A numerical model for the prediction of the electrical conductivity of nanofilled polymeric matrices

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Abstract.
This work describes a numerical approach aimed at predicting the electrical conductivity of polymeric matrices filled with carbon nano-tubes (CNT). The tunneling effect was modeled through a finite element, FE, approach. Each particle was schematized as a cluster of nodes connected by highly conductive elements, in compliance with the large conductivity of the CNTs. When two particles are in tunneling condition, a link was realized, whose electrical resistance was computed through a formula, involving, among the others, parameters like the mutual distance and the tunnel cross section area. The resulting system, a truss structure network contained within a cubic polymeric matrix, was then solved through a thermal analogy. The inward and outward currents passing through two opposite cube faces were simulated by applying thermal fluxes of opposite sign; the voltage drop caused by the global resistance was then estimated through a steady heat transfer analysis, giving the temperature gradient between the opposite faces. The ratio between the voltage (temperature) drop and the inward-upward current (thermal flux) was then assumed as resulting global resistance of the cube. A parametric investigation was finally performed, finding out the dependence of the gage factor (strain vs resistance variation) on CNT concentration and aspect ratio parameters (curvature, diameter-length ratio).