Anisotropic properties of MWCNT/polystyrene composite films in terahertz region

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Anisotropic properties of composite materials based on carbon nanotubes (CNT) and polystyrene were investigated in terahertz region. Particularly it was measured electromagnetic response (transmission and reflection spectra) of composite for two different polarizations of the electric field relative to preferential direction of composite. This direction was formed during samples preparation process by using repeated forge rolling. Dispersion function of CNTs was theoretically modelled, and dielectric permittivity was calculated. Anisotropy of dielectric response of composite indicated that the forge rolling resulted predominant orientation of CNTs in polymer matrix.

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BC3 nanotubes: elelctronic and structural properties

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Recently, classes of tubules, originating from hexagonal compounds, i.e. BN and BC2N have been proposed [1]. Total energy calculations imply that the hexagonal compound sheets are as likely to form tubules as the graphite sheets [2,3]. Indeed, tubule forms of the hexagonal compounds of B, C, N have been observed experimentally in an arc-discharge setup [2]. Using chemical analysis, it has been determined, that part of the samples has an atomic composition of B:C≈ 1:3. In this paper we present the results of theoretical research into the properties of boron-carbon nanotubes BCn, n=3 of hexagonal type within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme and density-functional theory. We studied the mechanism of BC3 nanotubes formation by rolling qusiplanar hexagonal BC3 layer. We used two structural modifications of BC3 tubes in which boron and carbon atoms occupy different positions, the so-called BC3 tubes of A or B types. We defined the optimal geometry of these structures and also their band structure. Analysis of the strain energies showed that the existence of tubule forms of BC3 is energetically favorable. The tubes of small diameter obtained by twisting a monolayer of boron are likely to be narrow-gap semiconductors.
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Influence of metal superlattice to boron nanotube

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In this paper we present the results of theoretical research into the properties of boron nanotubes (BNTs) of hexagonal type within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme. We studied the mechanism of sorption of Li, K and Na atoms on the external surface of single-walled boron arm-chair nanotubes. We defined the optimal geometry of the sorption complexes and obtained the values of the sorption energies. After these operations we considered the possibility of multiple regular adsorption of alkaline metal atoms on a BNT surface. We modeled the formation of superlattice from metal atoms above nanotube surface. Analysis of the band structure suggests that the band gap is insensitive to adsorption process. The electron density is located near boron atoms of the surface of the tube. The results suggest that the formation of metal-phase composites based on boron nanotubes is possible, which is promising for nano-based technology.

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