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Modelling the electro-mechanical properties of Ppy/epoxy conductive composites

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Abstract

Modern trends in materials dedicated for aircraft applications are focused on development of highly multifunctional materials that allow not only to carry mechanical loading, but also to possess several other types of functionality, e.g. be thermal resistant, electrically conductive, etc. The material of such a type, with a possibility of conducting electrical current without loss of mechanical properties is the main topic of presented research results. The work presented here deals with the determination of the overall stochastic mechanical and electrical properties of a blend of polypyrrole (Ppy) and epoxy. The material properties are obtained applying appropriate periodic boundary conditions (PBCs) to the representative volume elements (RVEs) of the material nano-structure. A strategy to model numerically the electrical percolation network in the framework of Finite Element Method (FEM) is proposed and discussed. Electrical and mechanical properties of the material are calculated as a function of the filler volume fraction. Finally, the numerical results are compared with experiments found in literature and an overall good agreement is found.

Key words:
A. Conductive blends, B. Representative Volume Elements (RVEs), C. Continuum percolation, D. Electro-mechanical properties, E. Polypyrrole (PPy)

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1 Introduction

While metals are well known to be conductive materials, Polymer Matrix Composites (PMCs) are essentially dielectric. This inherent characteristic limits their use in certain applications and usually leads to more complicated structural solutions where metals and composites are used together with the aim of achieving the fulfilment of several functions. This is the case, for example, of the fuselage of an aircraft that has a double functionality: structural and electrical. From the electrical point of view, the fuselage needs to be highly conductive for several reasons. First of all, because all the electrical circuits of the aircraft instrumentation needs to be connected to the fuselage that acts as electrical ground. Secondly, because the fuselage must behave as a Faraday cage to protect the passengers from the strong electric field generated by a lightening. In the event of lightening strike, the electrical charge redistributes on the outer skin of the fuselage maintaining the interior space uncharged and the passengers safe. A lightening strike can also provoke structural damage on the outer skin of a fuselage; increasing the conductivity of the fuselage would enable a faster dispersion of the electrical charge and, as a consequence, the reduction of the size of the damaged region.

The solutions which are currently used for the lightening strike protection in aircraft are based mainly on using of thin metal meshes and layers, metal-coated fibre or highly conductive metal fibre [1,2]. This, of course, complicates technological processes of manufacturing of aircraft structural parts and increase the manufacturing costs.

To achieve this multifunctional (structural and electrical) behaviour, aircrafts are usually manufactured following a semi-monocoque concept. The primary structure consists of a load-carrying shell structure reinforced with a metallic reticular frame satisfying both the structural and electrical requirements. If
composites would be conductive the structural complexity of an aircraft would
be enormously simplified and an integrated approach could be followed during
the aircraft design and manufacturing leading to a substantial reduction of
weight and costs.

Recent studies on electrically conductive composites cover several solutions.
The first group of such solutions is based on reinforcement of dielectric matrix
by conductive fibres or particles. One can mention here the studies of Taya
et al. [3], who studied short fibre/elastomer matrix composites; the authors
of [4,5] analysed electrical conductivity of carbon fibre-reinforced polymer
composites; while Chen et al. [6] investigated a conductivity of polyamide-6
with two types of conductive fillers – stainless steel fibres and carbon nan-
otubes. A comprehensive review on various combinations of natural materi-
als used for matrices and fillers of multifunctional conductive composites can
be found in [7]. The second group of aforementioned solutions consists thin
conductive films (see e.g. [8,9]) which can be potentially applied for cover-
ing of dielectric materials. Nevertheless, the mentioned combinations result
in mechanically and electrically heterogeneous materials which significantly
complicates a description of their behaviour.

While inorganic resins used for structural applications are dielectric, some or-
ganic resins are, on the contrary, conductive and could be used to increase
the conductivity of a composite structure. Intrinsically conducting polymers
(ICPs) are organic polymers able to conduct electricity [10,11]. Polyacety-
lene (PAC), polyaniline (PANI), polypyrrole (Ppy), polythiophene (PTh), and
their derivatives, are examples of conductive polymers. They are commonly
used in several applications as i) electromagnetic shielding, ii) microwave ab-
sorption, iii) static electricity dissipation, iv) heating elements, v) membrane
materials, vi) paint coatings for anticorrosion protection, and vii) sensor ma-
terials. ICPs, however, show inferior mechanical properties with respect to inorganic polymers (thermosets or thermoplastics) and for this reason they are not used as main component in composite primary structures.

On the other hand, it is possible to disperse ICP fillers in an inorganic matrix: the blend obtained would have intermediate properties between ICPs and inorganic polymers. The final product would preferably have a conductivity comparable to that of the ICP and mechanical properties comparable to inorganic resins which seems to be very attractive from the point of view of simplifying manufacturing processes of conductive composite structures.

It is common knowledge, in fact, that blends of ICPs with inorganic resins exhibit a metal-insulator transition with the variation of the volume fraction, $v_f$, of the conductive filler. At a given value of the volume fraction called percolation threshold, the conductivity of the blend shows a drastic jump-wise change and the blend become conductive. This phenomenon is explained using the percolation theory. Electrical percolation occurs when conductive particles are located at a short distance (lower than a critical value). When this happens the dielectric material between the particles became conductive, and its conductivity is the same that of the conductive particle: this phenomenon is also known as *tunnelling*. When this happens, no substantial resistance is offered to the passage of electrons from a conductive particle to another. The formation of the percolation networks increase drastically the conductivity of the blend.

In this paper, a method to obtain the overall stochastic electromechanical properties of conductive polymers is proposed. A blend of epoxy resin and polypyrrole (Ppy) is considered and the variation of the electromechanical properties is studied as a function of the volume fraction. Of course, the method is general and it can be applied to other blends of ICP/inorganic
resins. The Ppy was chosen because it allows to reach the percolation thresh-
old at very low volume fractions obtaining blends with mechanical properties
comparable with those of inorganic resin.

2 Numerical model

Ppy fillers may be modelled as spherical particles randomly dispersed in the
epoxy matrix. The position of the spheres is obtained using the algorithm
proposed in [12], while the Finite Element (FE) models are created in the
ments the aforementioned algorithm and that apply, automatically, the Pe-
riodic Boundary Condition (PBCs) to the exterior nodes of the RVE. The
coupled thermal-electrical-structural element Q3D4 (4-node linear displace-
ment, electric potential and temperature) is used to mesh the RVE.

2.1 Size of the RVE

It is well known that the elastic and electrical parameters will depend, in first
approximation, on the size of the RVE. Under the assumption of ergodicity,
however, if the size of the RVE is sufficiently large, its influence on the com-
puted electrical or mechanical properties can be mitigated or even eliminated.
On the other hand, large RVEs entail a very large number of elements and,
consequently, a very large computational time.

For this reason, a preliminary study on the optimal size of the RVE is per-
formed. It is assumed that the side of the cubic RVE reads \( L = N_f r \), where
\( r \) is the radius of the particle \( (r = 35 \text{ nm as reported in [15]} ) \) and \( N_f \) a scalar
that represent a dimensionless parameter that take into account the size of
the RVE. The volume fraction is considered varying between \( 0 \leq v_f \leq 0.15 \),
while the size of the RVE take the values $N_f = 5, 10, 15, 20, \ldots$ For every combination of the volume fraction, $v_f$, and the size of the RVE, $N_f$, 15 RVEs are created.

Figure

[Fig. 1 about here.]

The spherical particles have a radius of $r = 35 \text{ nm}$ [15], while the RVE side has a length of $L \approx 20r$.

To apply the PBC the mesh on two opposite faces must be conformal, or, in other words, meshes should be identical on opposite RVE boundaries. Unfortunately this condition is not meet when meshing the RVE using tetrahedral elements because the symmetries are lost and Abaqus is not able to mesh properly the RVE using its own built-in methods.

For this reason, an algorithm to mesh the RVE was implemented in the Python script and its efficacy has been demonstrated. The algorithm works as follows: i) the part is meshed using the Abaqus built-in free meshing algorithm; ii) the opposite mesh (that need to be conformal) are modified: adding/deleting nodes, changing the position of the nodes, etc., to obtain a conformal mesh. Figure 2 shows the mesh generated by the Abaqus built-in free meshing algorithm and by the proposed meshing algorithm on two opposite faces of the RVE. While the meshes generated using the Abaqus built-in are clearly non conformal (see Figure 2(a)), the meshes generated using the proposed algorithm allows the generation of a conformal mesh (meshes are superposable as shown in Figure 2(b)).

[Fig. 2 about here.]

Structural and electrical PBCs must be applied on the boundaries of the RVE. Faces, edges and vertices of the RVE are reported in Figure 3 with their numbering.
The structural PBCs [16] for opposite faces read:

\[
\begin{align*}
&u_i^1 - u_i^3 - \Delta_1 \varepsilon_{i1}^0 = 0 \\
&u_i^2 - u_i^4 - \Delta_2 \varepsilon_{i2}^0 = 0 \\
&u_i^6 - u_i^5 - \Delta_3 \varepsilon_{i3}^0 = 0
\end{align*}
\]

(1)

where \(u_i^n\) represents the degree of freedom \(i\) of node \(n\); \(\Delta_1, \Delta_2,\) and \(\Delta_3\) the size of the RVE along \(x, y,\) and \(z,\) respectively; and \(\varepsilon_{ij}^0\) represents the applied far–field strain component.

Similar equations are written for the edges:

\[
\begin{align*}
&u_i^2 - u_i^4 - \Delta_1 \varepsilon_{i1}^0 - \Delta_2 \varepsilon_{i2}^0 = 0 \\
&u_i^1 - u_i^3 - \Delta_1 \varepsilon_{i1}^0 + \Delta_2 \varepsilon_{i2}^0 = 0 \\
&u_i^6 - u_i^8 - \Delta_1 \varepsilon_{i1}^0 - \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^5 - u_i^7 - \Delta_1 \varepsilon_{i1}^0 + \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^{11} - u_i^9 - \Delta_2 \varepsilon_{i2}^0 - \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^{10} - u_i^{12} - \Delta_2 \varepsilon_{i2}^0 + \Delta_3 \varepsilon_{i3}^0 = 0
\end{align*}
\]

(2)

and for the vertices of the RVE:

\[
\begin{align*}
&u_i^3 - u_i^5 - \Delta_1 \varepsilon_{i1}^0 - \Delta_2 \varepsilon_{i2}^0 - \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^2 - u_i^8 - \Delta_1 \varepsilon_{i1}^0 - \Delta_2 \varepsilon_{i2}^0 + \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^7 - u_i^1 + \Delta_1 \varepsilon_{i1}^0 - \Delta_2 \varepsilon_{i2}^0 - \Delta_3 \varepsilon_{i3}^0 = 0 \\
&u_i^4 - u_i^6 - \Delta_1 \varepsilon_{i1}^0 + \Delta_2 \varepsilon_{i2}^0 - \Delta_3 \varepsilon_{i3}^0 = 0
\end{align*}
\]

(3)

In an analogous way the electrical PBCs are defined. For opposite faces the
PBCs read:

\[
\tilde{\phi}^1 - \tilde{\phi}^3 - \Delta_1 \tilde{E}_1^0 = 0 \\
\tilde{\phi}^2 - \tilde{\phi}^4 - \Delta_2 \tilde{E}_2^0 = 0 \\
\tilde{\phi}^6 - \tilde{\phi}^8 - \Delta_3 \tilde{E}_3^0 = 0
\]  

(4)

where \( \tilde{\phi}^n \) is the electrical potential of node \( n \) and \( \tilde{E}_i^0 \) is the applied far-field electrical field. For opposite edges the PBCs read:

\[
\tilde{\phi}^2 - \tilde{\phi}^4 - \Delta_1 \tilde{E}_1^0 - \Delta_2 \tilde{E}_2^0 = 0 \\
\tilde{\phi}^1 - \tilde{\phi}^3 - \Delta_1 \tilde{E}_1^0 + \Delta_2 \tilde{E}_2^0 = 0 \\
\tilde{\phi}^6 - \tilde{\phi}^8 - \Delta_1 \tilde{E}_1^0 - \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^5 - \tilde{\phi}^7 - \Delta_1 \tilde{E}_1^0 + \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^{11} - \tilde{\phi}^9 - \Delta_2 \tilde{E}_2^0 - \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^{10} - \tilde{\phi}^{12} - \Delta_2 \tilde{E}_2^0 + \Delta_3 \tilde{E}_3^0 = 0
\]  

(5)

while for opposite vertices it is obtained:

\[
\tilde{\phi}^3 - \tilde{\phi}^5 - \Delta_1 \tilde{E}_1^0 - \Delta_2 \tilde{E}_2^0 - \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^2 - \tilde{\phi}^8 - \Delta_1 \tilde{E}_1^0 - \Delta_2 \tilde{E}_2^0 + \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^7 - \tilde{\phi}^1 + \Delta_1 \tilde{E}_1^0 - \Delta_2 \tilde{E}_2^0 - \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^4 - \tilde{\phi}^6 - \Delta_1 \tilde{E}_1^0 + \Delta_2 \tilde{E}_2^0 - \Delta_3 \tilde{E}_3^0 = 0 \\
\tilde{\phi}^{11} - \tilde{\phi}^9 - \Delta_1 \tilde{E}_1^0 + \Delta_2 \tilde{E}_2^0 + \Delta_3 \tilde{E}_3^0 = 0
\]  

(6)

The application of the PBCs using equations (1)–(6) allows obtaining the elastic and electrical properties for the composite blend. The elastic properties, being the material isotropic, are obtained as:

\[
E = \frac{\langle \sigma_{ii} \rangle}{\varepsilon_0^{\varepsilon_0}} \quad G = \frac{\langle \sigma_{ij} \rangle}{2\varepsilon_0^{\varepsilon_0}}
\]  

(7)
where $\langle \cdot \rangle$ indicates the volume average. The electrical properties are obtained calculating the local electric flux vector $\mathbf{J}$ and the local electrical field $\mathbf{E}$ obtained as:

$$\mathbf{E} = -\nabla \phi$$

(8)

According to Ohm’s law the local electric flux vector reads:

$$\mathbf{J} = \sigma \mathbf{E}$$

(9)

therefore the conductivity (along the direction $i$) is obtained as:

$$\tilde{\sigma}_i = \langle \mathbf{J}_i / \mathbf{E}_i \rangle$$

(10)

It should be noted that the blend is mechanical and electrical isotropic, therefore the elastic parameters and the conductivities $\tilde{\sigma}_i$ calculated on the different directions (as in (7) and (10)) represent different estimations of the same physical quantity.

2.2 Modelling the electrical percolation

Electrical percolation occurs when a volume fraction of conductive particles is high enough to form a percolation cluster. This means that conductive particles belonged to this cluster are at a distance less than the hopping distance $H$.

Due to the fact that polymeric materials considered in a mixture have no organized structure it was suitable to apply a continuum percolation model with random distribution of particles. The applied percolation model was of hard-core soft-shell type which means that conductive particles (parametrized by their constant radius and spatial location parameters) were generated using the Poisson process of the constant concentration rate and the generated particles cannot interpenetrate each other, but their shells considered here as a
hopping distance can. After reaching the percolation threshold by a considered
system, these particles constitute an infinite percolation cluster. Considering
the fractal properties of a percolation cluster it is scale-invariant (see e.g. [17]),
i.e. the percolation occurs at every scale if a corresponding percolation thresh-
old is reached. This property allows to generalize proposed approach to the
macroscale problems. If this happens the dielectric material between two par-
ticles became conductive (same conductivity that the particles) and an electric
tunnel is originated between the particles. The hopping distance (see Figure 4)
is a characteristic parameter and for Ppy particles is equal to $H = 181$ nm as
calculated in [18].

Therefore, the following strategy can be applied. Once the RVE has been gen-
erated, different mechanical properties are assigned to conductive particles
and inorganic matrix. For the electrical properties, same conductivity is as-
signed to the conductive particles and to the elements of the RVE that lie
between particles that are electrically connected. Therefore, if two particles
with coordinates $C_1 (x_1, y_1, z_1)$ and $C_2 (x_2, y_2, z_2)$ are at a distance inferior to
$2H$, all the elements that lie in the cylinder with axis $C_1C_2$ and with radius
$r$ (where $r$ is the radius of the particle) are considering to be part of the
percolation network. To this elements, the same electrical properties of the
conductive particles are assigned. The mechanical and electrical parameters
of the Ppy and epoxy are reported in Table 1. It should be noticed that the
model is fully coupled and therefore it is possible to solve complex thermo-
electrical-structural analyses that can be used to optimize the material for
certain applications. At this stage however, only two studies are presented: i)
the determination of the elastic parameters, and ii) the determination of the
electrical parameters (i.e. the conductivity) neglecting the Joule heating. The
Joule heating is neglected because the steady-state solution of the coupled problem is not taken into account and it will be the object of further studies. However, the model presented, allows to face the fully coupled problem with no additional efforts and to consider the resistive heating and its effect in influencing the conductivity of the material.

[Table 1 about here.]

Figure 5 shows an example of the generated RVEs. The elements in red represent the conductive particles while the elements in ochre represent the percolation network (elements of the matrix that become conductive thanks to percolation). Additionally in white it is shown the inorganic matrix that is not affected by percolation and that will remain dielectric.

[Fig. 5 about here.]

Figure 6 shows the percolation networks in the RVEs as a function of the volume fraction $v_f$. It is observed that at $v_f = 0.05$ correspond the formation of the infinite cluster (the percolation network cross all the RVE) and that at $v_f = 0.1$ the blend is totally conductive.

[Fig. 6 about here.]

3 Results and discussion

The Young’s and shear moduli of the investigated blend are obtained applying a direct and shear remote strain, respectively. Figures 7(a) and 7(b) show the contour plots of $\varepsilon_{11}$ and $\sigma_{11}$ on the deformed RVE, while Figure 4 reports the Young’s modulus as a function of the volume fraction, $v_f$. It is observed that the Young’s modulus varies linearly with the volume fraction in the range investigated ($0 < v_f \leq 0.15$).

[Fig. 7 about here.]
Additionally, Figures 8(a) and 8(b) report the contour plots of $\gamma_{12}$ and $\tau_{12}$. The shear modulus too, show a linear behaviour varying the volume fraction $v_f$ (as reported in Figure 4).

Finally, the conductivity is calculated applying an electric potential difference on the boundaries of the RVE. Figures 10(a) and 10(b) show the contour plots of the electrical current density and the electrical potential gradient, respectively. Notice that at very low volume fraction, as the case showed in Figure 10, the presence of percolation networks not fully developed is clearly visible. For larger values of the volume fraction, the fields of the electrical current density and the electrical potential gradient are constant because the material becomes conductively homogeneous.

Finally, Figure 11 shows the conductivity of the blend as a function of the volume fraction, $v_f$, together with its standard deviation (reported in the error bars). Figure 11 emphasizes the drastic change, in the conductivity of the blend, due to the electrical percolation.

The formation of percolation networks occurs when the volume fraction is very small ($v_f < 0.05$) and this is consisted with experimental observation conducted by several authors [19,20]. Moreover, the percolation threshold is approximatively equal to $p_c \approx 0.001$ matching the estimation obtained by Katunin and Krukiewicz [18]. It should be observed that the standard deviation of the conductivity is quite large in the range of volume fractions $0.01 < v_f < 0.05$. This is essentially due to the fact that the percolation networks are not fully developed and are randomly oriented inside the RVE.
For this reason, the same RVE provides different values of the conductivity depending on whether the remote electric potential difference is applied along \( x \), \( y \), or \( z \).

It should be noted that the bigger scatter in the determination of the conductivity is obtained approximatively for a volume fraction of \( v_f \approx 0.25 \), and this correspond to the ascending portion of the curve reported in Figure 11. This is due essentially to the fact that when the transition from insulator to conductor occurs the material is not electrically homogeneous because the percolation networks that grow inside the material are totally random. Therefore, it can happen that the RVE is conductive in a given direction while it is not in another. This behaviour characterises the metal-insulator transition.

From a quick inspection of Figures 9 and 10, it is concluded that Ppy/epoxy blend could be used in primary structures. This blend in fact, allows to obtain a material fully conductive that has mechanical properties comparable with that of inorganic resins. In the investigated case, for example, when the volume fraction is \( v_f = 0.1 \) the material is fully conductive (\( \bar{\sigma} = 0.01 \text{S cm}^{-1} \)) and its mechanical properties are still comparable with that of pure epoxy (the reduction of the elastic properties is approximately 10%).

4 Conclusions

The results of this works may be summarize in the following concluding remarks:

- The application of the presented approach based on continuum percolation theory for finding the optimal volume fractions of conducting and dielectric polymers allows precise determination of percolation threshold(s) and can be generalized to arbitrary pairs of conductive/dielectric materials. Obtained
theoretical results, however, should be verified experimentally and corrected according to synthesis parameters.

- A fully coupled FE model of a blend of Ppy/epoxy was obtained in the commercial software Abaqus. A Python script was used to obtain several parametric models of the RVE. As well as generating the FE model using Abaqus built-in features, the Python script provides: i) the random distribution of particles using the algorithm developed in [12]; ii) a conformal mesh necessary to apply the PBCs; ii) apply the electrical and mechanical PBCs automatically on the RVE; run the analysis and extract the results.

- The model developed is general and can be easily adapted to other kind of ICP/inorganic resin blends, for example ICPs fillers with different dimensions or shape.

- The elastic and electric properties of the blend were calculated. As confirmed experimentally it was found that Ppy/epoxy blends could be used in primary structures because in spite of being electrically conductive the mechanical parameters are comparable with that of the pure resin.

- The methodology proposed to simulate the percolation networks allows to model the drastic change in conductivity that are observed when the volume fractions reach the percolation threshold.

- The model proposed can be used, with no effort, to study fully-coupled problems in electrically conductive blends considering not only the mechanical solicitations in the material, but also the applied electric potential difference. A first improvement would be considering the Joule heating effect and the variation of the conductivity with the temperature. Here these effects were neglected because the aim of the paper was only to show how to determine the overall stochastic parameters of the blend. However, these effects are crucial when the material needs to be optimized for certain ap-
Applications as using the material to improve the lightening strike protection of aircraft structures. In this case it will be unavoidable taking into account all these effects.

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<td>Young’s modulus (MPa)</td>
<td>4890 [21]</td>
<td>591 [22]</td>
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<td>Poisson’s modulus (–)</td>
<td>0.3</td>
<td>0.3</td>
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<td>7.9e-16 [18]</td>
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