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OMEGA POLYNOMIAL IN TITANIUM OXIDE NANOTUBES

M. GHORBANI[a*], M.A. HOSSEINZADEH[b], M.V. DIUDEA[c]

ABSTRACT. A new counting polynomial, called Omega $\Omega(G,x)$, was recently proposed by Diudea. It is defined on the ground of "opposite edge strips" *ops*. Two related polynomials: Sadhana $Sd(G,x)$ and Theta $\Theta(G,x)$ polynomials can also be calculated by ops counting. Close formulas for calculating these three polynomials in infinite nano-structures resulted by embedding the titanium dioxide pattern in plane, cylinder and torus are derived. For the design of titanium dioxide pattern, a procedure based on a sequence of map operations is proposed.

Keywords: *Titanium oxide, Omega polynomial, Sadhana polynomial, Theta polynomial*

INTRODUCTION

Nano-era is a suitable name for the period started with the discovery of C_{60} fullerene and carbon nanotubes [1-3]. It opened a new gate for the science and technology at nanometer scale with wide implications in the human activities. After the discovery of carbon nanotubes, the question about the possible existence of nanotubular forms of other elements was addressed by scientists and they tried to obtain inorganic nanostructures [4-6]. Various oxides, sulfides, selenides, borates, silicates, etc of many metals show very ordered structures at the nano-scale. Many of these compounds form nanotubes, similar to those of carbon: MX2, M=Mo, W, Ta, In, Zn, Ti, Cd, X=O, S, Se, Te, CB_x, BN, etc. In the last years, oxides and other above mentioned inorganic substances found applications in the design of nanostructured functional materials as films, nanorods, porous systems, nanoclusters and nanocrystallites or as nanofibers [7-13].

Among these nanostructures, the titanium nanotubular materials, called "titania" by a generic name, are of high interest due to their chemical inertness, endurance, strong oxidizing power, large surface area, high photocatalytic activity, non-toxicity and low production cost. The applications of TiO_2 nanotubes include photocatalysis, solar cells systems, nanoscale materials for lithium-ion batteries, etc. The titanium oxide nanotubes were synthesized using various methods and precursors [14-20], carbon nanotubes, porous alumina or polymer

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membranes as templates [21-27], anodic oxidation of Ti [28-30], sol–gel technique [31-35] or sonochemical synthesis [36]. Models of possible growth mechanisms of titanium nanotubes, the atomic structure of the nanotube walls and their stacking mode are discussed [19,20,35]. TiO_2 nanotubes are semiconductors with a wide band gap and their stability increases with increasing of their diameters. The numerous studies on the production and technological applications of nanotubular titania also require theoretical studies on stability and other properties, the topological ones included [37-42].

DESIGN OF TITANIUM OXIDE LATTICE

A map *M* is a combinatorial representation of a (closed) surface. Several transformations or operations on maps are known and used for various purposes. We limit here to describe only those operations needed here to build the TiO_2 pattern. For other operations, the reader is invited to consult refs [43-48].

Medial Med is achieved by putting new vertices in the middle of the original edges. Join two vertices if the edges span an angle (and are consecutive within a rotation path around their common vertex in *M*). Medial is a 4-valent graph and *Med*(*M*) = *Med*(*Du*(*M*)).

Dualization of a map starts by locating a point in the center of each face. Next, two such points are joined if their corresponding faces share a common edge. It is the (Poincaré) *dual Du*(*M*). The vertices of *Du*(*M*) represent faces in *M* and *vice-versa.*

Figure 1 illustrates the sequence of map operations leading to the TiO_2 pattern: *Du*(*Med*(6,6)), the polyhex pattern being represented in Schläfli's symbols. Correspondingly, the TiO_2 pattern will be denoted as: (4(3,6)), squares of a bipartite lattice of 3 and 6 connected atoms, while the medial pattern: ((3,6)4). Clearly, the TiO_2 pattern can be done simply by putting a point in the centre of hexagons of the (6,6) pattern and join it alternately with the points on the contour. It is noteworthy that our sequence of operations is general, enabling transformation of the (6,6) pattern embedded on any surface and more over, it provides a rational procedure for related patterns, to be exploited in cage/cluster building.

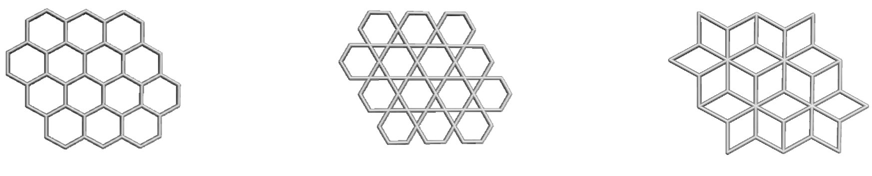

Figure 1. Way to TiO_2 lattice: (left) polyhex (6,6) pattern; (central) Med(6,6); (right) Du(Med(6,6))

OMEGA AND RELATED POLYNOMIALS

Let *G*(*V*,*E*) be a connected graph, with the vertex set *V*(*G*) and edge set *E*(*G*). Two edges *e* = *uv* and *f* = *xy* of *G* are called *codistant e co f* if they obey the following relation [49,50]:

$$d(v,x)=d(v,y)+1=d(u,x)+1=d(u,y) \quad (1)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e):=\{f\in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of *G*, *E*(*G*) being the union of disjoint orthogonal cuts: $E(G)=C_1\cup C_2\cup...\cup C_k,\ C_i\cap C_j=\varnothing, i\neq j$. Klavžar [51] has shown that relation *co* is a theta Djoković-Winkler relation [52,53].

Let *e* = *uv* and *f* = *xy* be two edges of *G* which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal cut *qoc* (*i.e.*, the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring. The length of *ops* is maximal irrespective of the starting edge.

Let *m*(*G*,*s*) be the number of *ops* strips of length *s*. The Omega polynomial is defined as [54]:

$$\Omega(G,x)=\sum_s m(G,s)\cdot x^s \quad (2)$$

The first derivative (in *x*=1) equals the number of edges in the graph

$$\Omega'(G,1)=\sum_s m(G,s)\cdot s=e=|E(G)| \quad (3)$$

A topological index, called Cluj-Ilmenau,[55] *CI*=*CI*(*G*), was defined on Omega polynomial

$$CI(G)=\{[\Omega'(G,1)]^2-[\Omega'(G,1)+\Omega''(G,1)]\} \quad (4)$$

An example is given in Figure 2, which illustrates just the pattern of TiO_2 lattice.

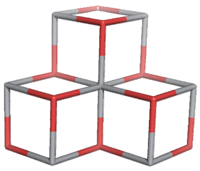

Figure 2. TiO_2 pattern; counting polynomial examples:

$$\Omega(G,x)=3x^3+3x^5;\ \Omega'(G,1)=24=e(G);\ CI(G)=474;$$

$$Sd(G,x)=3x^{19}+3x^{21};\ Sd'(G,1)=120=Sd(G);$$

$$\Theta(G,x)=9x^3+15x^5;\ \Theta'(G,1)=27+75=102=\Theta(G)$$

The Sadhana index *Sd*(*G*) was defined by Khadikar *et al*. [56,57] as

$$Sd(G)=\sum_s m(G,s)(|E(G)|-s) \quad (5)$$

where *m*(*G*,*s*) is the number of strips of length *s*. The Sadhana polynomial *Sd*(*G*,*x*) was defined by Ashrafi *et al*. [58] as

$$Sd(G,x) = \sum_s m(G,s) \cdot x^{|E(G)|-s} \quad (6)$$

Clearly, the Sadhana polynomial can be derived from the definition of Omega polynomial by replacing the exponent *s* by |*E*(*G*)-*s*|. Then the Sadhana index will be the first derivative of *Sd*(*G*, *x*) evaluated at *x*=1.

A third related polynomial is the Theta polynomial [59], defined in co-graphs as

$$\Theta(G,x) = \sum_s s \times m(G,s) \cdot x^s \quad (7)$$

The aim of this study is to compute the Omega and its related counting polynomials in TiO_2 lattice, embedded in the plane but also in the cylinder and torus.

RESULTS AND DISCUSSION

We begin with the 2-dimensional graph, named K, (Figure 3). The various types of ops are drawn by arrows.

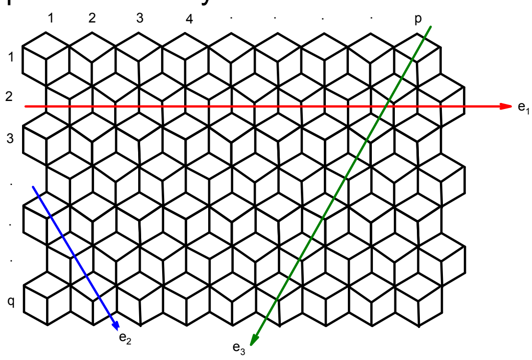

Figure 3. The ops strips of a 2-dimensional graph K of *Du*(*Med*(6,6)) TiO2 pattern.

By definition of Omega polynomial and Table 1 one can see that:

Table 1. The number of *ops* e_i, $1 \le i \le 6$ in the graph K.

No.	Number of *ops*	Type of *ops*
q	2p+1	e_1
2 ⋮ 2	$\begin{cases} 3 \\ 5 \\ \vdots \\ 2\min\{2p,q\}-1 \end{cases}$	e_2
$\begin{cases} 2p-q+1 \\ q-2p+1 \end{cases}$	$\begin{cases} 2q+1 & 2p \ge q \ge 1 \\ 4p+1 & q \ge 2p. \end{cases}$	e_3

Now, we can derive the following formulas for the counting polynomials in the infinite 2-dimensional graph K:

$$\Omega(K,x)=\begin{cases} qx^{2p+1}+2(x^3+x^5+...+x^{2q-1})+(2p-q+1)x^{2q+1} & 2p>q\geq 1 \\ qx^{2p+1}+2(x^3+x^5+...+x^{4p-1})+(q-2p+1)x^{4p+1} & q\geq 2p \end{cases} \quad (8)$$

$$Sd(K,x)=\begin{cases} qx^{|E(K)|-2p-1}+2(x^{|E(K)|-3}+x^{|E(K)|-5}+...+x^{|E(K)|-2q+1}) & \\ +(2p-q+1)x^{E(K)|-2q-1} & 2p>q\geq 1 \\ qx^{|E(K)|-2p-1}+2(x^{|E(K)|-3}+x^{|E(K)|-5}+...+x^{|E(K)|-4p+1}) & \\ +(q-2p+1)x^{|E(K)|-4p-1} & q\geq 2p \end{cases} \quad (9)$$

$$\theta(K,x)=\begin{cases} a(x)+2(3x^3+...+(2q-1)x^{2q-1})+(2p-q+1)(2q+1)x^{2q+1} & 2p>q\geq 1 \\ a(x)+2(3x^3+...+(4p-1)x^{4p-1})+(q-2p+1)(4p+1)x^{4p+1} & q\geq 2p \end{cases} \quad (10)$$

in which $a(x)=q(2p+1)x^{2p+1}$. Examples are given in Appendix.

We now consider the tubular structure G (Figure 4). Again the different cases of ops are drawn. One can see that $|S(e_1)| = 2p$ and $|S(e_2)| = 2q+1$. On the other hand, there are $q(e_1)$ and $2p(e_2)$ similar edges. This leads to the formulas

$$\Omega(G,x)=\mathrm{q}\cdot x^{2\mathrm{p}}+2\mathrm{p}\cdot x^{2\mathrm{q}+1} \quad (11)$$

$$Sd(G,x)=\mathrm{q}\cdot x^{|E(G)|-2\mathrm{p}}+2\mathrm{p}\cdot x^{|E(G)|-2\mathrm{q}-1} \quad (12)$$

$$\theta(G,x)=2\mathrm{pq}\cdot x^{2\mathrm{p}}+2\mathrm{p}(2\mathrm{q}+1)\cdot x^{2\mathrm{q}+1} \quad (13)$$

Figure 5 illustrates the case of a torus, denoted by H; it shows that there are two types of ops and their number is: $|S(e_1)| = 2p$, $|S(e_2)|=2pq$. On the other hand, there are 2q similar edges for each of e_1, e_2, respectively. With the above considerations we have the following formulas:

$$\Omega(H,x)=\mathrm{qx}^{2\mathrm{p}}+2\mathrm{x}^{2\mathrm{pq}} \quad (14)$$

$$Sd(H,x)=\mathrm{qx}^{|E(H)|-2\mathrm{p}}+2\mathrm{x}^{|E(H)|-2\mathrm{pq}} \quad (15)$$

$$\theta(H,x)=2\mathrm{pqx}^{2\mathrm{p}}+4\mathrm{pqx}^{2\mathrm{pq}} \quad (16)$$

CONCLUSIONS

Nano-structured titania can be described, in topological terms by the aid of counting polynomials, such as Omega, Sadhana and Theta polynomials.

Close formulas for calculating these three polynomials in infinite nano-structures resulted by embedding the titanium dioxide pattern in plane, cylinder and torus are derived. A procedure based on a sequence of map operations is proposed for the design of titanium dioxide pattern.

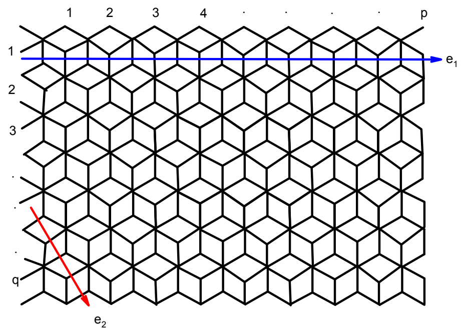

Figure 4. The ops strips of the nanotube G=TU[p,q].

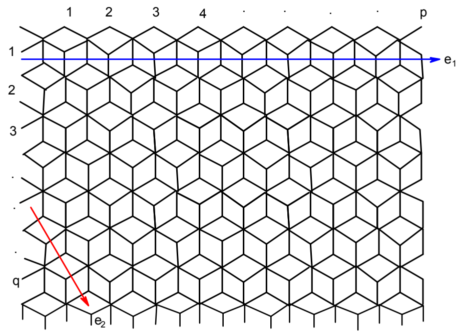

Figure 5. The ops strips of the nanotorus H=T[p,q].

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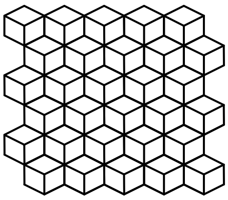
APPENDIX

Examples for calculating Omega polynomial.

1. Case of infinite 2-dimensional graph K.

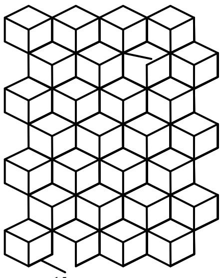
We have the Omega polynomial: $qx^{2p+1}+2(x^3+x^5+...+x^{2q-1})+(2p-q+1)x^{2q+1}$

1.1. Case: $2p > q > p, 2 | q,$
If q = 6, p = 5 then, the graph is:



and
$\Omega(G,x) = 6x^{11} + 2(x^3 + x^5 + x^7 + x^9 + x^{11}) + 5x^{13}$

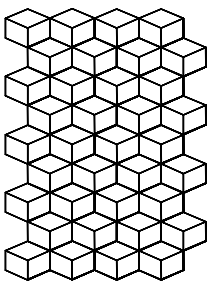
1.2. Case: $2p > q > p, 2 \nmid q,$
Now if p = 4, q = 7 then, the graph is:



and
$\Omega(G,x) = 7x^9 + 2(x^3 + x^5 + x^7 + x^9 + x^{13}) + 2x^{15}$

We have also $qx^{2p+1} + 2(x^3 + x^5 + ... + x^{4p-1}) + (q - 2p + 1)x^{4p+1}$

1.3. Case: $q \geq 2p$**.** If p = 4, q = 9 then, the graph is:

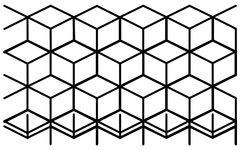


and
$\Omega(G,x) = 9x^9 + 2(x^3 + x^5 + x^7 + x^9 + x^{11} + x^{13} + x^{15}) + 2x^{17}$

2. Case of nanotubes G [p,q].

We have the Omega polynomial: $\Omega(G,x) = \mathrm{q}\mathrm{x}^{2\mathrm{p}} + 2\mathrm{p}\mathrm{x}^{2\mathrm{q}+1}$

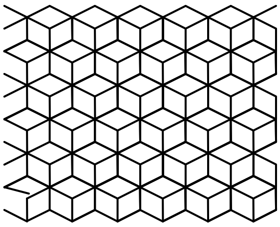
Now, if p = 5, q = 4 then, the graph is:



and

$\Omega(G,x) = 4x^{10} + 10x^{9}$

Or, if p = 6, q = 6 then, the graph is :



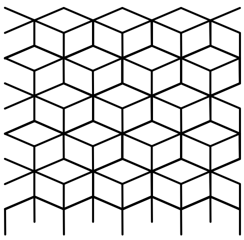
and

$\Omega(G,x) = 6x^{12} + 12x^{13}$

3. Case of nanotori H [p,q].

We have the Omega polynomial: $\Omega(H,x) = \mathrm{q}\mathrm{x}^{2\mathrm{p}} + 2\mathrm{x}^{2\mathrm{pq}}$

Now, if p = 4, q = 5 then, the graph is:



and

$\Omega(H,x) = 5x^{8} + 2x^{40}$