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Theoretical infrared phonon modes and band gap calculations of a bundle of two single walled carbon nanotubes

AH. Rahmani[a], M. Boutahir[a], B. Fakrach[a], H. Chadli[a] and A. Rahmani[a,*]

[a]Advanced Material and Applications Laboratory (LEM2A), University Moulay Ismail, FSM-ESTM, BP 11201, Zitoune,50000 Meknes, Morocco

Abstract

In this paper, we report the calculation results of infrared active modes in dimer of single-walled carbon nanotubes (SWCNTs). The spectra calculations are performed using the spectral moment's method (MMS). We present the evolution of the dimers of SWNCTs infrared spectrum as a function of the diameter and chirality of the two interacting nanotubes. We investigated the electronic properties of bundle of SWCNTs and the effect of coupling between nanotubes on charge transfer processes.The results are useful for the interpretation of the future experimental data of dimer of carbon nanotubes.

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Keywords: Carbon nanotube, Raman, Infrared, Dimer, charge transfer, MMS

1. Introduction

Since the discovery of carbon nanotubes [1], they are attracting growing interest from the international scientific community because of their intrinsic properties. Carbon nanotubes can be metallic or semiconducting, and offer many possibilities for creating nanoelectronics devices. Recently a bundle of two Single Walled Carbon Nanotubes (SWCNTs) have been synthesized using the chemical vapor deposition method and named this Nano system, dimer. The homogeneous (two identical SWCNTs) and inhomogeneous (non-identical SWCNTs) dimers of SWCNTs are

* Corresponding author: *E-mail address: a.rahmani@fs-umi.ac.ma*

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characterized by a weak van der Waals interaction between the neighboring carbons of its two constituting SWCNTs. Many experimental and theoretical studies have been conducted on their vibrational properties.

Carbon nanotubes field continue to grow since their discovery and these improvements are due to the development of synthesis techniques. Recently, the most promising method to produce carbon nanotubes on an industrial scale is the catalytic vapor chemical deposition (CVD) [2]. This method involves the decomposition of a carbon source in a gas phase, usually a hydrocarbon (methane, ethane, ethylene or acetylene are commonly used), carbon monoxide and ethanol on the catalyst particles metal (usually iron, cobalt or nickel). The method is very flexible since, depending on the catalyst system used and the operating conditions, it is possible to produce either nanofibers either single walled carbon nanotubes or multi-walled.

Raman spectroscopy is one of the most powerful tools for investigating the vibrational properties of materials in relation to their structural and electronic properties [3,4]. Infrared spectroscopy of carbon nanotubes has been neglected since the infrared activity is related to a dynamic dipole moment that is weak. Nevertheless, a number of optical phonons are active in infrared through transient dipole, creating a surprising number of phonon mode bands.

The objective of this work is to calculate the infrared active modes in dimers of carbon nanotubes. Calculations are performed for different possible configurations such as: armchair-armchair, zigzag-zigzag and armchrair-zigzag. We report the evolution of infrared spectrum dimers according to diameter, chirality and the length of the two interacted nanotubes. The results are useful in the interpretation of future experimental infrared data of dimers of SWCNTs.

Nomenclature

MMS spectral moment's method
SWCNT Single Walled Carbon Nanotube
dimer bundle of two Single Walled Carbon Nanotubes

2. Model and methods

A dimer consists of two SWCNTs greatly spaced by intermolecular distance d. The interactions between the carbon atoms at the surface of SWCNT are described using the force constants model introduced by Saito [5] and previously used to calculate the Raman and infrared spectra of SWCNTs [3,6,7,8]. Van der Waals interaction between the two tubes is described by the Lennard-Jones potential, given by the following expression:

$$U_{LJ} = 4\epsilon\left[(\sigma/R)^{12} - (\sigma/R)^{6})\right] \qquad (1)$$

The values of the Lennard-Jones parameters were chosen as ε=2.964 meV and σ=0.3407 nm. The energy calculations performed using the this potential show that the optimal SWCNT-SWCNT distance d in dimers is around 0.34 nm.

The intensity of the infrared absorption spectrum is given by the following expression:

$$I_\alpha(\omega) = \frac{\omega}{nc}\sum_j \frac{|a_{j\alpha}|^2}{2\omega_j}\left(\delta(\omega-\omega_j) - \delta(\omega+\omega_j)\right) \quad (2)$$

With

$$a_{j\alpha} = \sum_{k\alpha}\frac{q_k}{\sqrt{m_k}} e_j(k\alpha) \qquad (3)$$

Where n and c are the indice of the material and speed of light, respectively, ω_j and $e_j(k_\alpha)$ are respectively the frequency and the (k_α) component of the displacement amplitude for the k^{th} (α is cartesian coordinate) in the j^{th} mode. q_k is the effective charge and m_k is the mass of the k^{th} atom. To enhance the IR response of nanotubes, dynamical effective charges on tied carbon atoms were fixed at q_A=+1 and q_B=-1 for a given A-B bond.

The usual method to calculate the IR spectrum consists of injecting in the previous expressions the values of ω_j and $e_j(k_\alpha)$ obtained by direct diagonalization of the dynamical matrix of the system. However when the system contains a large number of atoms, as for long dimer of SWCNT, the dynamical matrix is very large and its