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Excessive Index of Boron and Carbon-Like Nanotubes

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ABSTRACT

Structures, devices, and systems having novel properties and functions due to the arrangement of their atoms on the 1 to 100 nanometer scale. Many fields of endeavor contribute to nanotechnology, including molecular physics, materials science, chemistry, biology, computer science, electrical engineering, and mechanical engineering. The study of Excessive index of matching has a number of applications particularly in scheduling theory to complete a process in the minimum possible time. The minimum number of perfect matching that covers the edge set of a graph G is known as excessive index of G. In this paper, we determine the excessive index for Boron Triangular Nanotube, $TUHC_6[2p, q]$ nanotube and $HC_5C_7[p, q]$ nanotube.

Keywords: Nanotubes, Perfect Matching, Excessive Index.

1. INTRODUCTION

Nanotechnology is defined as the study and use of structures between 1 nanometer (nm) and 100 nanometers in size. Nanotechnology creates many new materials and devices with a wide range of applications in medicine, electronics, computer, chemistry, energy, agriculture, communication and heavy industry. Nanotube was accidently discovered by a Japanese researcher at NEC in 1990 while making Buckyballs[8]. It involves different structures of nanotubes. The most significant nano structures are carbon nanotubes, boron triangular nano-

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tubes. Nanotubes are three dimensional cylindrical structures formed out of the two dimensional sheets.

Nanotubes can easily penetrate membrances such as cell walls. In fact, the long, narrow shape of nanotubes make them look like miniature needles, thus it makes sense that they can function like a needle at the cellular level. Medical researchers are using this property by attaching molecules to the nanotubes that are attracted to cancer cells to deliver drugs directly to diseased cells[13]. Also, Nanotechnology is having an impact on several aspects of food science, from how food is grown to how it is packaged. Companies are developing nanomaterials that will make a difference not only in the taste of food, but also in food safety, and the health benefits that food delivers.

Scheduling is the process of deciding how to commit resources between a variety of possible tasks. Determining excessive index has important applications in scheduling[5]. In this paper, we determine the excessive index for Boron Triangular Nanotube, $TUHC_6[2p, q]$ nanotube and $HC_5C_7[p, q]$ nanotube.

2. GENERAL RESULTS

Let G be a simple molecular graph without multiple edges and loops and with set of vertices $V(G)$ and set of edges $E(G)$. In a molecular graph, each vertex represents an atom of the molecule and an edge represents bond between corresponding atoms. A *Matching* in a graph $G = (V, E)$ is a subset M of edges, no two of which have a vertex in common. A matching M is said to *perfect* if every vertex in G is an endpoint of one of the edges in M [3]. Thus a perfect matching in G is a 1-*regular spanning subgraph* of G. In the literature it is also known as a 1-*factor* of G. A *near-perfect* matching covers all vertex but not exactly one vertex. The perfect matching problem is known to be in randomized *NC*.

A graph G is 1-*extendable* if every edge of G belongs to at least one 1-factor of G. A 1-*factor cover* of G is a set $\mathcal{F}$ of 1-factors of G such that $\bigcup_{F \epsilon \mathcal{F}} \mathcal{F} = E(G)$. A 1-factor cover of minimum cardinality is called a *excessive factorization*. An excessive near 1-factorization of a graph G is minimum set of near 1-factors whose union contains all the edges of G [7]. The *Excessive index* of a graph G is the minimum number of perfect matching that covers the edge set of G. The *excessive index* of G, denoted $\chi'_e(G)$, is the size of an excessive factorization of G. We define $\chi'_e(G) = \infty$ if G is not 1-extendable. A graph G is 1-*factorizable* if its edge set $E(G)$ can be partitioned into edge-disjoint 1-factors. The problem of determining whether a regular graph G is 1-factorizable is NP-complete.

Mazzuoccolo proves that the well known Berge-Fulkerson conjecture can be stated in terms of the excessive index of cubic graphs[11]. Bonisoli and Cariolaro observed that the problem of determining the excessive index for regular graph is NP-hard[4]. Cariolaro and Fu determined the excessive index of complete multipartite graphs, which proved to be a challenging task[6]. The excessive index of a bridgeless cubic graph has been studied by Fouquet *et al.*[9].

Theorem 1: Let G be a graph. Then $\chi'_e(G) \geq \Delta$[4].

Theorem 2: Let G be a regular graph with even order. Then $\chi'_e(G) = \Delta(G)$ if and only if G is 1-factoriable.

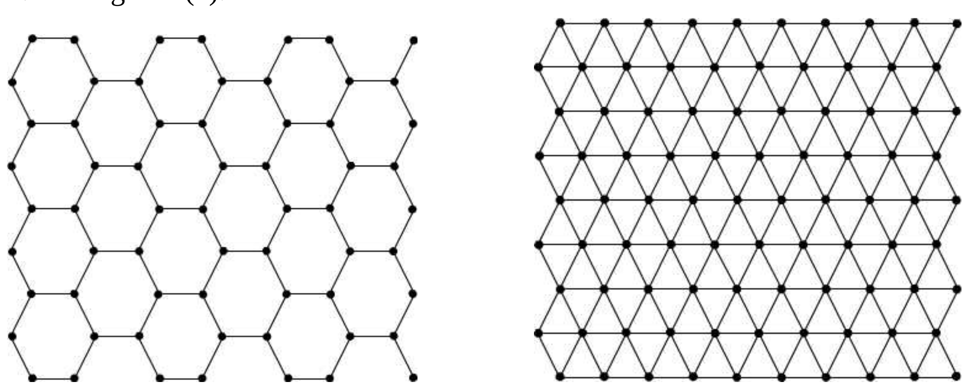
Theorem 3: A carbon hexagonal nanotube has only odd number of rows and even number of columns[12].

3. BORON TRIANGULAR NANOTUBE

There are different shapes of carbon nanotubes such as armchair, chiral and zigzag based on the rolling of 2D carbon hexagonal sheet. Kunstmann and Quandt hypothesize that zigzag boron nanotubes do not exist[10]. Hence in this graph, we do not discuss zigzag boron nanotubes and focus only on armchair model of carbon nanotubes. The boron triangular nanotube was created in 2004[10] and obtained from a carbon hexagonal nanotube by adding an extra atom to the center of each hexagon.

Definition1: A *carbon hexagonal nanotube* of order $n \times m$ is a tube obtained from a carbon hexagonal sheet of n rows and m columns by merging the vertices of last column with the respective vertices of first column. A carbon hexagonal nanotube of order $n \times m$ has nm vertices and $m(3n-2)/2$ edges[12]. See Figure 1(a).

Definition2: A *boron triangular nanotube* of order $n \times m$ is obtained from a hexagonal nanotube of order $n \times m$ by adding a new vertex at the center of each hexagon of the hexagonal nanotube. A boron triangular nanotube of order $n \times m$ has $3nm/2$ vertices and $3m(3n-2)/2$ edges[12]. See Figure 1(b).



(a) (b)

Figure1: (a) Carbon Hexagonal Sheet, (b) Boron Triangular Sheet.

Theorem1: Let G be the Boron triangular nanotube. Then $\chi'_e(G) = 6$.

Proof:

Input: A Boron Triangular Nanotube of dimension $n \times m$.

Algorithm:

i) All horizontal independent edges constitute M_1.

ii) The horizontal edges left in M_1 will be comes under M_2 together with acute edges in column 1 induced by row i and row $i+1$, $i\ even$, $2 \leq i \leq n-1$.

iii) All Obtuse edges induced by row i and row $i+1$, $i\ even$, $2 \leq i \leq n-1$ and horizontal edges in row 1 constitute M_3.

iv) All acute edges induced by row i and row $i+1$, $i\ even$, $2 \leq i \leq n-1$, except the acute edges in column 1 together with the horizontal edges of row 1 left in M_3 constitute M_4.

v) All obtuse edges induced by row i and row $i+1$, $i\ odd$, $1 \leq i \leq n-2$ and the horizontal edges of n^{th} row comes under M_5.

vi) All acute edges induced by row i and row $i+1$, $i\ odd$, $1 \leq i \leq n-2$ and the horizontal edges of n^{th} left in M_5 comes under M_6.

End Excessive Index $\chi'_e(BT(n,m))$
Output $\chi'_e(BT(n,m)) = 6$.

4. $TUHC_6[2p,q]$ NANOTUBE

Let us consider a zig-zag polyhex lattice and p be the number of vertical lines in first row and q be the number of horizontal "zig-zag" lines[1].

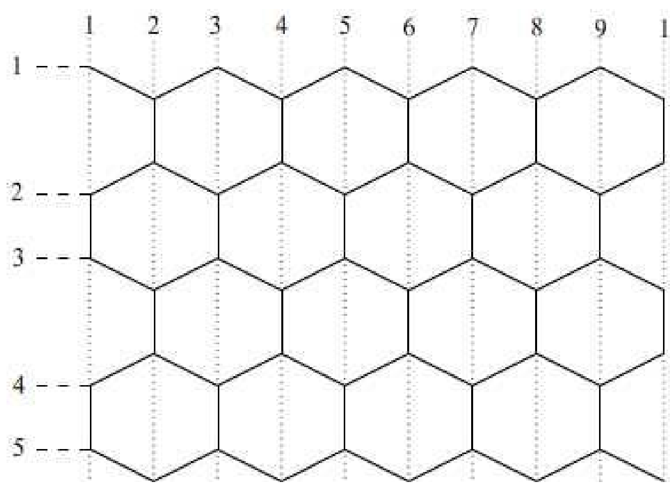


Figure 2: Zig-Zag $TUHC_6[2p,q]$, $p = 9, q = 5$.

Theorem 2: Let G be the $TUHC_6[2p,q]$ nanotube. Then $\chi'_e(G) = 6$.
Proof:
Input: $TUHC_6[2p,q]$ nanotube.

Algorithm:
i) All the acute edges constitute M_1.

ii) All the obtuse edges constitute M_2.
iii) All the vertical edges constitute M_3.

End Excessive Index $\chi'_e(TUHC_6[2p,q])$
Output $\chi'_e(TUHC_6[2p,q]) = 3$.

5. $HC_5C_7[p,q]$ NANOTUBE

The $HC_5C_7[p,q]$ nanotube consists of heptagon and pentagon nets[2]. See Figure 3. We denote the number of heptagons in the first row by p. In this nanotube the four first rows of vertices and edges are repeated alternatively, we denote the number of this repetition by q. In each period there are $16p$ vertices and $2p$ vertices are joined to the end of the graph, and hence the number of vertices in this nanotube is equal to $16pq + 2p$.

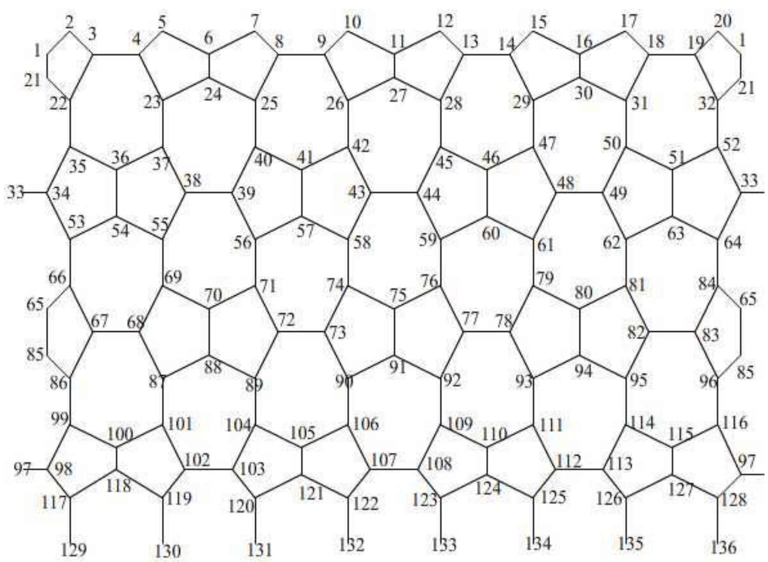


Figure 3: $HC_5C_7[p,q]$ nanotube

Theorem 3: Let G be the $HC_5C_7[p,q]$ nanotube. Then $\chi'_e(G) = 3$.
Proof:
Input: $HC_5C_7[p,q]$ nanotube

Algorithm:

i) All the Horizontal and the Vertical edges of C_7 and vertical edges of C_5 constitute M_1.
ii) All the obtuse edges of C_5 and C_7 constitute M_2.
iii) All the acute edges of C_5 and C_7 constitute M_3.

End Excessive Index $\chi'_e(HC_5C_7[p,q])$
Output $\chi'_e(HC_5C_7[p,q]) = 3$.

6. CONCLUSION

In this paper, we determine the excessive index for Boron Triangular Nanotube, $TUHC_6[2p,q]$ nanotube and $HC_5C_7[p,q]$ nanotube. It would be an interesting line of research to determine the excessive index for other nanotubes since scheduling theory is the process of deciding how to commit resources between a variety of possible tasks.

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