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Numerical Simulations on Piezoresistivity of CNT/Polymer Based Nanocomposites

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Summary

In this work, we propose a 3 dimensional (3D) numerical model to predict the piezoresistivity behaviours of a nanocomposite material made from an insulating polymer filled by carbon nanotubes (CNTs). This material is very hopeful for its application in highly sensitive strain sensor by measuring its piezoresistivity, i.e., the ratio of resistance change versus applied strain. In this numerical approach, a 3D resistor network model is firstly proposed to predict the electrical conductivity of the nanocomposite with a large amount of randomly dispersed CNTs under the zero strain state. By focusing on the fact that the piezoresistivity of the nanocomposite is largely influenced by the tunnelling effects among neighbouring CNTs, we modify this 3D resistor network model by adding the tunnelling resistance between those neighbouring CNTs within the cut-off distance of tunnelling effect, i.e., 1nm in this study. The predicted electrical conductivities by this modified 3D resistor network model are verified experimentally. Furthermore, to analyze the piezoresistivity of nanocomposite under various strain levels, this modified 3D resistor network model is further combined with a fibre reorientation model, which is used to track the orientation and network change of rigid-body CNTs in the nanocomposite under applied strain. This combined model is employed to predict the piezoresistivity of the nanocomposite iteratively corresponding to various strain levels with the experimental verifications. Some key parameters, which control the piezoresistivity behaviour, such as, cross sectional area of tunnel current, height of barrier, orientation of CNTs, and electrical conductivity of CNTs and other nanofillers, are systematically investigated. The obtained results are very valuable, which can provide a guidance for designing the strain sensor of this nanocomposite with enhanced sensitivity.