Effect of nitrogen doping on the polarizability of carbon nanotubes

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Anisotropic polarization properties of carbon nanotubes (CNTs) are important for development of chemical sensors, electromechanical systems, antennas, detectors and sources of electromagnetic radiation in terahertz region, and shielding composite materials. These properties can be modified by inserting nitrogen atoms in the CNT walls in the results of decomposition of nitrogen-containing precursor. The content as well as the chemical state of incorporating nitrogen is dependent on the synthetic conditions. The nitrogen concentration in single-walled CNTs (SWCNTs) is limited to ~ 1at.% while it may exceed ~3-5 at.% in multi-walled CNTs (MWCNTs). Here we use density functional theory (DFT) for calculation of the substitutional energy for nitrogen atoms in CNT and the static polarizability of models. It is found that static polarizability is sensitive to the position of nitrogen atoms in CNT wall. The thermodynamically most preferable configuration, when the nitrogen atoms occupy the sites in pentagonal rings near the closed CNT tip, provides the largest gain in polarizability especially for the longitudinal component. Formation of such rings in graphitic network promotes closing of nanotube that could explain bamboo-like structure of nitrogen-doped MWCNTs. Assembly of conical graphitic segments containing nitrogen near the cone tip should give much higher longitudinal polarizability of nitrogen-doped MWCNTs as compared with the undoped counterparts or nitrogen-doped SWCNTs. High anisotropy of polarizability response expected for nitrogen-doped MWCNTs would open their utilization for development of electromagnetic protecting materials.

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Simulation of Electromechanical Pproperties of Ordered Carbon Nanotube Arrays

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Carbon nanotube arrays are shown to have interesting mechanical resonant properties which manifest themselves in electromechanical phenomena such as excitation of resonant vibrations of nanotubes in electromagnetic fields due to the action of ponderomotive forces. Hierarchical simulation approach to the modeling of such arrays is necessary including quantum mechanical, molecular-dynamical and continual description levels. Elastic properties of carbon nanotubes can be calculated by molecular dynamics simulations and then be used for continual modeling of nanotube arrays electromechanical behaviour by multiphysics methods. This program was realized for electromagnetic fields of radio and UHF regions both for individual nanotubes and arrays. Possible applications of resonant behaviour of the arrays are discussed.

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