Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 139 (2015) 380–384

Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.elsevier.com/locate/saa

Optical properties of two-dimensional zigzag and armchair graphyne nanoribbon semiconductor

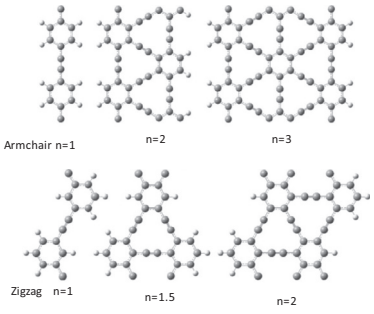
Mohamad Asadpour [a], Mahmoud Jafari [a,*], Milad Asadpour [b], Maryam Jafari [c]

[a] Department of Physics, K.N. Toosi University of Technology, Tehran, Iran
[b] Sardarjangal Higher Education Institute, Rasht, Iran
[c] Department of Industrial Engineering, K.N. Toosi University of Technology, Tehran, Iran

HIGHLIGHTS

- We examine changes in the width of nano ribbons.
- Increasing nano ribbons width will decrease optical band gap.
- Increasing nano ribbons width will increase dielectric constant.
- Increasing nano ribbons width will increase energy loss spectroscopy.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 16 September 2014
Received in revised form 21 November 2014
Accepted 10 December 2014
Available online 25 December 2014

Keywords:
Graphyne nanoribbon
Optical band gap
Electron energy loss spectroscopy
Dielectric constant
Static refractive index

ABSTRACT

Optical properties of zigzag and armchair graphyne nanoribbon (GNR) sheet were investigated. Effect of increasing the width of nanoribbon on optical properties and optical band gap in particular was also studied. Calculations were based on density functional theory (DFT) and the results showed that these structures were semiconductors with the optical band gap of about 1–3.5 eV; this value was higher than for the armchair than zigzag structures. With increasing the width of the ribbons, optical band gap decreased in both structures and maximum electron energy loss spectroscopy (EELS) and dielectric constant increased for the zigzag and armchair structures. Moreover, for the armchair structure, maximum optical reflectivity versus GNR width was a linear function, while it showed a teeth behavior for the zigzag structure.

Introduction

In recent years, many studies have been performed on carbon structures, most of which are on the two-dimensional ones [1–3]. Graphene is the most well-known carbon structure made of carbon atoms which has similar hybridization-SP_2. This issue is due to the unique physical properties of two-dimensional structures of carbon atoms that are formed with strong sigma bonds. As a result of unique electronic properties, graphene is used instead of other materials in different industries [4].

Experimental investigations are always considered by researchers to improve the properties of structures. Experimental investigations are carried out on the elastic properties of graphene. Using atomic force microscopy, stiffness of 340 ± 50 N/m was obtained for graphene [5]. By mechanical cutting, a single layer of graphite in the form of graphene nanoribbon has been experimentally provided in [6–8]. Production of these nanoribbons leads to building transistors and electronic components with smaller dimensions and better performance [9–11].

* Corresponding author. Tel.: +98 2122853308; fax: +98 2122853650.
E-mail address: jafari@kntu.ac.ir (M. Jafari).

http://dx.doi.org/10.1016/j.saa.2014.12.020
1386-1425/

Baughman et al. suggested structures like graphene which contained triple carbon–carbon bonds in addition to the conventional bonds of the graphene structure. This new structure, called graphyne, was introduced in three types of alpha, beta, and gamma graphyne [12]. These new structures were synthesized in the form of carbon nanotubes and graphyne sheets by chemical vapor deposition [13–15]. Investigation of various properties of graphyne nanoribbons has been recently performed. These structures are semiconductors with the band gap of less than 1.7 eV [16]. By impurity doping of boron or nitrogen for one of these nanoribbons, the band gap was decreased [17]. Investigation of the optical properties of these structures by increasing the width of nanoribbons has not been done yet and thus became the goal of the present study.

In this paper, optical properties of zigzag and armchair gamma graphyne nanoribbons with different widths were examined. These graphyne nanoribbons were two-dimensional sheets which were developed in one direction [16]. Semiconductors with different band gaps will be applicable in solar cells technology due to the complete absorption of light by successive layers [18]; thus, GNR with different widths was investigated.

Results and calculation details

The calculations were carried out using quantum espresso code [19] based on density functional theory using plane wave. Separate unit cells for the ribbons with various widths were considered (Fig. 1) and the optimized bond length was obtained after the optimization of structures by local density approximation (LDA). This approximation has been found to be appropriate for homogeneous semiconductor structures [4,20,21].

The vacuum of about 10 Å was considered between the ribbons. The k point was considered by $1 \times 10 \times 1$ for NSCF and $1 \times 7 \times 1$ for SCF calculation in the brillouin zone. The optimized bond lengths (Table 1) were in agreement with those of the previous papers [17,22,23] and minimum bond length was related to triple carbon–carbon bond (1.21 Å).

Simulation and calculation were performed for the nanoribbons with width of $n = 1$ (4.34 Å), $n = 2$ (10.29 Å), and $n = 5$ (28.14 Å) for the armchair and $n = 1$ (8.45 Å), $n = 1.5$ (11.89 Å), $n = 3.5$ (25.63 Å) for zigzag structures (Fig. 1), where n denotes the number of chains of hexagonal carbon rings.

Optical properties of solid structures were investigated using dielectric function [24]. Electron energy loss spectroscopy (EELS), absorption, reflectivity, and refractivity indexes were obtained from the imaginary parts of the dielectric function [25,26].

Table 1
The optimized bond length.

The optimized bond length	
Label	Zigzag and armchair
A (Å)	1.42
B (Å)	1.41
C (Å)	1.21

Dielectric function of a material describes the electrical and optical properties versus energy, wavelength, or frequency. Investigation results of the imaginary part of dielectric function (ε_2) showed that the optical band gap decreased with increasing width of the nanoribbons in both zigzag and armchair structures (Fig. 2). In the armchair nanoribbon with the width of 4.34 Å, optical band gap was 3.44 eV and, with increasing width to 28.14 Å, the band gap decreased to 0.88 eV. Also, in the zigzag with the width of 8.45 Å, optical band gap was 2.68 eV and, with increasing width to 25.63 Å, it decreased to 1.04 eV. In these structures, a decrease of optical band gap with increasing width of the nanoribbons was completely in line with the decrease of the band gap in the electronic band structure [16]. At lower widths, changes of optical band gap were faster. Optical band gap of the zigzag nanoribbons was more than that of the armchair at a specific width (Fig. 2).

As can be seen in Fig. 3, for each of the structures, the peak of EELS increased with increasing width. At all widths, the energy loss function of the armchair nanoribbon was greater than that of the zigzag, except for the width of 22.19 Å (Fig. 4). Finally, energy of volume-Plasmon (EELS max-peak) shifted to higher energies with the increasing width.

Results of the real part (ε_1) of dielectric function are shown in Fig. 5. This quantity is the dielectric constant at zero energy. These results showed that, with increasing the width of the nanoribbon, dielectric constant was increased. The dielectric constant values are presented in Table 2. At equal widths, dielectric constant was higher for the armchair nanoribbon because of being more symmetric than the zigzag. Furthermore, the real part of dielectric function described the electric polarization of the material and it was higher for the armchair than zigzag.

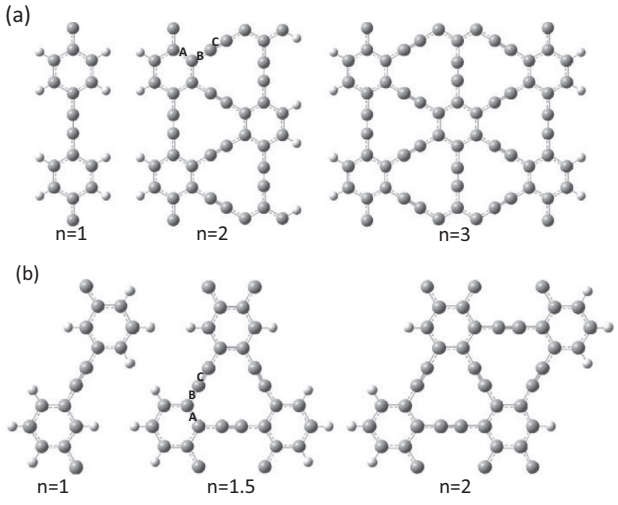


Fig. 1. (a) Armchair-edged GNR with widths $n = 1, 2, 3$, (b) zigzag edged GNR with widths $n = 1, 1.5, 2$.

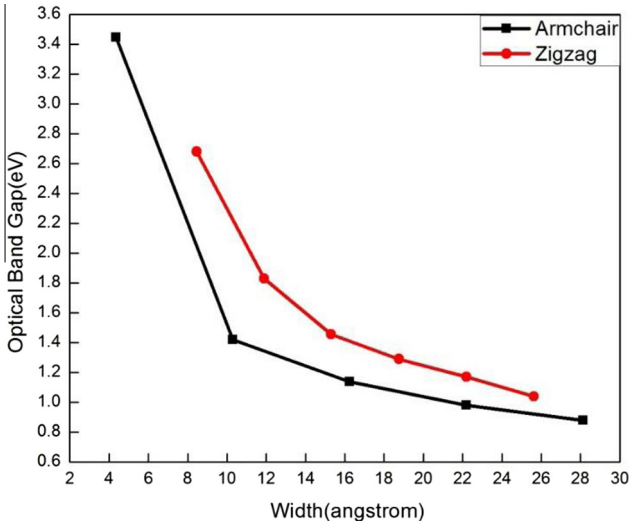


Fig. 2. Variation of optical band gap as a function of the ribbon width for zigzag and armchair GNR.