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Packing of Certain Nanotubes and Nanosheet

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Abstract

Molecules arranging themselves into predictable designs on silicon chips could lead to microprocessors with much smaller circuit elements. Mathematically, assembling in predictable patterns is equivalent to packing in graphs [1]. An *H-packing* of a graph G is a set of vertex disjoint subgraphs of G, each of which is isomorphic to a fixed graph H. In this paper, we investigate that the three layered and six layered Titania Carbon Nanotubes admit a perfect packing and thus determine their packing numbers. We also investigate the packing numbers of H-Naphtalenic Nanosheet.

1 Introduction

Carbon nanotubes are one of the most commonly mentioned building blocks of nanotechnology. Carbon nanotubes based sensors have shown many benefits over their past counterparts and are suitable candidates for wireless sensor nodes [5] which are used in many applications, ranging from military target tracking to industrial monitoring. H-packing, is of practical interest in the areas of scheduling, wireless sensor tracking, wiring-board design, code optimization [3] and many others.

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Definition 1.1. *[2] An $H-$packing of a graph G is a set of vertex disjoint subgraphs of G, each of which is isomorphic to a fixed graph H. The maximum number of vertex disjoint copies of H in G is called the packing number and is denoted by $\lambda(G, H)$.*

Determining the maximum $\lambda(G, H)$ is called the maximum $H-$packing problem in G. The vertices belonging to the subgraph H of an $H-$packing are said to be saturated by the $H-$packing and the other vertices are said to be unsaturated. A packing that saturates every vertex of G is said to be a perfect packing.

2 Titania Nanotubes

Titania, TiO_2, attracts considerable technological interest due to its unique properties in biology, optics, electronics, and photo-chemistry. Titanium nanotubes have been observed in two types of morphologies: single-walled titanium (SW TiO_2) nanotubes and multi-walled (MW TiO_2) nanotubes.

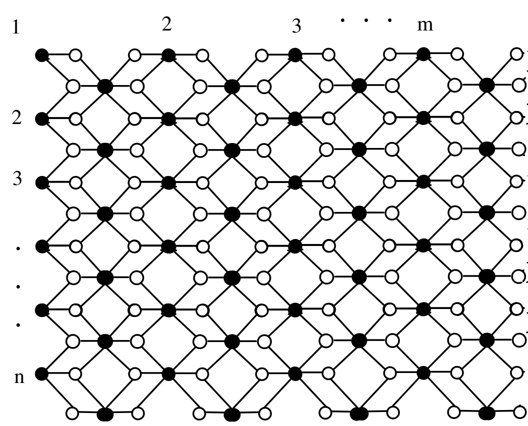

Figure 1: $TNT_3[m, n]$

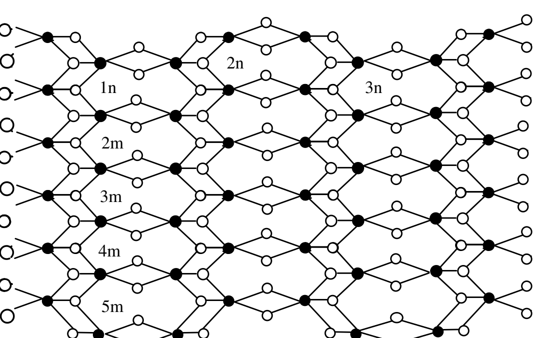

Figure 2: $TNT_6[5, 3]$

In the three-layered titania nanotube $TNT_3[m, n]$, m and n represent the number of titanium atoms in each row and column, respectively (Figure 1). The sixlayered singlewalled titania nanotube $TNT_6[m, n]$, m denotes the number of octagons in a column and n denotes the number of octagons in a row (figure 2). Black dots correspond to titanium atoms, whereas white dots correspond to oxygen atoms, and edges represent bonds [4].

2.1 Packing with P_3

Theorem 2.1. *The three layered titania nanotube* $TNT_3[m,n]$ *admits a perfect* H*-packing with* $2mn$ *copies of* H, *where* $H \simeq P_3$ *for all* $m \geq 2,\ n \geq 2$.

Proof. The three layered titania nanotube $TNT_3[m,n]$ has $6mn$ vertices where m and n represent the number of titanium atoms in each row and column, respectively (See figure 1). A single molecule of titanium dioxide consists of one atom of titanium bonded with two atoms of oxygen on either sides. In graph theoretical terms this arrangement of oxygen-titanium-oxygen corresponds to a path P_3 on 3 vertices. $TNT_3[m,n]$ can be decomposed into $\frac{6mn}{3}$ copies of P_3 each corresponding to an horizontal arrangement of *O–Ti-O*. Due to the structural arrangement of $TNT_3[m,n]$ and since the total number of vertices is $6mn$, a multiple of 3, it admits a perfect packing with P_3 and $\lambda(TNT_3[m,n],P_3) = 2mn$ for all $m \geq 2,\ n \geq 2$. □

Theorem 2.2. *The six layered titania nanotube* $TNT_6[m,n]$, $m \geq 2,\ n \geq 2$ *admits a perfect* H*-packing with* $2(m+1)(n+1)$ *copies of* H *when* $n \equiv 1\ (mod\ 2)$, *where* $H \simeq P_3$.

Proof. The six layered titania nanotube $TNT_6[m,n]$ has $6(m+1)(n+1)$ vertices, where m denotes the number of octagons in a column and n denotes the number of octagons in a row. The structural arrangement of $TNT_6[m,n]$ nanotube consist of $n+1$ alternating strips of A and B (figure 3) linked by $m+1$ pairs of oxygen atoms between each of the strips forming parallelograms alternating with octagons.

The strip A consists of a series of parallelograms arranged sequentially in which each parallelogram alternates with its mirror image. In strip A consider the diagonal lines α drawn across only the parallelograms arranged in the same direction aligning with the first. Strip B is the mirror image of strip A and let the diagonal lines of the corresponding parallelograms be called as β.

In $TNT_6[m,n]$ nanotube structure every pair of titanium atoms are either joined by an α line or a β line. Now with the titanium atom at the centre consider the path P_3 formed by adjoining two oxygen atoms from its either sides as shown in figure 4. This completely decomposes the $TNT_6[m,n]$ nanotube structure into $2(m+1)(n+1)$ number of copies of H. Hence $\lambda(TNT_6[m,n],P_3) = 2(m+1)(n+1)$ for all $m \geq 2,\ n \geq 2$ and $n \equiv 1 \pmod 2$. □

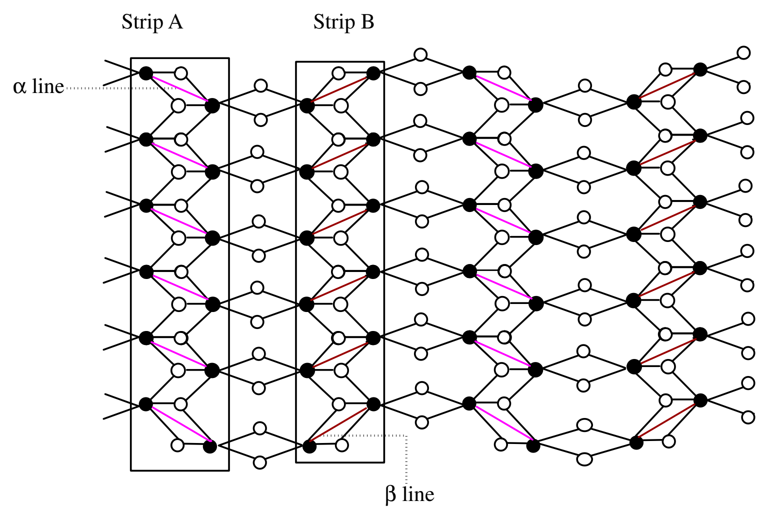

Figure 3: $TNT_6[5,3]$

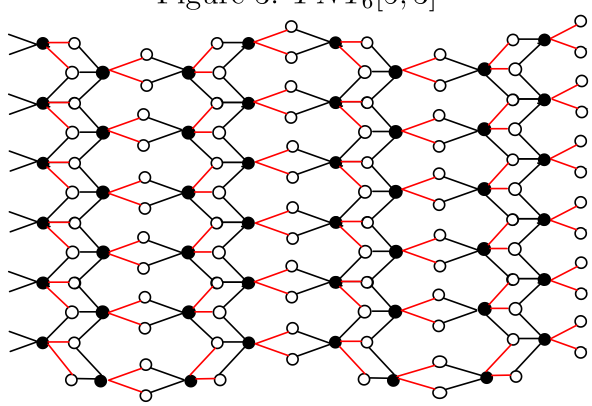

Figure 4: P_3 packing of $TNT_6[5,3]$

2.2 Packing with Y tree

The Y tree is an acyclic connected graph on six vertices as given in figure 5.

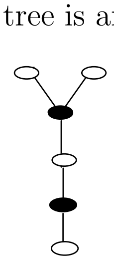

Figure 5: Y tree

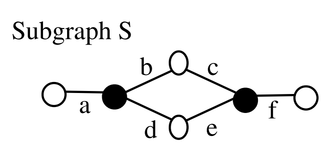

Figure 6:

Theorem 2.3. *The six layered titania nanotube $TNT_6[m,n]$, $m \geq 2$, $n \geq 2$ admits a perfect H-packing with $(m+1)(n+1)$ copies of H when $n \equiv 1\ (mod\ 2)$, where $H \simeq Y$ tree.*

Proof. In $TNT_6[m,n]$, consider the $OTiO-O-TiO$ structural arrangement given by figure 6 and call it as graph S say. The entire padding of $TNT_6[m,n]$ consist $(m+1)(n+1)$ number of such graphical structures S joined together by pairs of acute and obtuse parallel lines or chemical bonds. In the subgraph S of $TNT_6[m,n]$, removing any of the edges b, c, d or e results in the graph $H \simeq Y$ tree. This demonstrates that the $TNT_6[m,n]$ nanotube structure admits a perfect H-packing with $(m+1)(n+1)$ copies of H when $n \equiv 1$ (mod 2). □

2.3 Packing with Octagons C_8

Theorem 2.4. *Let $G \simeq TNT_6[m,n]$, $m \geq 2$, $n \geq 2$ and $H \simeq C_8$. Then for $n \equiv 1\ (mod\ 2)$*

$$\lambda(G,H) = \begin{cases} (n+1)(\lfloor m/2 \rfloor) & m \equiv 0\ (mod\ \ 2) \\ (n+1)(\lfloor m/2 \rfloor + 1) & m \equiv 1\ (mod\ \ 2) \end{cases}$$

Proof. The six layered titania nanotube $TNT_6[m,n]$ has $m(n+1)$ octagons, where m denotes the number of octagons in a column and n denotes the number of octagons in a row and the tube formation yields one more octagon in each row. Each octagons in the i^{th} row $(1 \leq i \leq m)$ shares two vertices with the octagon in the $(i-1)^{th}$ row and two vertices with the octagon in the $(i+1)^{th}$ row and for octagons in the first and m^{th} row shares only two vertices with the octagons in the next and previous rows respectively. Hence, perfect packing of $TNT_6[m,n]$ with C_8 is not possible.

Case 1: $m \equiv 0$ (mod 2)

When $m \equiv 0$ (mod 2), there is an even number of rows in the nanotube with $n+1$ number of octagons in each row. Now pack the octagons in the odd rows starting from first to the $(m-1)^{th}$ row which gives a total of $\lfloor \frac{m}{2} \rfloor$ odd rows. Hence, the total numbers of octagons packed out of $m(n+1)$ octagons are $\lfloor \frac{m}{2} \rfloor (n+1)$ and the total number of saturated vertices are $8\lfloor \frac{m}{2} \rfloor (n+1)$. Therefore $\lambda(G,H) = (n+1)(\lfloor \frac{m}{2} \rfloor)$ for $m \equiv 0$ (mod 2).

Case 2: $m \equiv 1$ (mod 2)

When $m \equiv 1 \pmod 2$, there is odd number of rows in the nanotube with $n+1$ number of octagons in each row. Now pack the octagons in the odd rows starting from first to the m^{th} row which gives a total of $\lfloor \frac{m}{2} \rfloor + 1$ odd rows. Hence, the total numbers of octagons packed out of $m(n+1)$ octagons are $(\lfloor \frac{m}{2} \rfloor + 1)(n+1)$ and the total number of saturated vertices are $8(\lfloor \frac{m}{2} \rfloor + 1)(n+1)$. Therefore $\lambda(G, H) = (n+1)(\lfloor \frac{m}{2} \rfloor + 1)$ for $m \equiv 1 \pmod 2$.
□

3 *H*-Naphtalenic Nanosheet *(2n, 2m)*

A H-Naphtalenic Nanosheet*[2m,2n]* is a trivalent decoration made by alternating squares C_4, pair of hexagons C_6 and octagons C_8 and it is a bi-regular graph with m number of rows and n number of columns. The H-Naphtalenic Nanosheet*[2m,2n]* has $10mn$ vertices [6].

3.1 Packing with Pentane (P_5)

Theorem 3.1. *The H-Naphtalenic Nanosheet(2n, 2m) admits a perfect H-packing with $2mn$ copies of n-pentane(P_5) for all values of m and n.*

Proof. For $m = 1$ and $n = 1$ the H-Naphtalenic Nanosheet*[2,2]* consist of a single pair of hexagon with 10 vertices. Hence the $10mn$ vertices of the H-Naphtalenic Nanosheet*[2m,2n]* is contributed by the n pair of hexagons in each of the m rows joined together by vertical and horizontal pairs of edges or chemical bonds. This proves that if we have to ascertain that the H-Naphtalenic Nanosheet*(2n, 2m)* admits a perfect H-packing with $2mn$ copies of n-pentane(P_5) for all values of m and n, it is sufficient to show that the H-Naphtalenic Nanosheet*[2,2]* admits a perfect H-packing with 2 copies of n-pentane(P_5).

The H-Naphtalenic nanosheet*[2,2]* can be split into two pairs of n-pentane when the three vertical edges that bonds them are eliminated. Generalizing this for all values of m and n, the H-Naphtalenic Nanosheet*(2n, 2m)* can be split into $2mn$ pairs of n-pentane when the all the vertical and horizontal edges that bonds them are eliminated. Hence, if $G \simeq H$-Naphtalenic Nanosheet$(2n, 2m)$ and $H \simeq P_5$, then $\lambda(G, H) = 2mn$ for all $m \geq 1, n \geq 1$.
□

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