About the relevance of waviness, agglomeration, and strain on the electrical behavior of polymer composites filled with carbon nanotubes evaluated by a Monte-Carlo simulation

Por: Roman, S (Roman, Sebastian)[1] ; Lund, F (Lund, Fernando)[2] ; Bustos, J (Bustos, Javier)[3] ; Palza, H (Palza, Humberto)[1]

MATERIALS RESEARCH EXPRESS
Volumen: 5
Número: 1
Número de artículo: 015044
DOI: 10.1088/2053-1591/aaa531
Fecha de publicación: JAN 2018
Tipo de documento: Article
Ver impacto de la revista

Resumen

In several technological applications, carbon nanotubes (CNT) are added to a polymer matrix in order to develop electrically conductive composite materials upon percolation of the CNTnetwork. This percolation state depends on several parameters such as particle characteristics, degree of dispersion, and filler orientation. For instance, CNT aggregation is currently avoided because it is thought that it will have a negative effect on the electrical behavior despite some experimental evidence showing the contrary. In this study, the effect ofCNTwaviness, degree of agglomeration, and external strain, on the electrical percolation of polymer composites is studied by a three dimensional Monte-Carlo simulation. The simulation shows that the percolation threshold of CNT depends on the particle waviness, with rigid particles displaying the lowest values. Regarding the effect of CNT dispersion, our numerical results confirm that low levels of agglomeration reduce the percolation threshold of the composite. However, the threshold is shifted to larger values at high agglomeration states because of the appearance of isolated areas of high CNTconcentrations. These results imply, therefore, an optimum of agglomeration that further depends on the waviness and concentration of CNT. Significantly, CNT agglomeration can further explain the broad percolation transition found in these systems. When an external strain is applied to the composites, the percolation concentration shifts to higher values because CNT alignment increases the inter-particle distances. The strain sensitivity of the composites is affected by the percolation state ofCNTshowing a maximum value at certain filler concentration. These results open up the discussion about the relevance in polymer composites of the dispersion state ofCNTand filler flexibility towards electrically conductive composites.

Palabras clave

Palabras clave de autor:carbon nanotube composites; Monte-Carlo simulation; percolation process; filler agglomeration
KeyWords Plus:PERCOLATION-THRESHOLD; FIBROUS NETWORKS; CONDUCTIVITY; NANOCOMPOSITES; DISPERSION; SENSOR; FUNCTIONALIZATION; CRYSTALLIZATION; NANOSTRUCTURES; POLYCARBONATE

Información del autor

Dirección para petición de copias: Palza, H (autor para petición de copias)

+ Univ Chile, Fac Ciencias Fis & Matemat, Dept Ingn Quim & Biotecnol, Santiago, Chile.

Direcciones:

+ [1] Univ Chile, Fac Ciencias Fis & Matemat, Dept Ingn Quim & Biotecnol, Santiago, Chile
+ [2] Univ Chile, Fac Ciencias Fis & Matemat, Dept Fis, Santiago, Chile
+ [3] Univ Chile, NIC Labs, Santiago, Chile

Direcciones de correo electrónico:hpalza@ing.uchile.cl

Financiación

Entidad financiadora	Número de concesión
CONICYT	FONDECYT 1150130 FONDECYT 1160823

Ver texto de financiación

Editorial

IOP PUBLISHING LTD, TEMPLE CIRCUS, TEMPLE WAY, BRISTOL BS1 6BE, ENGLAND

Información de la revista

- **Impact Factor:** Journal Citation Reports

Categorías / Clasificación

Áreas de investigación: Materials Science
Categorías de Web of Science: Materials Science, Multidisciplinary

Información del documento

Idioma: English
Número de acceso: WOS:000423194900006
ISSN: 2053-1591