A GRAND CANONICAL MONTE CARLO SIMULATION STUDY OF CARBON STRUCTURAL AND ADSORPTION PROPERTIES OF IN-ZEOLITE TEMPLATED CARBON NANOSTRUCTURES

Th. J. Roussel
CRMCN, Université de la Mediterranée, Marseille, France

Abstract
We have used the Grand-Canonical Monte-Carlo technique (GCMC) to simulate the vapor deposition of carbon in the porosity of various zeolitic nanopores (silicalite, AlPO4-5, faujasite). The carbon-carbon interactions is described within a Tigh-Binding formalism (TB) and the carbon-matrix interactions are assumed to be physisorption. Depending on the pore size and topology, various carbon structures can be obtained. For instance, we show that narrowest single wall nanotube can be synthetized in the cylindrical channel of AlPO4-5 zeolite (pore diamater 7 A) in agreement with the experimental work of Tang (ref...). We further show that this ultra small nanotube is defective but stable after template removal. We also demonstrate that a zeolite such as silicalite with smaller pores (pore diameter 5 A) does not allow obtaining nanotubes but a mesh of intercrossing carbon chains. The pore topology of faujasite (made of tetrahedrally coordinated spherical cavities) allows making a highly porous ordered carbon material that was sunsequently tested for H2 storage along with other perfect nanostrucutres (graphene layers, bundles ...) for comparison.

J. Chem. Phys 2003 reject

STRUCTURAL STABILITY AND ENERGETICS OF SINGLE-WALLED CARBON NANOTUBES UNDER UNIAXIAL STRAIN BY O(N) TIGHT-BINDING MOLECULAR-DYNAMICS SIMULATION

Cem Ozdogan
Computer Engineering, Cankaya University, Ogretmenler Cad,.Ankara, Turkey

Abstract
The O(N) and parallelization techniques have been successfully applied in tight-binding MD simulations of SWNT's of various chirality. The accuracy of the O(N) description is found to be enhanced by the use of basis functions of neighboring atoms (buffer). (10,10) SWNT consisting of 400 atoms with 20 layers is simulated under tensile loading using our developed O(N) parallel TBMD algorithms. It is observed that the simulated carbon nanotube is able to carry the strain up to 122% of relaxed tube length in elongation and up to 93% for compression. The Young's modulus, tensile strength and Poisson ratio are calculated and the values found are 0.311 TPa, 4.92 GPa and 0.287, respectively. The frequency of vibration for the pristine (10,10) carbon nanotube in radial direction is 4.71*10^3 GHz and it is sensitive to the strain rate.

CARBON NANOTUBES AS COMPOSITE COMPONENTS FOR SOME NONORGANIC NANOTUBES

L. A. Chernozatonskii
Institute of Biochemical Physics of RAS, Moscow, 119991 Russia

Abstract
Structures, stability, electronic and mechanical properties of carbon @ nonorganic (nO) double nanotubes are considered. We have investigated next nO nanotube components: BN, AlN, GaN and dioxides MO2(M=Si, Ge, Sn, Pb). The nitride nanotubes have hexagon atomic lattice like graphite. The dioxide nanotubes have quasiquadroon atomic lattice [1]. We study structural stability of C-nO double nanotubes, and their mechanical properties by molecular dynamics methods. All nO nanotubes are piezo- dielectrics, that is why their piezoelectric effects are investigated. Electronic properties of metallic C @ MO2 double nanotubes are studied by DFT methods: the changing of metallic spectra of pure carbon nanotubes in of C-nO DNThas been obtained, but nevertheless the nO nanotubes can be work good isolator for metallic CNT. Ways of C-nO DNT synthesis similar C-BN nanotube one [2] and their applications are considered also.
1. L. A.Chernozatonskii. JETP Lett. 80 (2004) 732.
2. D. Golberg et al., MRS Bull. 29 (2004) 38.