Temperature-induced transition in carbon nanotube on a substrate

M.A. Kovaleva
A.V.Savin
Semenov Federal Research Semenov Federal Research Center of Chemical Physics of Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia
makovaleva@chph.ras.ru

CNTs attract interest of researchers in physics, material science, electronics and biotechnology and nanotechnology due to their unique thermal, mechanical, optical and biological properties. We present the study of single-walled carbon nanotube (CNT) interacting with a plane substrate. We characterize the energy of interaction with the substrate using effective Lennard-Jones-type potential.
Nanotubes have high longitudinal (axial) and relatively weak transverse (radial) stiff ness. Because of this, at sufficiently large diameters, nanotubes due to the weak noncovalent interaction of atoms can transform from a hollow cylindrical shape to a collapsed state.

We find energy of the homogeneous open and collapsed states depending on the radius of the carbon nanotube and report on the bi-stability in some range of the CNT diameters. The energy profile of the transition between these two states can be found numerically; for that we solve the problem on the minimum of energy for each fixed value of the distance between the substrate plane and the center of the upper side of the nanotube.
Using the molecular -dynamical simulations we look at the evolution of the CNT with the initial half-opened, half-collapsed state.
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With use of the molecular dynamics modelling we demonstrate that the transition area from one state to another is spatially localized and has the features of topological soliton. The transition of a nanotube from one stationary state to another can be described qualitatively as the motion of a kink (topological soliton) in the φ-4 model with an asymmetric double-well potential having one, narrow deep hole corresponding to the collapsed state and a second, wide hole higher in energy corresponding to the open state of the nanotube. We show that the value and the direction of the front propagation speed depend significantly on the CNT diameter as well as on the temperature of the system. We discuss the mechanism of the process using a model of effective oscillator in a double-well potential.

REFERENCES

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FIGURES

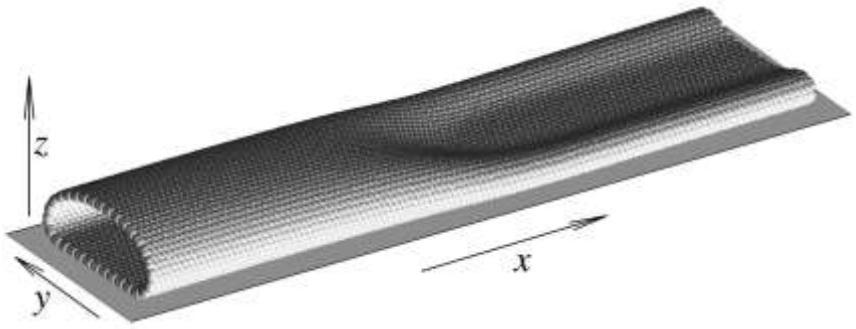

Figure 1: View of a carbon nanotube with a chirality index (31,31) located on a substrate formed by the surface of a silicon carbide crystal 6HSiC (0001). The left end of the nanotube is in an open stationary state (the cross-section of the nanotube has the shape of a convex drop), the right end is in a collapsed stationary state (the cross-section has the shape of an asymmetric dumbbell with a at two-layer central part).
In the middle part of the nanotube, a localized region of its smooth transition from one stable stationary state to another is formed.