

Universal and Anisotropic Simulation Platform for the Study of Electrical Properties of Conductive Polymer Composites

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Abstract: In order to carry out a study on the synergistic relationship of variables which could affect the electrical properties of CPC, a universal and anisotropic platform of simulation, containing three simulation modules is explored. The simulation modules are: FEM (finite element modeling), PTM (percolation threshold modeling) and ENM (electrical networks modeling).

Key words: Conductive polymer composites, finite elements method, simulation.

1. Introduction

Due to easy fabrication, tunable properties and a broad range of applications, the research area of CPCs (conductive polymer composites), consisting of insulating polymers and conductive fillers (CB (carbon black), CFs (carbon fibers), graphene, etc.) has increasingly gained more attention in the last decade [1]. CPCs with good flexibility exhibit a variety of sensing responses when subjected to external strain. The sensing mechanism is mainly based on the destruction and reconstruction of conductive networks. Therefore a variation of conductivity can be linked to the amount of exposure by external stimuli.

Recently, CPCs with good flexibility have been considered as satisfactory candidates to develop flexible strain sensors. Utilizing the advantages of the polymer matrices, CPCs can show excellent stretching ability and quick response to external stress [2-4]. Elastomers, such as vinylidene

fluoride-hexafluoropropylene copolymer [5], PDMS (polydimethylsiloxane) [6], SR (silicone rubber) [7-9] or TPU (thermoplastic polyurethane) [10-12] are typically used as polymer matrices. However, the application of CPCs based strain sensors still faces severe challenges, e.g., unstable signal output and insufficient reversibility. In particular, due to different demands for the strain sensing behavior in different applications, CPCs with tunable strain response patterns are urgently needed.

2. Background

Besides the experimental investigation, simulations can provide an effective way of understanding the dynamic mechanism [13-15]. A surplus of theoretical studies carried out by simulations has already been conducted in order to investigate the relationship between the geometry of fillers and electrical properties [16-18]. However, most of these studies assumed an idealized isotropic orientation of the fillers, represented by using just one parameter for the spatial orientation [19, 20]. If the geometrical factors are considered, as for example the aspect ratios of the fillers and the filler inclination, the influence on the

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electrical properties can be studied thoroughly.

Besides the experimental investigation, simulation can provide an effective way of understanding the dynamic mechanism. Many excellent theoretical studies via simulations have already been conducted [1-3] in order to investigate the relationship between the geometry of fillers and electrical properties. However, most of these studies assumed an idealized isotropic orientation of the fillers, and focused on only one variable of geometrical distribution. Considering the geometrical factors, i.e. fillers' aspect ratios and filler inclination might influence the electrical properties [21, 22]. Therefore, a systematic theoretical study on the influence of the geometrical distributions and filler dimensionality, especially for the 3-dimensional fillers, would still be scientifically necessary.

3. Model

For the simulation and modeling, the influence of different parameters on the electrical conductivity, particularly on the electrical percolation filler fraction was discussed in relation to experimental data [23]. In order to carry out a study on the synergistic relationship of these variables, a universal and anisotropic platform of simulation, containing three simulation modules had been explored [24]. The simulation modules contain FEM (finite element modelling), PTM (percolation threshold modeling) and ENM (electrical networks modelling). After constantly updating, the simulation platform performs the following features:

- Anisotropy (orientation);
- High degree of flexibility;
- High degree of automation;
- High efficiency: Under the same magnitude of mesh and computing environment, our platform needs only 1/3 the time of other similar simulation program;
- High accuracy: All parameters and results can be accurate up to 12 decimal places;
- Very low error rate (less than 0.01%).

The mesh strategy is the key of simulation. For simulation with different settings and conditions, it is necessary to bring different mesh strategy when facing diverse models. In the platform of simulating CPCs, the mesh strategy is always optimized and updated.

4. Experimental

The ordinate axis shows the number of elements, and the abscissa shows the ratio of current mesh quality and the smallest mesh quality [25]. For the 3D model, it could also be approximated as the reciprocal of the ratio of the minimum element volume to the current element volume. This distribution is a practical tool for judging the quality of the mesh and the authenticity of the simulation results. A curve that satisfies the normal distribution represents a suitable meshing.

Finite element modelling (FEM) in 3 dimensions was used in order to examine how the electrical conductivity of polymeric fiber composites is influenced by the orientation, aspect ratio, filler fraction and material of the fibers, with the primarily intention to confirm the reliability of equations 10-12. The FEM modelling strategy presented in this paper was an improved version of the model previously presented in Nilsson et al. [21, 24]. An overview of the simulation process is presented in Fig. 1.

The typical number of mesh elements for a composite comprising 30 fiber sections is about 250,000 tetrahedrals. Figs. 2 and 3 show typical meshes of a small model composite.

After constantly updating and improving in the past years, the simulation platform performs with high degree of flexibility, high degree of automation, high efficiency and high accuracy. Fig. 4 shows the mesh quality control of the simulation. Within the platform, all the factors could be controlled as either constant or variable, and a deeper understanding of the relationship between different factors is comprehended. An experimental consideration with multiple levels of variables is carried out, and the synergistic relationship

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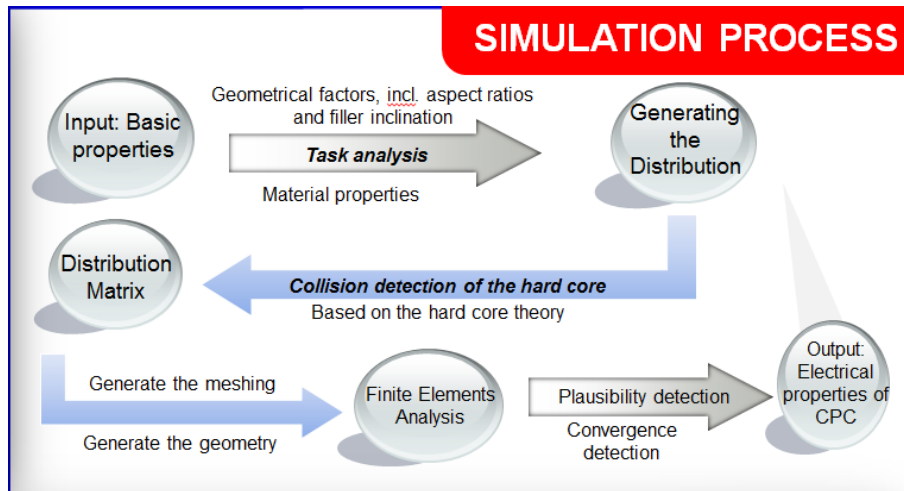


Fig. 1 Process of the simulation set in the platform.

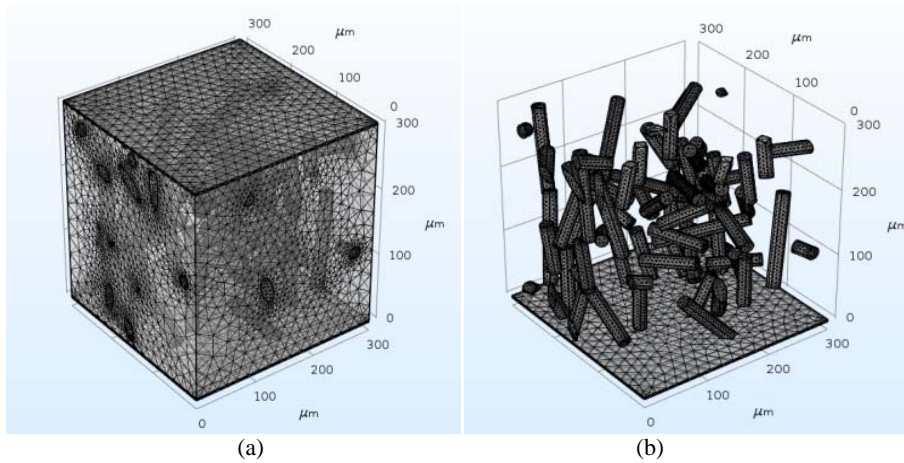


Fig. 2 (a) Mesh strategy for the simulation with 1~150 fillers, with the top and bot-voltage blocks a coefficient of geometry scale 0.3. The coefficient of the space and the fillers is 1.0. The mesh operation over the geometry is set to be free tetrahedral. (b) Mesh of the conductive filler, with the top voltage block and the space set to be hidden.

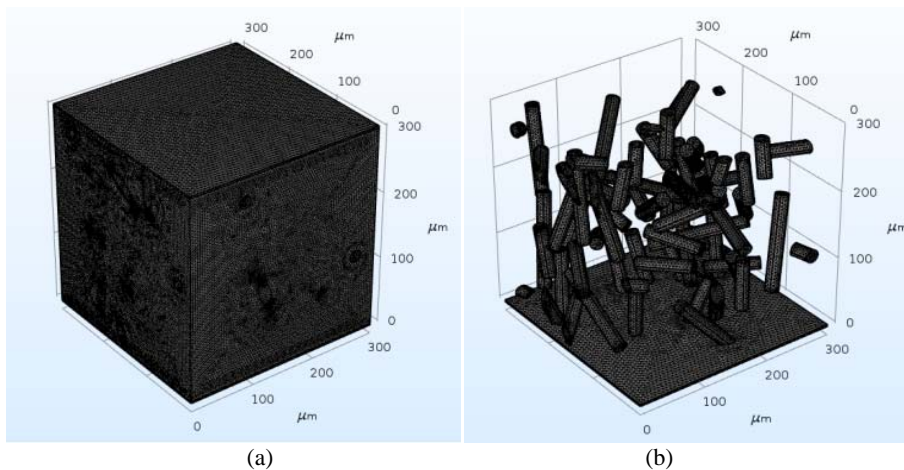


Fig. 3 (a) Mesh strategy for the simulation with > 150 fillers, with the top and bot-voltage blocks a coefficient of geometry scale 2.0. The coefficient of the space and the fillers is 10.0. The mesh operation over the geometry is set to be free tetrahedral. (b) Mesh of the conductive filler, with the top voltage block and the space set to be hidden.

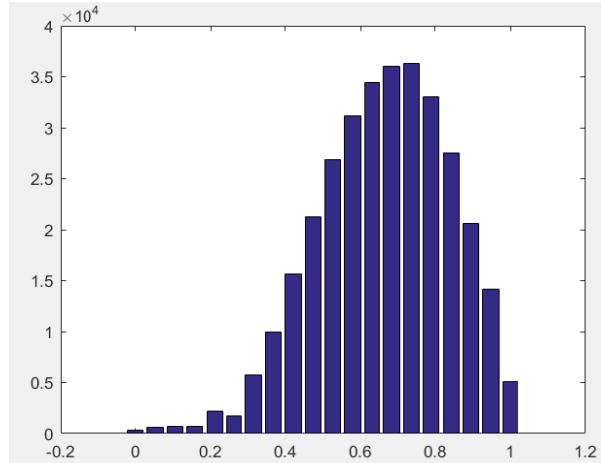


Fig. 4 Mesh quality control.

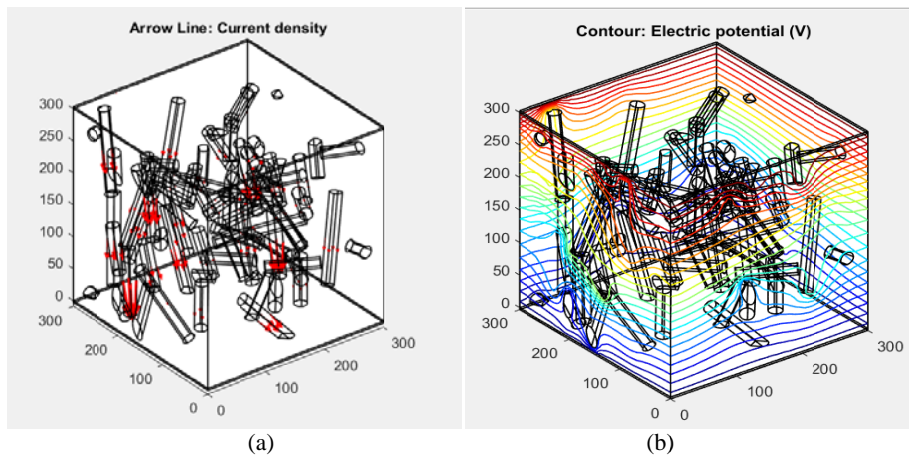


Fig. 5 Output of the current density and the electric potential.

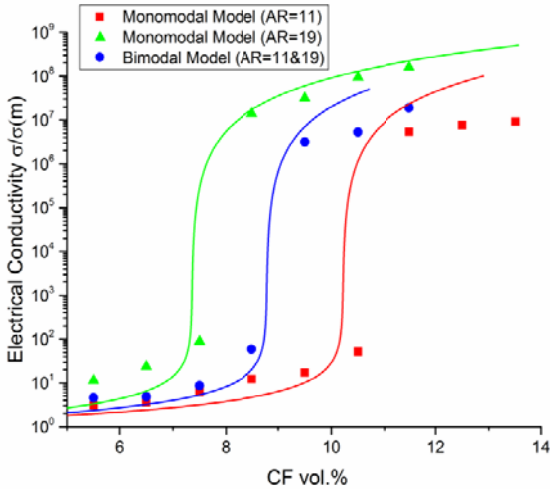


Fig. 6 Logarithm of conductivity vs. CF volume fraction for the composites from different aspect ratios, as well as the bimodal model. The filler fraction of the both kinds of CFs in the bimodal model is set to be 50%. With the change in composition, the conductivity of the CPCs as well as the percolation threshold will also show a corresponding change.

of the variables could be systematic studied. The trend of change in each variable under different environmental settings is clearly displayed and systematically studied by the simulation platform.

In Fig. 5, the arrow line of current density shows automatically the path built by the conductive fillers, the denser the red arrows, the greater is the current flow, which also indicates the less resistance of the path. This output is significant at showing the electrical flow within the matrix according to the distribution of the fillers. After collecting more than 1,000 groups of data and calculating the median value out of it, a McLachlan Fit has been done according to the function.

Fig. 6 shows the McLachlan Fit of the data, and the mono modal with aspect ratio 19 has a lowest percolation threshold of 7.6%; the group with AR = 11

has the highest percolation threshold of 10.2%. With a bimodal model of a certain ratio between the both kinds of fillers (1:1), the percolation threshold could be adjusted to an intermediate value 8.4%. With more data from the simulation platform, a preparation method with a fixed percolation threshold will be determined.

5. Conclusions

A significant research aiming at the difficulties of simulating CPCs is carried out as the first phase of the simulation. The platform will be systematically updated for a better performance and efficiency, especially the PTM (percolation threshold method) module and the “high conductive layer” feature. Through the whole working phase, all the factors with high research value will be controlled as either constant or variable, and a deeper understanding of the relationship between different factors will be comprehended. An experimental consideration with multiple levels of variables will be carried out, and the synergistic relationship will be systematically studied. Combined with experimental data, the trend of change in each variable under different environmental settings will be clearly displayed by the simulation platform.

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