Modeling the electrical and mechanical properties of CNT/polymer nanocomposites

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It is well known that the addition of carbon allotropes to a polymeric matrix affect its mechanical and electrical properties. The changes can be significant even at small weight fractions of the reinforcement. Among the carbon allotropes carbon nanotubes (CNT) have received considerable attention [1]. This is due to their aspect ratio that enables the production of conductive composites with a low weight fraction of reinforcement and also enabling an improvement in the composite's mechanical properties.

In the work, a numeric model has been employed to investigate the mechanical and electrical properties of polymer/CNT nanocomposites material subjected to a deformation. To achieve a better understanding of phenomena occurring at the smaller scales, an electrostatic model is used [2] as well as the molecular dynamics (MD) method [3]. The two models are then coupled in an iterative procedure, enabling the prediction of the micro-scale constitutive response, which is related to the local microstructure. The electrostatic model is based on ''hard-core'' cylinders model and the prescribed conduction mechanism is hopping between nearest neighbours.

In this work, it is also demonstrated how the conductivity of a polymer/CNT composite changes with the applied stress to the composite, effectively providing the ability to simulate and predict strain-dependent electrical behaviour of CNT nanocomposites, and useful insights for tailoring the structure of active/smart materials for specific properties.

It is also shown that the mechanical behaviour of a computer generated material depends on the fiber length, their initial orientation in the polymeric matrix, and their concentration. The fiber concentration has a significant effect on the properties, with higher loadings corresponding to higher stress levels and higher stiffness, as could be expected from experimental work.

References

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