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Physics Letters A 338 (2005) 366–372
PHYSICS LETTERS A
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Bond distortions in armchair type single wall carbon nanotubes

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Received 9 November 2004; received in revised form 20 February 2005; accepted 21 February 2005

Available online 19 March 2005

Communicated by R. Wu

Abstract

The energy band gap structure and stability of $(3,3)$ and $(10,10)$ nanotubes have been comparatively investigated in the frameworks of the traditional form of the Su–Schrieffer–Heeger (SSH) model and a toy model including the contributions of bonds of different types to the SSH Hamiltonian differently. Both models give the same energy band gap structure but bond length distortions in different characters for the nanotubes.

Keywords: SSH Hamiltonian; Armchair nanotube; Constraint; Bond alternations

1. Introduction

A single-wall carbon nanotube (SWCNT) is an empty tube of graphene consisting of hexagonally arranged carbon atoms. In graphene, there are two different rim shapes, armchair and zigzag. For an armchair SWCNT, the hexagon rows are parallel to the tube axis. The π-electronic structure of an armchair SWCNT arises from the π-structure of graphene. Each carbon atom in graphene contributes to the structure with one electron in the $2p_z$ orbital perpendicular to the plane of the sheet. Generally, the overlap of π-orbitals due to the curvature in nanotubes are neglected for moderate curvatures. If n is the number of two-carbon sites (dimers), i.e., the nearest neighbors on polyacetylene (PA) chain which is the prototype polymer of graphene, the nanotube is labeled as (n,n). One of the most important properties of armchair nanotubes is that they show metallic behavior [1].

In the present treatise the tight-binding approximation, which is sometimes known as the method of linear combination of atomic orbitals, is used. This approximation deals with the case in which the overlap of atomic wave functions is enough to require corrections to the picture of isolated atoms but not so much as to render the atomic description completely irrele-

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0375-9601/$ – see front matter © 2005 Published by Elsevier B.V.
doi:10.1016/j.physleta.2005.02.033

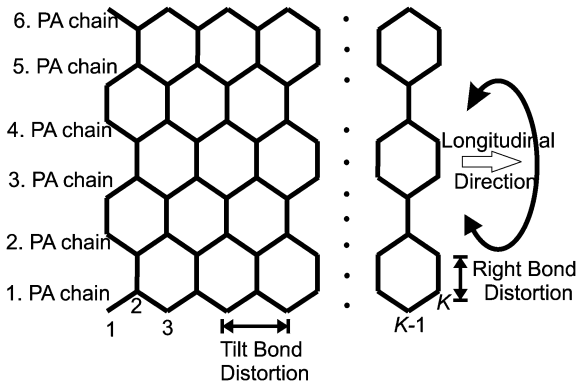

Fig. 1. Inter-chain coupling structure of a (3, 3) armchair type nanotube and bond distortions.

vant. It is mostly used for describing the energy bands arising from the partially filled d-shells of transition metal atoms and for describing the electronic structure of insulators. Moreover, the tight-binding approximation provides an instructive way of viewing Bloch levels complementary to that of the nearly free electron picture, permitting a reconciliation between the apparently contradictory features of localized atomic levels on the one hand and free electron-like plane-wave levels on the other [2].

The tight-binding approximation was originally developed by Su–Schrieffer–Heeger (SSH) [3] for conducting polymers (1D systems) and then extended to two-dimensional systems by Harigaya [4,5]. Harigaya's model preserves the fixed-length constraint of one-dimensional polymer chain and hence it contains a single Lagrange multiplier. In most applications of this model to graphene and to tubes constructed from graphene, the constraint has still been used in the same form, that is all bond distortions are summed without considering the type of bonds and this sum is assumed to vanish. However, two different types of bonds appear in graphene and so in tubes, tilt and right (see Fig. 1). It would also be worthwhile to point out that bond length difference of hexagon structure have been reported by the calculations on graphene and nanotubes [5,6].

Considering this fact, in this work on armchair type nanotubes, we present for the first time the modification in Harigaya's model by taking the contributions of bonds of different types to the SSH Hamiltonian differently. This automatically leads us to separate the constraint into two constraints, vanishing of the sum of right bond distortions and vanishing of the sum of tilt bond distortions. In this way we build a toy model which provides more freedom for lattice relaxations. We have already mentioned the very preliminary results of this toy model in our work in [7]. In our second work [8], we evaluated the electronic band structure of (3, 0) nanotube with periodic boundaries in the framework of this toy model and in the Harigaya's model comparatively. We observed that the tiny energy gap appearing in Harigaya's model was lost when our toy model has been used. This result consists with the fact that zigzag nanotubes $(n, 0)$ are metallic when n is any multiple of 3, and semiconducting when n cannot be divided by 3. This is determined by whether the K and K′ points of the graphite meet with the one-dimensional Brillouin zones determined by the geometry or not.

The (n, n) armchair nanotubes are always metallic for all the integers n and metallic behavior of (3, 3) armchair nanotube has also experimentally being shown [9,10]. Recently, Li et al. [11] have grown free-standing SWCNTs. Their diameter is as small as 0.4 nm. The (3, 3) armchair nanotubes are among the possible structures of this size [11]. This is why we deal with here with (3, 3) armchair nanotube in the framework of our toy model. On the other hand, the commonly observed diameter of SWCNT by experiments is known as about 1.4 nm which corresponds to that of (10, 10) SWCNT. Therefore, we also test our toy model with this larger diameter nanotube.

2. Model

The SSH model Hamiltonian

$$H_{\mathrm{SSH}} = -\sum_{\langle i,j\rangle,\sigma}\left[t_0 - \alpha\left(u_i^{(j)} - u_j^{(i)}\right)\right]\left(c_{i,\sigma}^{\dagger}c_{j,\sigma} + \mathrm{h.c.}\right) + \frac{\kappa}{2}\sum_{\langle i,j\rangle}\left[\left(u_i^{(j)} - u_j^{(i)} - C\right)^2 - (C)^2\right], \qquad (1)$$

which had originally been written for 1D systems, was directly applied to 2D systems without any modification by Harigaya [5]. Here, $\langle i, j\rangle$ is the nearest-neighbor carbon–carbon atom pairs and t_0 is the hopping integral of the undimerized system. The second term represents the dimerization due to σ skeleton