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Mechanical and ElectroProperties of CNT/Polymer Composite with High Aspect ratio CNT

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Carbon nanotubes (CNTs) are expected to be a new functional material because they have outstanding mechanical, electrical and thermal properties, compared with conventional carbon fiber. However recent reports indicate that mechanical properties, such as Young's modulus and tensile strength of CNT/polymer composite could not be improved as they are expected. One of the reasons seems that commercial CNTs donft have enough length for reinforcement of mechanical properties at the point of rule of mixture. In order to investigate the effect of CNT length on mechanical properties of composite, CNT aligned along the vertical direction was synthesized by rf plasma CVD method to obtain the uniform length CNT. CNTs of 10nm in diameter, up to 800um in length could be synthesized and the length could be changed by changing the synthesizing time. After melt mixing, tensile test specimens of in-house CNT/polymer composite were fabricated by hot press in a vacuum chamber. As the results of tensile tests, Young's modulus increased by 25% and tensile strength increased by 45% under the condition of 620*f*Êm length and 1wt% CNT loaded. It is found the Young's modulus and tensile strength could be improved by using longer CNT.

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Effects of physical properties of multiwall carbon nanotube (MWCNT) on electrical conductivity and electrical conduction stability of MWNT nanocomposite

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We report major parameters of MWCNT composites to get the high electrical conductivity. To evaluate these parameters, composite samples were prepared by mixing silicone rubber with different kind of multiwall carbon nanotubes, and the electrical conductivities of the composites were discussed in terms of the waviness, crystallinity and the aspect ratio. It was shown how these physical properties of MWCNT affect the electrical conductivity in the viewpoint of the percolation scaling law. And we also investigate the change of electrical conductivity by static/cyclic heating and its underlying mechanism in the nanotube composite.

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Thermal boundary resistance in polymer-nanotube composites: a molecular modelling study

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We present numerical simulations of the thermal boundary (or Kapitza) resistance of single wall carbon nanotubes (CNTs) embedded in an amorphous polyethylene (PE) matrix. The polymer matrix was first prepared using a coarse-grained lattice model to fully relax the chain conformation near the nanotube-polymer interface, followed by reverse-mapping [1] of an atomistic model. The thermal boundary resistance (TBR) of the CNT-PE system was then calculated via a lumped heat capacity method [2] using the temperature difference between the CNT and PE matrix obtained from non-equilibrium molecular dynamics simulations. The results show that the TBR increases with stiffness of the CNT, indicating elastic heat transport at the interface. On the other hand, TBR decreases with increasing temperature, indicating an increasing contribution of inelastic heat transport. We discuss the implications of these for the production of CNT-polymer composites with more efficient heat transfer at the interfaces. [1] K.R. Haire, T.J. Carver, A.H. Windle, Comput. Theoret. Polym. Sci., 11, 17-28 (2001). [2] C.F. Carlborg, J. Shiomi, S. Maruyama, Phys. Rev. B, 78, 205406 (2008).

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Electronic and thermal properties of graphene-diamond hybrid structures

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We have theoretically investigated electronic and thermal properties of a graphene-diamond hybrid structure consisting of a graphene covalently bonded to the diamond surfaces. In our simulations, the edge structure of graphene at the graphene-diamond interfaces was chosen as Fujita type. The energetics and electronic structures of the hybrid system have been simulated by the ab-initio calculation based on the density-functional theory, and their thermal transport properties have been calculated by the nonequilibrium molecular-dynamics (NEMD) method with Tersoff-Brenner bond order potential. From the ab-initio calculation, we found that the hybrid structure is stable and that the edge state appears at the graphene-diamond interfaces. On the other hand, form the NEMD simulations, we found that the heat flows efficiently from the graphene to the diamond, but it does not flow efficiently in the opposite direction. This is contrary to the fact that the electrical current does not flow from graphene (diamond) to the diamond (graphene). We propose that the graphene-diamond hybrid structure is a potential candidate for novel transmission lines with low energy consumption.

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Identification of Substitutional Boron in doped Single-Walled Carbon Nanotubes

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Substitutional doping of B in single-walled carbon nanotubes (SWCNTs) is a well known functionalization path. Here, it is expected that B atoms substitute C atoms without additional atomic rearrangement, leading to the formation of an acceptor state in the SWCNT electronic structure even at very low B concentrations. These nanotubes have recently gained major attention. Interestingly, superconductivity was reported in thin films containing this material. B substitution in the SWCNT lattice is not necessarily uniform, and the formation of B nano-domains has been considered for a long time. For this reason, quantifying the amount and bonding environments of B in the SWCNT lattice has been challenging, particularly when the doping concentration is below 1at%. In B doped samples similar to those used in this study, EELS studies carried out in a TEM failed to detect the substituted B in the C network. For this reason, B induced changes in the intensity of the RBM and shifts in G' band have been used as indirect proof of substituted B in the SWCNT lattice. Here I will present the direct detection of B in the SWCNT lattice from the core level signal recorded with high resolution x-ray photoelectron spectroscopy. I will show how the corresponding line shape analysis is utilized to identify the different B bonding environments and to correlate the changes in the electronic properties of B doped SWCNTs with Raman spectroscopic studies, elucidating the site selective bonding environments with unprecedented detail even when the B concentration is below 1at%.

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Influence of purification and covalent functionalization on the electrical conductivity of singlewall carbon nanotube composites

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