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OMEGA POLYNOMIAL IN P-TYPE SURFACE NETWORKS

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ABSTRACT. Design of two crystal-like networks was achieved by embedding a zig-zag Z-unit and its corresponding armchair A-unit, of octahedral symmetry, in the P-type surface, by means of the original software Nano Studio. The hypothetical networks, thus obtained, were characterized in their topology by Omega counting polynomial**.**

Keywords: *crystal-like networks, Omega polynomials, topology*

INTRODUCTION

In the last two decades, novel carbon allotropes have been discovered and studied for applications in nano-technology. Among the carbon structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) were the most challenging [1,2]. Inorganic clusters, like zeolites, also attracted the attention of scientists. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [3-8].

The present study deals with two hypothetical crystal-like nano-carbon structures, of which topology is described in terms of Omega counting polynomial.

BACKGROUND ON OMEGA POLYNOMIAL

In a connected graph $G(V,E)$, 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 relation [9]:

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

which is reflexive, that is, *e co e* holds for any edge *e* of *G*, and symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive; if "*co*" is also transitive, thus it is 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 [10] has shown that relation *co* is a *theta* Djoković-Winkler relation [11,12].

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We say that edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Note that the relation *co* is defined in the whole graph while *op* is defined only in faces. Using the relation *op* we can partition the edge set of *G* into *opposite* edge *strips, ops.* An *ops* is a quasi-orthogonal cut *qoc*, since *ops* is not transitive.

Let *G* be a connected graph and $s_1, s_2, ..., s_k$ be the *ops* strips of *G*. Then the *ops* strips form a partition of *E(G)*. The length of *ops* is taken as maximum. It depends on the size of the maximum fold face/ring F_{max}/R_{max} considered, so that any result on Omega polynomial will have this specification.

Denote by *m*(*G*,*s*) the number of *ops* strips of length *s* and define the Omega polynomial as [13-15]:

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

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

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

On Omega polynomial, the Cluj-Ilmenau index [9], *CI*=*CI*(*G*), was defined:

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

The Omega polynomial partitions the edge set of the molecular graph into opposite edge strips, by the length of the strips.

OMEGA POLYNOMIAL IN TWO P-SURFACE CRYSTAL NETWORKS

Design of two crystal-like networks was achieved by identifying the opposite open faces of a zig-zag Z-unit and its corresponding armchair A-unit (Figure 1), of octahedral symmetry and embedding them in the P-type surface, with the help of original software Nano Studio [16] .

Omega polynomials for the repeat units of the Z_P and A_P structures (Figure 2) herein discussed are listed in Table 1. The polynomials are calculated at $R_{max}[8]$ as follows.

In the Z_P structure, the term at exponent 1 counts the edges in odd faces/rings that are not counted in even rings. The exponent 2 refers to isolated even rings while the exponent 4 represents strips of three even-membered faces/rings.

In the A_P structure, there are no odd faces so the polynomial has no terms at exponent 1. The exponent 6 represents strips of five even-membered faces/rings.

Figure 1. Units of the Z_P (left) and A_P (right) crystal-like structures

The polynomials are calculated on a cubic lattice of dimension (k,k,k), at $R_{max}[8]$; following similar considerations and analyzing the calculations made by our original Nano Studio [16] software, we derived the formulas, listed in Table2, and provided examples for some k-values, as well.

Figure 2. The Z_P (left) and A_P (right) crystal-like structures

Table 1. Topological data for the units of Z_P and A_P structures

Octahedral structure	Vertices	Edges	Faces f_8	Open Faces	Omega Polynomial $R_{max}[8]$	CI
Z_P	120	168	12	6	$48X^1+36X^2+12X^4$	27840
A_P	144	192	12	6	$12X^2+24X^4+12X^6$	36000

In the Z_P and A_P network structures, the term at exponent 8 represent the number of edge strips of length 8; these strips cross only f_8 when link 4 Z_P units, and cross faces f_8 and f_6 when link 4 A_P units respectively, so it is present starting with k=2. In case of Z_P net, the term at exponent 8 counts the large hollows, ordered as in zeolites, natural alumino-silicates, used as molecular sieves or in chemical catalysis.

Table 2. Omega polynomial in Z_P and A_P networks

	Formulas for Z_P network	
	$\Omega(X,k,R_{\max}[8]) = 48k^2X^1 + 12k(4k^2-2k+1)X^2 + 3k(5k^2+3k-4)X^4 + 3k(k-1)^2X^8$	
	$\Omega'(1) = 48k^2 + 2\cdot 12k(4k^2-2k+1) + 4\cdot 3k(5K^2+3k-4) + 8\cdot 3k(k-1)^2 = 12k^2(15k-1)$	
	$\Omega''(1) = 12k(37k^2-23k+4)$	
	$CI(k) = 48k(675k^5-90k^4+3k^3-13k^2+6k-1)$	
	Formulas for A_P network	
	$\Omega(X,k,R_{\max}[8]) = 12kX^2 + 12k(k+1)X^4 + 3k(k-1)^2X^8 + 12k^2X^{5k+1} + 24k\sum_{i=2}^{k} X^{4(2i-1)}$	
	$\Omega'(1) = 12k^2(15k+1)$	
	$\Omega''(1) = 4k(203k^3+33k^2-80k+12)$	
	$CI(k) = 4k(8100k^5+1080k^4-167k^3-78k^2+77k-12)$	
k	Omega polynomial: examples	*CI*
	$R_{max}[8]$, Z_P network	
1	$48X+36X^2+12X^4$	27840
2	$192X+312X^2+132X^4+6X^8$	1933728
3	$432X+1116X^2+450X^4+36X^8$	22567104
4	$768X+2736X^2+1056X^4+108X^8$	128288064
5	$1200X+5460X^2+2040X^4+240X^8$	492768960
6	$1728X+9576X^2+3492X^4+450X^8$	1478124000
	$R_{max}[8]$ A_P network	

Table 2-continuation

1	$12X^2+24X^4+12X^6$	36000
2	$24X^2+72X^4+6X^8+48X^{11}+48X^{12}$	2199792
3	$36X^2+144X^4+36X^8+72X^{12}+108X^{16}+72X^{20}$	24609456
4	$48X^2+240X^4+108X^8+96X^{12}+96X^{20}+192X^{21}+96X^{28}$	136947840
5	$60X^2+360X^4+240X^8+120X^{12}+120X^{20}+300X^{26}+120X^{28}+120X^{36}$	519300960
6	$72X^2+504X^4+450X^8+144X^{12}+144X^{20}+144X^{28}+432X^{31}+144X^{36}+144X^{44}$	1544324400
7	$84X^2+672X^4+756X^8+168X^{12}+168X^{20}+168X^{28}+756X^{36}+168X^{44}+168X^{52}$	3882737712

Formulas for the number of atoms in the two networks are given in Table 3.

Table 3. Number of atoms $v = |V(G)|$

Z_P network structures $v_k = 120 \cdot k^3$			A_P network structures $v_k = 144 \cdot k^3 - 24 \cdot k^2(k-1)$			
k	1	2	3	4	5	6
v for Z_P	120	960	3240	7680	15000	25920
v for A_P	144	1056	3456	8064	15600	26784

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