Elasticity at the nanoscopic scale

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Aside from new physics governed by quantum mechanics, some classical concepts may survive in the nanoworld. Elasticity is one of the fields of materials science that can reasonably be applied to nanostructures. Care should be taken, however, to stay with well-defined quantities. Not all the elastic constants keep on their meaning when transposed to the nanoscopic scale. For instance, Young modulus of about 5 TPa has been predicted for single-walled nanotube. The fact is that this modulus has no significance at the atomic level. Other elastic coefficients, by contrast, can be defined unambiguously at the atomic level and can be measured experimentally. The task is not easy, in general, which explains why available values, if any, may differ significantly from each other. Ab-initio calculations can be a substitute to experiment for providing the input data needed by classical mechanics. That is important because mechanical properties of nanostructures can be predicted from elasticity if and only if reliable data exist. It will be shown that the simple Kirchoff-Love theory of thin plates can be extrapolated top down by providing constitutive equations that remains well-defined for an atomic sheet. This approach will be illustrated for the case of graphene and nanotubes. A critical review on how to obtain the constitutive parameters will be proposed, which will permit to address interesting questions on the mechanical properties of these fascinating nanomaterails, among which: graphene sheet buckling, nanotube bending, structural instability of nanocarbons.

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Session «Quantum chemistry simulation»

Electron structure of pure and doped nanotubes calculated using linear augmented cylindrical wave method

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In the terms of muffin-tin and DFT theory, we developed a linear augmented cylindrical wave (LACW) method for electronic structure of the single- and double-wall nanotubes. We calculated the band structures of the nanotubes up to the chiral (100, 99) tubule. The electronic spectrum of nanotubes is governed by the electrons movement in interatomic space of cylindrical layers, by scattering on the atomic spheres, and tunneling between the layers. A model for electronic structure of nanotubes embedded in a crystal matrix is developed too. The LACW-Green function theory is elaborated for the nanotubes with point defects. A first-principles numerical method for calculation of the electronic structure of the point impurities in the single-walled carbon nanotubes nanotubes based on a Green's function technique is developed. The host nanotubes electron Green's function is calculated using a linear augmented cylindrical wave theory. The Green's function of the impurities is calculated in the terms of matrix Dyson equation. The impurities are described by the single-site perturbed muffin-tin potentials in otherwise perfect nanotubes with the rotational and helical symmetries. Due to the account of these symmetry properties, the method is developed applicable to any tubule including the chiral nanotubes with point defects independent of the number of atoms in translational unit cell of the host systems. Finally, a relativistic version of the LACW method is elaborated and applied to calculating the spin-orbit coupling effects in the armchair nanotubes. This study was performed in the frames of the Program “Researches and developments on priority directions of scientific-technological complex of Russia in 2007-2012”. It was supported by RFBR (11-03-00691).

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