Graphene-Nanotube Composite with an Island Structure for flexible stretchable electronics: Ab Initio Study

M.M. Slepchenkov, Pavel V. Barkov, O.E. Glukhova,

Saratov State University, Russia

Objective

In this work, in silico methods are used to study the effect of tensile deformation on the electrical properties of hybrid graphene-nanotube films.

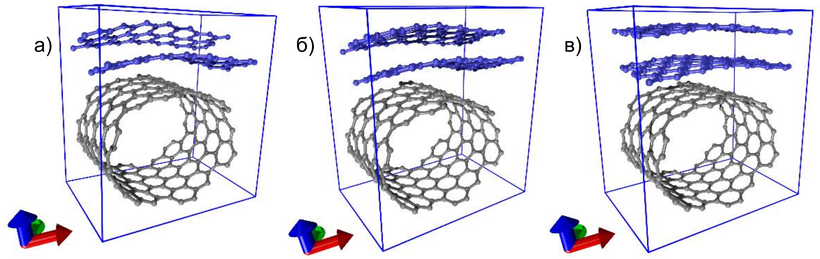
Methods and approaches

The calculation of the atomic structure of hybrid graphene/SWCNT films was carried out using the SCC-DFTB method implemented in the DFTB+ version 20.2 open access software package. The electrical conductivity was calculated within the framework of the Landauer-Buttiker formalism.

Conclusions

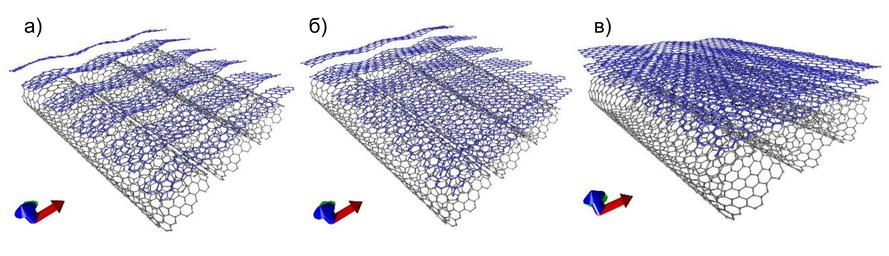
It has been established that for the topological models under study, a pattern of elastic deformation is observed in almost the entire range of tensions under consideration. The exception is the V1 model with the minimum width of the zigzag nanoribbon (2 hexagons) in the supercell. For this model, at 10% tension, the presence of a phase transition of the structure was revealed, which accompanies the transformation of the planar configuration of bilayer graphene into a wave-like one. The V2 model with a graphene nanoribbon width of 3 hexagons as part of a supercell showed the best ability to maintain high electrically conductive properties under tension. The electrical resistance for this model in both directions of current transfer changed by several tenths of kΩ during stretching. The V3 model with a graphene nanoribbon width of 4 hexagons in the composition of the supercell turned out to be the least sensitive to deformation in the considered stretching range.

The work was supported by a grant from the President of the Russian Federation (project MK-2289.2021.1.2)



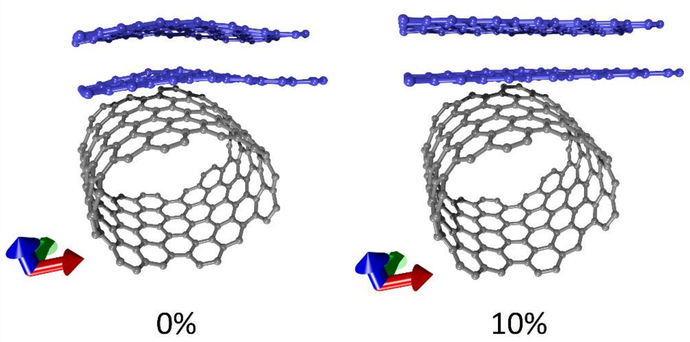
Atomistic models of supercells of hybrid films formed by bilayer graphene and SWCNTs (12,6):

a) model V1; b) model V2; c) V3 model

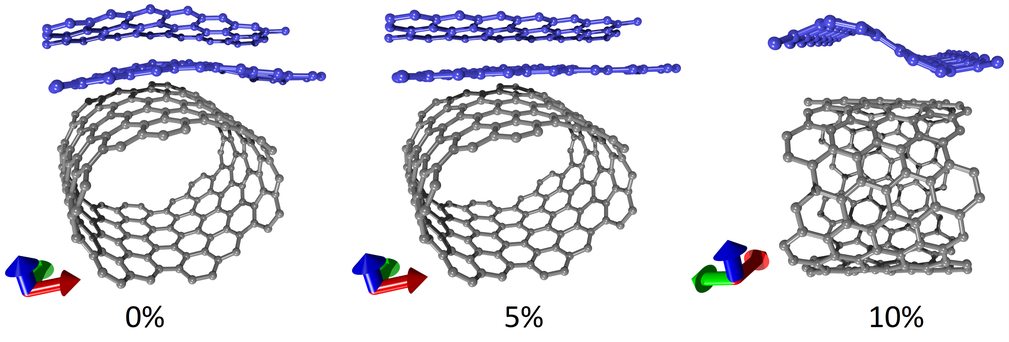


Atomistic models of extended fragments of hybrid films formed by bilayer graphene and SWCNTs (12,6):

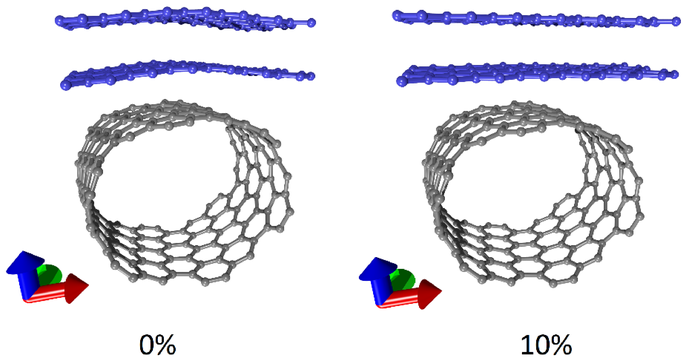
a) model V1; b) model V2; c) V3 model



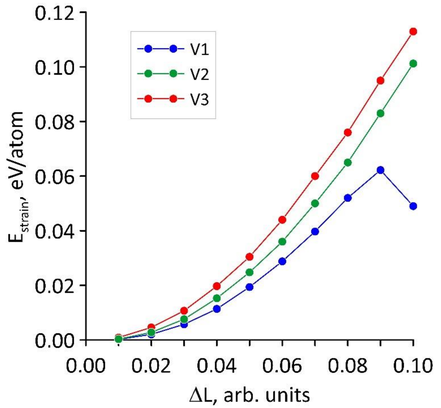
Changes in the Atomic Structure of the Supercell of Hybrid Films Formed by Bilayer Graphene and SWCNTs (12,6) under Model V3 Tensile Deformation



Changes in the Atomic Structure of the Supercell of Hybrid Films Formed by Bilayer Graphene and SWCNTs (12,6) under Model V1 Tensile Deformation



Changes in the Atomic Structure of the Supercell of Hybrid Films Formed by Bilayer Graphene and SWCNTs (12,6) under Model V2 Tensile Deformation



Graph of dependence of strain energy on strain value in relative units

Electrical resistance values of hybrid graphene/SWCNT(12,6) films under axial tension by different percentages

	V1	V2	V3
stretching 0%			
R_x, kOhm	7.53	6.22	125.89
R_y, kOhm	6.58	5.95	16.31
stretching 1%			
R_x, kOhm	8.39	6.53	128.38
R_y, kOhm	6.50	5.90	15.87
stretching 5%			
R_x, kOhm	7.68	6.00	64.19
R_y, kOhm	6.42	5.85	9.20
stretching 10%			
R_x, kOhm	218.28	5.98	34.95
R_y, kOhm	10.154	5.75	7.179