation

\[
\bar{\alpha} = \alpha_z \langle \sin^2 \theta \rangle + \alpha_\eta \langle \cos^2 \theta \rangle, \tag{17}
\]

where, as before, the angular brackets denote the averaging over the orientations of inclusions which is determined by their specific arrangement.

The quantity \(F_z(z, r')\) in Eq. (16) can be represented in terms of the 2D Fourier integral

\[
F_z(z, r') = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_z(z', k_x, k_y) e^{i k_x (x-x')} e^{i k_y (y-y')} dk_x dk_y, \tag{18}
\]

where \(f_z(z', k_x, k_y)\) is the 2D Fourier transform, \(k_x\) and \(k_y\) are the spatial frequencies along the \(x\) and \(y\) axes, respectively, and \((x, y, z)\) and \((x', y', z')\) are the Cartesian coordinates of the observation point and dipole location, respectively. The local field can be written in a similar way as follows

\[
E_z(r) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e_z(z', k_x, k_y) e^{i k_x (x-x')} e^{i k_y (y-y')} dk_x dk_y. \tag{19}
\]

In the quasi-static limit, which is realized in electrical engineering, where \(d \ll L_1, L_2 \ll \lambda\) with \(\lambda\) being the wavelength associated with the operating frequency, the Fourier transform of the field susceptibility is reduced to

\[
f_z(z', k_x, k_y) \approx \frac{4\pi}{\varepsilon_0 d}. \tag{20}
\]

In this approximation \(E_z\) does not depend on the coordinates and is given by

\[
E_z \approx \frac{E_0}{1 - (4\pi/\varepsilon_0) N\bar{\alpha}}. \tag{21}
\]

This result can be rewritten in the form

\[
E_z \approx \frac{E_0}{1 - f\bar{\beta}}. \tag{22}
\]

where \(f = (4\pi/3)Na^2c\) is the volume fraction of inclusions and

\[
\bar{\beta} = \beta_z \langle \sin^2 \theta \rangle + \beta_\eta \langle \cos^2 \theta \rangle \tag{23}
\]

with

\[
\bar{\beta} = \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_h + L_z (\varepsilon_i - \varepsilon_h)} \tag{24}
\]

and

\[
\beta_\parallel = \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_h + L_z (\varepsilon_i - \varepsilon_h)} \tag{25}
\]

As it is seen from Eq. (2), the quantity \(\bar{\beta}\) equals to the volume density of the inclusion polarizability, averaged over the orientations of inclusions, up to a factor of \(\varepsilon_i/4\pi\).

One can also derive from the above the effective dielectric permittivity of the nanocomposite which determines the capacitance of the nanocomposite capacitor. This quantity is defined as

\[
\varepsilon = \frac{D_z}{E_0} = \frac{(\varepsilon_h + 4\pi N\bar{\alpha})E_z}{E_0} = \varepsilon_h + f\bar{\beta}, \tag{26}
\]

which is reduced to the previously obtained result in the case of spherical inclusions.

The applicability of Eq. (26) is limited by the point dipole approximation for the inclusions. Its range of validity can be derived as follows. The electric field produced by the dipole moment of an inclusion, induced by the external field \(E_0\), at the distance \(R_0\) in the host dielectric is estimated as \(E \sim \bar{\alpha} E_0/\varepsilon_h R_0^3\) with \(\bar{\alpha}\) being the average polarizability of inclusions. The maximum variation of the field across the inclusion, in case of a prolate spheroid, is found as \(\Delta E \sim 6\bar{\alpha}c E_0/\varepsilon_h R_0^3\). Making here the substitution \(\bar{\alpha} = (\varepsilon_i/4\pi) V\bar{\beta}\) with \(V\) being the volume of an inclusion according to Eq. (2) and considering \(R_0\) as the mean distance between the inclusions one obtains \(\Delta E/E_0 \sim 3f\bar{\beta}/(2\pi R_0)\). As it was shown for spherical metal nanoparticles, for which \(|\varepsilon_i| \gg \varepsilon_h\) and \(\bar{\beta} = 3\), the point dipole approximation is reasonably good if their radius, \(R\), satisfies the inequality \(R \leq R_0/3\) or in terms of the volume fraction \(f \leq 0.2\) that gives \(\Delta E/E_0 \leq 0.6/(2\pi) \approx 0.1\). For spheroids one should take \(c \leq R_0/3\) and accordingly \(\Delta E/E_0 \leq f\bar{\beta}/(2\pi)\). It is reasonable to assume that in a general case this approximation works well under the same condition for the variation of the field \(E\), i.e. \(\Delta E/E_0 \leq f\bar{\beta}/(2\pi) \leq 0.6/(2\pi)\) that puts an upper limit \(f\bar{\beta} \leq 0.6\) provided that \(f \leq 0.2\). The same result is obtained for oblate spheroids.

### III. ANALYSIS OF THE SHAPE IMPACT

The impact of the nanoinclusions shape on the capacitance of a nanocomposite capacitor emerges through the dependence of the effective dielectric permittivity of the nanocomposite, Eq. (26), on the depolarization factors which enter the
quantities \( \beta_\perp \) and \( \beta_\parallel \), Eqs. (24) and (25), respectively. Their average \( \bar{\beta} \), which is determined by the orientations of inclusions, dictates the rate of the dielectric permittivity increase with the volume fraction of inclusions.

Some important conclusions follow from the analysis of Eq. (23). For random orientations of inclusions in the volume of the nanocomposite, \( \langle \sin^2\theta \rangle = \langle \cos^2\theta \rangle = 1/2 \) and \( \bar{\beta} = (\beta_\perp + \beta_\parallel)/2 \). For the alignment parallel to the \( xy \) plane and random orientations within this plane, \( \theta = \pi/2 \) and \( \bar{\beta} = \beta_\perp \). For an alignment along the \( z \) axis, \( \theta = 0 \) and \( \bar{\beta} = \beta_\parallel \). One can notice that the first of the above values equals the arithmetic mean of the last two values.

Another observation which can be deduced from Eqs. (24) and (25) is valid in the limiting case where \( \varepsilon_i \gg \varepsilon_h \) and the depolarization factors are not too small, so that \( L_i \varepsilon_i \gg \varepsilon_h \). In such a case \( \beta_\perp \approx L_\perp^{-1} \) and \( \beta_\parallel \approx L_\parallel^{-1} \). In particular, for spherical inclusions \( \beta = 3 \), for cylindrical inclusions aligned parallel to the \( xy \) plane \( \beta \approx 2 \) and aligned parallel to the \( z \) axis \( \beta \gg 1 \). In a general case the relation of \( \bar{\beta} \) with the depolarization factors is more complicated. For random orientations of inclusions, it is demonstrated in Figs. 2 and 3 where the relative dielectric permittivity of the nanocomposite is plotted for both prolate and oblate spheroids against their aspect ratio. One can see that this behaviour largely depends on the dielectric contrast between the inclusion and the host polymer, \( \varepsilon_i/\varepsilon_h \). For a small contrast, \( \varepsilon \) slightly varies with the aspect ratio, while for a large contrast an increase in \( \varepsilon/\varepsilon_h \) can be an order of magnitude. The prolate spheroids are characterized by a larger increase in \( \varepsilon \) than the oblate ones for the same value of the aspect ratio, the enhancement being more significant for a larger dielectric contrast. In both cases the spheroidal inclusions provide larger values of \( \varepsilon/\varepsilon_h \) than the spherical ones. One can also observe that at some values of the aspect ratio \( \varepsilon/\varepsilon_h \) gets saturated and does not increase further. Such a saturation occurs at larger values of the aspect ratio for a larger dielectric contrast.

Figures 4 and 5 demonstrate the dependence of the quantity \( \varepsilon/\varepsilon_h \) on the volume fraction of inclusions for prolate and oblate spheroids, respectively. One can observe a more rapid increase of the effective dielectric permittivity for larger aspect ratio, the increase being more significant for prolate spheroids.

### IV. COMPARISON WITH EXPERIMENTS

The expression for the effective dielectric function of the nanocomposite, Eq. (26), can be rewritten in the form

\[
g(\varepsilon) = \bar{\beta} f \tag{27}
\]

with \( g(\varepsilon) = (\varepsilon - 1)/(\varepsilon + 1) \) and \( \varepsilon = \varepsilon/\varepsilon_h \), which facilitates a comparison with experimental data. According to the above criterion, one can expect that Eq. (27) is applicable if \( g(\varepsilon) \leq 0.6 \) provided that \( f \leq 0.2 \). The NWs fabricated in experiments have a cylindrical shape and for them the aspect ratio (AR) is defined as the length to diameter ratio.

Figure 6 shows the experimental data obtained for the dielectric permittivity of a nanocomposite capacitor, in which the nanocomposite is represented by lead zirconate titanate (PZT) NWs with the aspect ratio \( AR \approx 14 \) dispersed in polyvinylidene fluoride (PVDF) matrix and recalculated to the quantity \( g(\varepsilon) \). The three sets of data correspond to random orientations of NWs, alignment of NWs perpendicularly to the \( z \) axis and alignment parallel to the \( z \) axis. The linear fits of the dependence of \( g(\varepsilon) \) against \( f \) have the slopes \( \bar{\beta} = 1.4 \pm 0.1, 0.5 \pm 0.2 \) and \( 2.22 \pm 0.06 \), respectively. The arithmetic mean of the latter two slopes is equal to \( 1.4 \pm 0.1 \), in excellent agreement with the above theoretical prediction. On the other hand, the failure to predict the values of \( \bar{\beta} \) from the depolarization factors signifies that the value of \( \varepsilon_i \) is not too large.
The dielectric permittivity found here for non-modified NW shapes from spheroids which were used for modelling. The data recalculated to the function $g(\tilde{\varepsilon})$ for different NW aspect ratios are well fitted by straight lines in agreement with Eq. (27) and their slopes are given in Table I. Equation (23), being applied to random orientations of NWs, allows one to deduce the effective values of $\varepsilon_i$ from the obtained results which are shown in Table I as well. Some discrepancy between $\varepsilon_i$ deduced for the BaTiO$_3$/PDMS nanocomposites with different aspect ratios of NWs can originate from a distinction of the NW shapes from spheroids which were used for modelling. The dielectric permittivities found here for non-modified BaTiO$_3$ NWs are comparable with those deduced from the experimental data on electrical breakdown in polymer nanocomposites containing BaTiO$_3$ nanoparticles. Such low values of $\varepsilon_i$ indicate that in both nanoparticles and nanowires the ferroelectric phase responsible for giant dielectric permittivity is largely destroyed. On the other hand, the surface-modified BaTiO$_3$ NWs demonstrate significantly larger values of the dielectric permittivity that indicates a remarkable role of the interface polarization.

V. CONCLUSION

In the present paper, we have theoretically investigated the influence of the aspect ratio and orientations of spheroidal
The quantity $g(\bar{\varepsilon})$ calculated for different nanocomposites containing BaTiO$_3$ NWs as a function of the volume fraction of NWs. The aspect ratios of NWs are shown in the brackets. The straight lines are the best linear fits to the experimental data shown by symbols and taken from: Figure 4b in Ref. 20 for BaTiO$_3$/PDMS(3,6,15), Figure 3 in Ref. 22 for BaTiO$_3$/PVDF-TrFE(15) and Figure 7a in Ref. 29 for BaTiO$_3$/PVDF(9.3). Only the data which satisfy the applicability criterion of Eq. (27) are used for fitting. The experimental error bars for BaTiO$_3$/PVDF(9.3) nanocomposite are comparable with the symbol size, while in the other cases they are not available.

inclusions on the effective dielectric permittivity of a nanocomposite enclosed between two parallel metallic electrodes. We have shown that the dielectric permittivity and hence the capacitance of a nanocomposite capacitor is fully described by an average inclusion polarizability density, $\beta$, and we have found its dependence on the aspect ratio and orientations of inclusions in an analytical form. We have demonstrated that our theoretical predictions are in excellent agreement with the available experimental data. The results obtained in the paper substitute the Maxwell Garnett approximation, which is not applicable in electrical engineering.

The model developed in this paper can be extended to the case where NWs are coated with a layer of a different phase.\textsuperscript{12} Then, instead of Eq. (2), one should use the expression for the polarizability of a coated ellipsoid.\textsuperscript{43} The model can also treat a mixture of inclusions with different dielectric permittivities.\textsuperscript{14} In such a case the polarization of inclusions, Eq. (7), should include the contributions from all components.

It should be stressed that the approach adopted in this paper follows from first principles. Although being limited in its applicability, it provides nevertheless a proper starting point for the nanocomposite capacitor design. The other theoretical models which have been developed to calculate the effective dielectric permittivity of nanocomposites (see, e.g., Refs.\textsuperscript{12,45}) are based on different ways of the field averaging and none of them consider the field reflected from the nanocomposite boundaries.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

V.G. Bordo: Conceptualization; Methodology; Formal analysis; Software; Writing original draft. T. Ebel: Conceptualization; Funding acquisition; Project administration; Writing review and editing.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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