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A newly defined envelope function for nano particles - carbon nano tube

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Dangling bonds on CNT (Carbon NanoTube) surface induce the spurious surface states. These dangling bonds can be bonded by incoming nano particles which is associated wave function with different characters (localization at the surface) in respect to real quantized states. When the translational symmetry is broken, we can limit the calculation to an area like a ring or a super cell. This can be achieved by several theoretical methods. The most widely used theoretical tools to deal with nano structures are based on the envelope function. The envelope of the nano structure wave function is relied on several approximations which have been widely debated in the literature. These approaches have experienced a great success mainly due to a fair compromise between simplicity of the method and reliability of the results. By applying the Bloch theorem for CNT structure and defining the periodic boundary conditions, we can find a newly defined envelop wave function for nano particles in CNT structure by making two approximations, namely by smooth variation of the perturbation potential and the effective mass approximation. For this purpose, we need to consider appropriate boundary conditions in order to allow such flux of particles. The obtained results show that the equation fulfills all wave vectors and how nano particles perturb CNT structure.

Key words: Thin films, carbon nano tube, nano particles, envelop wave function.

INTRODUCTION

CNTs have attracted rapidly an increasing attention of the scientific community in the last decade for several reasons (Iijima et al., 1993). It has played an enormous role in the success of nano electronic device due to their outstanding properties. The unique electrical, thermal, mechanical properties cause many scientists to investigate about this interesting material. Because of small size of this structure and problems that exist in measurement of electrical properties, theoretical methods have improved more than experimental methods. Therefore, special experimental, analytical methods and computational tools are needed to study the interaction of incoming nano particles and CNT structure for particular functionalities. These interactions between nano particles and CNT structure can be directly understood from the desorption energy of a single walled carbon nanotube (SWCNT) which represents an elegant illustration of

Bloch's theorem at the level of individual wave functions (Li and Chou, 2003).

Recently, some researchers have calculated the Van der Waals free energy and force between an incoming atom (molecule) like hydrogen atom and carbon nano tubes (CNTs) by using Lifshitz - type formulation (Bahari, 2009; Dai, 2002; Bahari et al., 2006b; Bahari et al., 2008; Bahari, 2008). Modern technology, however, has pushed nano structures to dimensions where Lifshitz approximation may not be as accurate as one requires. Moreover, this concept has to be substituted for instance by other approaches, the complexity of the problem becomes rapidly intractable. It has also been an important fundamental question regarding how interaction between nano particles and CNT affects CNT electrical properties. The point is the wave functions in CNT structure which are not generally Bloch wave functions. For this purpose, we assume that these interactions between incoming nano particles and CNTs are not so strong and they can just perturb the CNT structure. These issues are critical to the future advancement of nanotube science and techno-

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logy, and are being actively pursued by researchers (Nakhei and Bahari, 2009; Bahari and Amiri, 2009; Bahari et al., 2005; Morgen et al., 2005; Bahari et al., 2006a).

In this work, we have studied nano particles interactions with CNT structure. The mechanism can be understood by considering these interactions. These features and mechanisms bear certain resemblance to conventional hydrogen sensors based on semiconductor field effect transistors.

Graphene sheet and CNT structure

There is a variety of ways to formulate the deformation of SWCNTs (Li and Chou, 2003). Their results have been shown that deformation is so critical in studying CNT's properties, because it can change carbon atom positions.

CNTs are tube-like structures that result from a special arrangement of carbon atoms. These nanometer-wide tubular arrangements of sp² orbital are formed at 1200 to each other within a plane. A CNT is thereby formed when one single layer of graphite is wrapped onto itself and the resulting edges joined. The structure of a nano tube can be defined using a roll-up vector C(n, m) or chirality that are named chiral vector. The chiral vector and the diameter of the nanotube are defined as;

$$C_n = n_{a1} + m_{a2}$$

$$D = \frac{\sqrt{3}}{\pi} a \sqrt{n^2 + m^2 + nm}$$

Where a₁ and a₂ denote unit vectors in a 2D graphite lattice. The C-C bond length, a, is 0.142 nm. SWCNT is named a zigzag (armchair), if n ≠ 0 and m = 0 (n = m). Otherwise is known chiral.

As mentioned above, carbon atoms in this sheet are arranged in a hexagonal ring and tubes are also capped by a hemisphere section drawn from a spherical (fullerene) arrangement of carbon atoms. A SWCNT can be a metal, semiconductor or small - gap semiconductor depending on the structural parameters (Nakhei and Bahari, 2009; Bahari and Amiri, 2009).

The graphene sheet lattice structure is not a Bravais lattice by itself, because two nearest atoms in its unit cell do not have the same orientation, but can be regarded as an underlying square (oblique) Bravais lattice with a two - atoms basis.

Furthermore, for a graphene sheet, the conduction and valence bands touch each other at the six corner points of the first Brillouin zone in that these states are filled with the highest energy (Fermi's energy) of electrons. But, the electronic states of an infinitely long nanotube are parallel lines in K space, continuous along the tube axis and quantized along the circumference. This is because the band shift due to charge transfer interactions does not change the density of states at the Fermi - level

for a metallic tube.

The interactions between nano tube and nano particles are important because of variation of CNT's structure and its properties with this interaction. It is known that in three - dimensional bulk materials, different metals exhibit different interactions with carbon.

Theory

Many of researchers have pursued the analysis of CNTs by theoretical modeling. These models include atomistic and continuum models which can be classified into classical molecular dynamic (MD), tight-binding molecular dynamic (TBMD) and density functional theory (DFT). In general, any problem associated with atomic motions can be simulated by these modeling, but due to enormous computations, applications of these modeling are limited to systems with a few numbers of atoms that usually are short-lived phenomena. Periodicity in r - space generates a reciprocal lattice in k - space through the basic relation

$$e^{iK.R} = 1 \quad (1)$$

Where R is translational vector and the reciprocal lattice vectors K may be expressed in terms of primitive translations b_j in where

$$K = \sum_{j=1}^3 n_j b_j \quad (2)$$

Where n_j = 0, ± 1, ± 2...

Discreteness of the k - space is achieved by imposing on the crystal, then the periodic boundary conditions imply

$$\frac{1}{L} \sum_{R \in V} e^{iK.R} = \sum_K \delta_{k,K}$$

$$\frac{1}{L} \sum_{R \in V} e^{iK.R} = \delta_{R_0,0}$$

Where V = Lv is the crystal volume, L is the number of k - points contained in first Brillouin zone (Z) and v_i are integers in where

$$k_i = \frac{v_i}{2L_i}; -L_i + 1 \leq v_i \leq L_i; i = 1,2,3$$

Of course, R is not restricted to V. Equations 1, 2 express, respectively, orthonormality modulo a vector K and closure in Z of the plane wave fields. The one - body Hamiltonian in a perfect crystal indicates a periodic potential U(r) = U (r+R). For just one electronic band and

the perturbed structure, the Schrodinger equation can be written as

$$H\psi(r) = E\psi(r) \tag{3}$$

For simplicity, we suppose these interactions perturb CNT structure in which the perturbation potential, $V_p(r)$ is taken into account in Hamiltonian. We also assume that the structure is most commonly called a honeycomb lattice due to the hexagonal arrangement of carbon atoms.

In the confinement directions, the translational symmetry is broken and Bloch theorem thus can be applied. Such boundary condition, as usual, allows a reduction of the problem to the unit cell which results in a reduction of the number of atoms considered.

$$H = \frac{-\hbar^2}{2m} \nabla^2 + V_s(r) + V_p(r) \tag{4}$$

Where $V_s(r)$ and $V_p(r)$ are CNT structure potential and perturbed potential, respectively. Since all elements in Equation 4 commute with each other, the wave functions $\psi(r)$ is the Schrodinger equation form a one-dimensional unitary representation of this group which may be parameterized by a wave vector $k \in Z$. Thus the action of the translation by R is:

$$\psi_k(r + R) = e^{iK \cdot R} \psi_k(r)$$

By applying the orthonormality condition in the crystal volume V , we have

$$H|k\rangle = \epsilon_k|k\rangle$$

$$\langle k|k\rangle = \delta_{k,k'}$$

$$L \int_C d^3r U_{nk}^*(r) U_{n'k'}(r) = \delta_{n,n'}$$

The system wave function, $\psi(r)$, is also expressed as a linear combination of unperturbed band, $u(k',r)$

$$\psi(r) = \sum_{k'} a_{k'} u(k',r) \tag{5}$$

We substitute Equations 4, 5 into Equation 3 and multiply

it by $u^*(k',r)$, so that

$$\sum_{k'} a_{k'} \langle u(k,r) | \frac{-\hbar^2}{2m} \nabla^2 + V_s(r) | u(k',r) \rangle + \sum_{k'} a_{k'} \langle u(k,r) | V_p(r) | u(k',r) \rangle = E a_{k'}$$

Integrating above equation over the whole structure gives

$$\epsilon_k a_{k'} + \sum_{k'} a_{k'} \langle u(k,r) | V_p(r) | u(k',r) \rangle = E a_{k'}$$

We put into integrals running over structure, in which V_p varies slowly on the CNT and is constant within each ring. Translational vector, R , is defined

$$\sum_{k'} a_{k'} \langle u(k,r) | V_p(r) | u(k',r) \rangle = \sum_R V_p(r) \int_{ringR} U^*(k,r) U(k',r) d^3r$$

From elementary solid state physics, unperturbed band, $u(k,r)$ obey Bloch's theorem, that is,

$$u(k,r) = v_k(r) e^{ik \cdot r}$$

Where v_k has the periodicity of the hexagonal rings. According to the Fourier theorem (6)

$$\sum_{k'} a_{k'} \langle v(k,r) e^{ik \cdot r} | v(k',r) e^{ik' \cdot r} \rangle = \sum_{G,R} g(G) V_p(r) \int_{ringR} e^{i(k'-k)(r+R)} v_k^*(r+R) v_k(r+R) d^3r$$

$$\sum_{k'} a_{k'} \langle v(k,r) e^{ik \cdot r} | v(k',r) e^{ik' \cdot r} \rangle \approx \sum_{G,R} g(G) V_p(R) e^{i(k'-k) \cdot R} V_{ring} \delta_{G,0}$$

Where

$$\int_{ringR} e^{iG \cdot r} d^3r = V_{ring} \delta_{G,0} \tag{7}$$

Here we assume that $k' - k = G$ is so small. By inserting Equation 7 into Equation 6, we have

$$\sum_{k'} \langle u(k,r) | V_p(r) | u(k',r) \rangle = g(0) \sum_{G,R} V_p(r) e^{i(k'-k) \cdot R} \tag{8}$$

So that

$$g(0) = \frac{1}{V} \int_V v_k'(r) v_k(r) d^3r \approx \frac{1}{V}$$

Where V is the volume of CNT.

Now, we sum up it on all rings by getting integral over the whole CNT structure

$$\sum_{k'} \langle u(k,r) | V_p(r) | u(k',r) \rangle = \frac{1}{V} \int_V V_p(r) e^{i(k'-k) \cdot r} d^3r \tag{9}$$

We substitute Equation 9 into Equation 8 and use the effective mass approximation for the unperturbed

structure

$$\varepsilon_k = E_C + \frac{-\hbar^2 k^2}{2m^*}$$

Such that

$$\frac{-\hbar^2 k^2}{2m^*} a_k + [E_C - E] a_k + \frac{1}{V} \sum_{k'} a_{k'} \int V_p(r) e^{i(k'-k).r} d^3 r = 0$$

Now, we define the envelop wave function as bellow

$$a_k = \frac{1}{\sqrt{V}} \sum_{k'} a_{k'} \delta(k - k') = \frac{1}{\sqrt{V}} \int \Lambda(r) e^{-ik.r} d^3 r$$

And

$$k^2 a_{k'} = \sum_{k'} k^2 a_{k'} \delta(k - k') = \frac{1}{\sqrt{V}} \int \sum_{k'} k'^2 a_{k'} e^{i(k'-k).r} d^3 r$$

$$\frac{1}{\sqrt{V}} \int \sum_{k'} k'^2 a_{k'} e^{i(k'-k).r} d^3 r = \int (-\nabla^2 \Lambda(r)) e^{-ik.r} d^3 r$$

This description leads naturally to the notion of an electron movement in the crystal. The equations

$$\int e^{-ik.r} \left[\frac{-\hbar^2}{2m^*} \nabla^2 + E_C - E + V_p \right] \Lambda(r) d^3 r = 0$$

Is obtained, which is fulfilled for all K only if

$$\int e^{-ik.r} \left[\frac{-\hbar^2}{2m^*} \nabla^2 + E_C - E + V_p \right] \Lambda(r) d^3 r = 0$$

This is the envelop wave equation. Although this definition is still too general to be useful, the crucial step (in the future) is to define the creation and annihilation operators for a complete system (Morgen et al., 2005).

Conclusion

For systematic studies of the interaction between SWCNTs and nano particles, we use an analytical method. This method can be suggested for evaluating the electronic band energy of SWCNTs and clearly describing nanostructures based on the effective mass approximation.

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