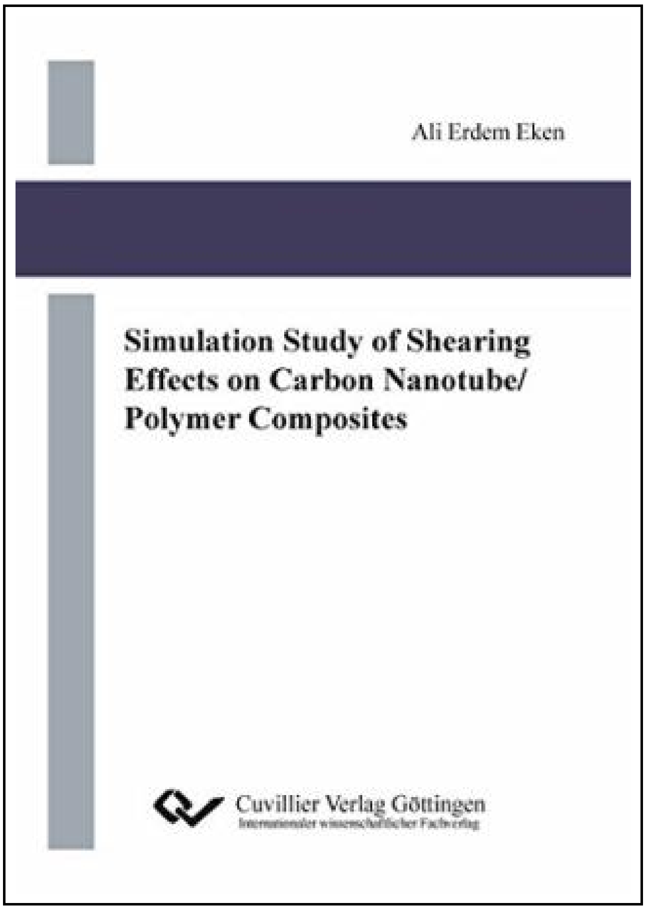
Simulation Study of Shearing Effects on Carbon Nanotube/Polymer Composites



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SIMULATION STUDY OF SHEARING EFFECTS ON CARBON NANOTUBE/POLYMER COMPOSITES

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Cuvillier Verlag Aug 2012, 2012. Taschenbuch. Book Condition: Neu. 213x147x12 mm. Neuware - During processing of carbon nanotube (CNT)/polymer composites, materials are exposed to significant deformation that changes the microstructure and affects the properties of the final products. In order to improve the material properties and manufacturing process, a clear understanding of how these materials react to the flow fields is required. Single carbon nanotubes cannot be observed during processing with commercial characterization methods. Therefore simulations are the only way to get insight the movement of the carbon nanotubes in polymer melts. In this thesis, fiber-level simulation technique is employed to simulate CNT/polymer composites in simple shear flow. This model incorporates CNT flexibility, irregular CNT equilibrium shapes and CNT interactions. The combined effects of carbon nanotube properties such as aspect ratio, curvature and tunneling length, as well as shear rate on the microstructure and electrical conductivities of CNT/polymer composites are investigated. Electrical conductivities are calculated using a resistor network algorithm. Results for percolation thresholds in static systems agree with theoretical predictions and experimental measurements. Imposed shear flow decreases the electrical percolation threshold by facilitating the formation of conductive aggregates. In agreement with previous research lower percolation thresholds are obtained for nanotubes with high aspect ratio. The effect of nanotube shape is different for sheared and non-sheared suspensions. Increasing nanotube curvature increases the percolation threshold in the non-sheared suspensions while this effect is reversed in the sheared suspensions such that increasing nanotube curvature decreases the percolation threshold. Increasing nanotube curvature favors the formation of agglomeration in sheared suspensions which leads to network formation. Alignment studies show that when nanotubes are aligned, percolation threshold increases due to the decrease of tube-tube contact occurrence probability. Another prediction of the simulations is that a greater tunneling length causes a decrease in percolation threshold of...

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