

RESUMO N° 310

INTERACTION BETWEEN CARBON NANOTUBES AND IONIC LIQUIDS

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In the last decade, mechanical and structural properties of isolated and embedded Carbon Nanotubes (CNT) have been extensively studied using classical Molecular Dynamics (MD). CNTs have been embedded in polymeric, metallic and ceramic matrices, primarily as mechanical reinforcements, but simulation results scarcely agree with experimental results. One of the problems resides in the fact that CNTs tend to form bundles resulting in very poor dispersion and consequent reduction of the contact area between CNTs and the matrix composite. MD simulation models do not usually take this in account. In recent years, CNTs have been modeled as embedded in more complex media, such as ionic liquids. These mixtures are expected to display novel dynamic and structural properties, arising from the pronounced nanostructuration of ionic molecules around the CNTs, including effective dispersion of CNTs bundles. In this work, MD simulations were used to model the insertion of CNTs in an ionic liquid matrix. The ionic liquids modeled were parameterized using the well-known CL&P forcefield. The effect of CNT polarizability was introduced in order to assess its influence on the formation of the nanostructures. Polarizability was introduced directly using the Tersoff potential with the core-shell model and indirectly using AIREBO potential with carefully modified Lennard-Jones non-bonded interactions parameters. The nanostructured pattern, obtained from different ionic liquids and CNTs with different diameters, was characterized using cylindrical distribution functions and density profiles. Interaction energies were obtained and compared between polarizability models. Different ionic liquids were also compared with respect to their capability to disperse (or not) CNT bundles. This work is part of a wider research project which aims to shed light on the interactions between ionic liquids and carbon nanoagglomerates.