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Role of transition metal dopants on spin dependent electronic behavior of nanotubes

Serkan Caliskan
Fatih University, Turkey

Spintronics is a developing and attractive field in both science and engineering due to possible new interesting applications. It plays an important role in nanotechnology and industrial applications. This field is related to role of spins or manipulation of spins through the nanostructures. Nanostructures (including nanotubes, nanowires and atomic wires) upon combining with spintronics, lead to new type devices with multifunctional and superior properties. Concerning the applications, detailed understanding of properties of these structures and interactions between electrons and the medium in which they move; and therefore, investigation of spin polarized transport (electron movement), evaluation of spin polarized quantities, examination of dependencies on other factors (topological disorder, electronic correlations, temperature, impurities, external field, etc.) are required. In the present study, we perform density functional theory calculations on boron nitride nanotubes (BNNTs), which are containing substitutional transition metal (TM) dopants, to reveal the spin dependent electronic structure properties. The dopants are chosen as TM atoms to be able to induce possible spin dependent behavior and/or to emerge the spin polarization in the structures. Both optimized pure and doped several zigzag nanotubes with infinite lengths are investigated. We mainly concentrate on electronic structure and magnetic properties in terms of chiral vector describing the doped zigzag nanotubes. Hence we extract the impact of chirality and dopants on the spin dependent energy gap and other relevant quantities for relaxed nanotubes. BNNTs and carbon nanotubes are compared and obtained results are discussed for the possible applications of these nanotubes, as fundamental structures, in the field of spintronics.

caliskan34@gmail.com

Formation of ripples in graphene as a result of interfacial instabilities

A R Harutyunyan
Honda Research Institute USA Inc., USA

Formation of ripples on a supported graphene sheet involves interfacial interaction with the substrate. In this work, graphene was grown on a copper foil by chemical vapor deposition from methane. On thermal quenching from elevated temperatures, we observed the formation of ripples in grown graphene, developing a peculiar topographic pattern in the form of wavy grooves and single/double rolls, roughly honeycomb cells, or their combinations. Studies on pure copper foil under corresponding conditions but without the presence of hydrocarbon revealed the appearance of peculiar patterns on the foil surface, such as dendritic structures that are distinctive not of equilibrium solidified phases but arise from planar and/or convective instabilities driven by solutal and thermal capillary forces. We propose a new origin for the formation of ripples in the course of graphene growth at elevated temperatures, where the topographic pattern formation is governed by dynamic instabilities on the interface of a carbon catalyst binary system. These non-equilibrium processes can be described based on Mullins-Sekerka and Benard-Marangoni instabilities in diluted binary alloys, which offer control over the ripple texturing through synthesis parameters such as temperature, imposed temperature gradient, quenching rate, diffusion coefficients of carbon in the metal catalyst, and the miscibility gap of the metal catalystcarbon system.

AHarutyunyan@oh.hra.com