THE EFFECT OF NANOTUBE WAVINESS ON THE ONSET OF PERCOLATION IN CARBON-NANOTUBE REINFORCED COMPOSITES

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Electrical conductivity in nanotube-reinforced polymers follows a classic percolation-like behavior (e.g. [1]). Thus, the study of percolation in these materials is of high interest and is motivated by the potential for their use as electrically and/or thermally conductive systems with an extremely low concentration of nanotubes. The classic percolation models for sticks in three dimensions are often applied to the prediction of percolation onset in nanotubes-reinforced composites. In these numerical and analytical studies nanotubes are modeled as straight, rigid, capped cylinders, or spherocylinders (e.g. [2]). The excluded volume rule [3] which states that the number of objects at percolation is inversely proportional to the object's excluded volume is also widely applied, with a constant of proportionality of one since the nanotubes are of high aspect ratio [4].

It is well documented that embedded nanotubes are not straight but rather are curved or wavy; however the extent to which waviness affects percolation has not been explored. The objectives of this work were thus to investigate the effect of fiber waviness on the onset of percolation for three-dimensional networks of randomly oriented fibers, and to determine the applicability of the excluded volume rule to systems of wavy fibers.

Fibers were modeled as capped helices instead of straight cylinders. A numerical method was used to determine the excluded volume of fibers of different degrees of waviness and aspect ratios and the analytical percolation threshold found for each case. The percolation threshold for systems of wavy fibers of was also found using Monte Carlo simulations and the results compared with the inverse of the excluded volume and with the straight fiber results.

Our results show that for high aspect ratio fibers, the inverse proportionality between percolation threshold and excluded volume holds, independent of fiber waviness. This suggests that for systems of high aspect ratio fibers, including nanotubes-reinforced composites, an analytical solution for the percolation threshold can be derived from an expression for excluded volume. Further, we show that for high aspect ratios, the percolation threshold of the wavy fiber networks is directly proportional to the analytical straight fiber solution. Thus, the onset of percolation can be adequately modeled by applying a factor based on fiber geometry to the analytical straight fiber solution.

References

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