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Oscillation characteristics of carbon nanotori molecules along carbon nanotubes under various system parameters

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Abstract. In this paper, mechanics of carbon nanotori molecules oscillating along the exterior of carbon nanotubes (CNTs) is fully investigated. On the basis of the continuum approximation in conjunction with the 6-12 Lennard-Jones (LJ) potential function, new semi-analytical expressions are given in terms of double integrals to evaluate van der Waals (vdW) potential energy and interaction force between the two interacting molecules. Furthermore, suction energy and acceptance condition, which are the two main characteristics of nanotube-based systems for applications such as drug delivery and so forth, are determined. Using the actual distribution of vdW force, the equation of motion is solved numerically to obtain time-dependent variables of system. Moreover, considering flexible nanotori and CNT molecules, the molecular dynamics (MD) simulations are conducted to assure the validity of the time history of system obtained from the continuum method. A novel semi-analytical expression is also proposed for the precise evaluation of oscillation frequency into which the effects of both geometrical parameters and initial conditions are incorporated. With respect to the present formulation, a comprehensive study into the effect of system parameters on the oscillation frequency is carried out. Numerical results demonstrate that the operating frequency of nanotori-CNT oscillator is in the gigahertz (GHz) range.

Keywords: A. Nanostructures

1. Introduction

Sparking a significant breakthrough in materials science and nanotechnology has led to the next industrial revolution to begin. Owing to the extraordinary mechanical and electromechanical properties of carbon nanotubes (CNTs) [1], this new class of nanomaterials is identified as the building block of nanotechnology with extensive applications in nanoelectromechanical systems (NEMS) [2, 3]. Amongst

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