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OMEGA AND SADHANA POLYNOMIALS IN P-TYPE SURFACE NETWORKS

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ABSTRACT. Design of a hypothetical carbon crystal lattice, embedded in the P-type surface, was performed by identifying two opposite open faces of a unit, of octahedral symmetry, by the aid of Nano Studio software. The topology of the net and its co-net, thus obtained, was characterized by Omega and Sadhana counting polynomials.

Keywords: *Omega polynomial, Sadhana polynomial, P-type surface networks*

INTRODUCTION

Among the carbon allotropes, discovered in the nano-era, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) were the most challenging [1,2]. Inorganic compounds including oxides, sulfides, selenides, borates, silicates, etc. of many metals, also found applications as nano-structured functional materials [3-12].

Zeolites are natural or synthetic alumino-silicates with an open three-dimensional crystal structure. Zeolites are micro-porous solids known as "molecular sieves." The term molecular sieve refers to the property of these materials to selectively sort molecules, based primarily on a size exclusion process. This is due to a regular structure of pores, of molecular dimensions, forming channels [13-17].

The rigorous and often aesthetically appealing architecture of crystal networks attracted the interest of scientists in a broad area, from crystallographers, to chemists and mathematicians.

The present study deals with a hypothetical carbon crystal-like nanostructure, of which topology is described in terms of Omega and Sadhana counting polynomial.

NETWORK DESIGN

The hypothetical carbon crystal network herein discussed was built up by identifying two opposite open faces of a unit (Figure 1, left), of octahedral symmetry, by the aid of Nano Studio software [18], also enabling their embedding in the P-type surface [1,2], belonging to the space group P_n 3 *m*.

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As any net has its co-net, this was identified to the structure presented in Figure 1, right. Indeed, when constructing the two infinite networks (Figure 2), a perfect superposition (Figure 2, central) can be evidenced: in fact is one and the same infinite network, differences appearing only at the boundaries. Thus, the topological characterization will be done on cubic (k,k,k) domains, separately, for the net and its co-net (see below).

v=98; e=120; f_6=8; f_8=12 v=144; e=192; f_6=20; f_8=24

Figure 1. Units of the net (left) and co-net (right)

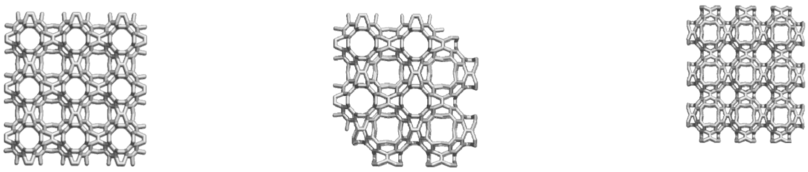

Figure 2. The net (3,3,3- left), superimposed net&co-net (2,2,2-central) and co-net (3,3,3- right) in a cubic (k,k,k) domain.

COUNTING POLYNOMIALS

A counting polynomial [19] is a representation of a graph *G*(*V*,*E*), with the exponent *k* showing the extent of partitions *p*(*G*), $\cup p(G) = P(G)$ of a graph property *P*(*G*) while the coefficient $p(k)$ are related to the number of partitions of extent *k*.

$$P(x) = \sum\nolimits_k p(k) \cdot x^k \quad (1)$$

Let *G* be a connected graph, with the vertex set *V*(*G*) and edge set *E*(*G*). Two edges *e*=(*u*,*v*) and *f*=(*x*,y) of *G* are called *codistant* (briefly: *e co f*) if the notation can be selected such that [20]:

$$d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \quad (2)$$

where *d* is the usual shortest-path distance function. The above relation *co* is reflexive (*e co e*) and symmetric (*e co f*) for any edge *e* of *G* but in general is not transitive.

A graph is called a *co-graph* if the relation *co* is also transitive and thus an equivalence relation.

Let $C(e) := \{f \in E(G);\ f\ co\ e\}$ be the set of edges in *G* that are codistant to $e \in E(G)$. The set *C*(*e*) can be obtained by an orthogonal edge-cutting procedure: take a straight line segment, orthogonal to the edge *e*, and intersect it and all other edges (of a polygonal plane graph) parallel to *e*. The set of these intersections is called an *orthogonal cut* (*oc* for short) of *G*, with respect to *e*.

If *G* is a *co-graph* then its orthogonal cuts $C_1, C_2, ..., C_k$ form a partition of *E*(*G*): $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \emptyset, i \neq j$.

A subgraph *H*⊆*G* is called *isometric*, if $d_H(u,v) = d_G(u,v)$, for any $(u,v) \in H$; it is *convex* if any shortest path in *G* between vertices of *H* belongs to *H*. The relation *co* is related to ~ (Djoković [21]) and Θ (Winkler [22]) relations [23,24].

Two 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*. Then *e co f* holds by the assumption that faces are isometric. The relation *co* is defined in the whole graph while *op* is defined only in faces/rings. Note that John *et al*. [20] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI*.

Relation *op* will partition the edges set of *G* into *opposite* edge *strips ops*, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) In a plane graph, the inner dual of an *ops* is a path, an open or a closed one (however, in 3D networks, the ring/face interchanging will provide *ops* which are no more paths); (iv) The *ops* is taken as maximum possible, irrespective of the starting edge. The choice about the maximum size of face/ring, and the face/ring mode counting, will decide the length of the strip.

Also note that *ops* are *qoc* (quasi orthogonal cuts), meaning the transitivity relation is, in general, not obeyed.

The Omega polynomial [25-27] $\Omega(x)$ is defined on the ground of opposite edge strips *ops* $S_1, S_2, ..., S_k$ in the graph. Denoting by *m*, the number of *ops* of cardinality/length *s*=|*S*|, then we can write

$$\Omega(x) = \sum_s m \cdot x^s \tag{3}$$

On *ops*, another polynomial, called Sadhana *Sd*(*x*) is defined [28,29]:

$$Sd(x) = \sum_s m \cdot x^{|E(G)|-s} \tag{4}$$

The first derivative (in *x*=1) can be taken as a graph invariant or a topological index (e.g., *Sd'*(1) is the Sadhana index, defined by Khadikar *et al*. [30]):

$$\Omega'(1) = \sum_s m \cdot s = |E(G)| \tag{5}$$

$$Sd'(1) = \sum_s m \cdot (|E(G)| - s) \tag{6}$$

An index, called Cluj-Ilmenau [20], *CI*(*G*), was defined on $\Omega(x)$:

$$CI(G) = \left\{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\right\} \tag{7}$$

In tree graphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent *s*=1.

POLYNOMIALS IN THE P-TYPE SURFACE NETWORKS

Omega and Sadhana polynomials are herein calculated at $R_{max}[6]$. Formulas for the two infinite networks are listed in Tables 1 and 2, with examples at the bottom of these tables.

In the discussed network, one can see that the coefficient $a(X^1)$ gives the number of octagons, by counting the edges not enumerated in the even faces. Next, $a(X^2)/3$ provides the number of hexagons while $a(X^4)/4$ counts the number of tubular necks (each bearing four anthracene units) joining the nodes of the net. In the co-net, the most informative is $a(X^4)/12$, giving the total number of the nodes while $(a(X^4)/12)^{1/3}=k$, the co-net parameter.

Table 1. Omega and Sadhana polynomials in the net

Formulas

$$\Omega(X,R_{\max}[6]) = k^2(72+12(k-1))X + 24k^3X^2 + 12k^2(k-1)X^4$$
$$= 12k^2(k+5)X + 24k^3X^2 + 12k^2(k-1)X^4$$
$$\Omega'(1) = 12k^2(9k+1)\,;\ \Omega''(1) = 48k^2(4k-3)$$
$$CI(G) = 12k^2(972k^4 + 216k^3 + 12k^2 - 25k + 11)$$
$$Sd(X,R_{\max}[6]) = k^2(72+12(k-1))X^{e-1} + 24k^3X^{e-2} + 12k^2(k-1)X^{e-4}$$
$$= 12k^2(k+5)X^{12k^2(9k+1)-1} + 24k^3X^{12k^2(9k+1)-2} + 12k^2(k-1)X^{12k^2(9k+1)-4}$$
$$Sd'(1) = 12k^2(9k+1)(48k^3+48k^2-1) = e(48k^3+48k^2-1)$$

k	Omega polynomial: examples	*e*(*G*)	*CI*(*G*)
1	$72X^1+24X^2$	120	14232
2	$336X^1+192X^2+48X^4$	912	829872
3	$864X^1+648X^2+216X^4$	3024	9137664
4	$1728X^1+1536X^2+576X^4$	7104	50449728

	Sadhana polynomial: examples	*Sd'*(1)
1	$72X^{119}+24X^{118}$	11400
2	$336X^{911}+192X^{910}+48X^{908}$	524400
3	$864X^{3023}+648X^{3022}+216X^{3020}$	5222448
4	$1728X^{7103}+1536X^{7102}+576X^{7100}$	27272256

The number of atoms in the cubic domains (k,k,k) of the two lattices can be calculated by the formulas given in Table 3; some examples are available.

Table 2. Omega and Sadhana polynomials in co-net

Formulas

$$\Omega(X,R_{\max}[6]) = k^2(96+12(k-1))X + 24k^3X^2 + 12k^3X^4$$
$$= 12k^2(k+7)X + 24k^3X^2 + 12k^3X^4$$
$$\Omega'(1) = 12k^2(9k+7)\,;\ \Omega''(1) = 192k^3$$
$$CI(G) = 12k^2(972k^4 + 1512k^3 + 588k^2 - 25k - 7)$$
$$Sd(X,R_{\max}[6]) = k^2(96+12(k-1))X^{e-1} + 24k^3X^{e-2} + 12k^3X^{e-4}$$
$$= 12k^2(k+7)X^{12k^2(9k+7)-1} + 24k^3X^{12k^2(9k+7)-2} + 12k^3X^{12k^2(9k+7)-4}$$
$$Sd'(1) = 12k^2(9k+7)(48k^3+84k^2-1) = e(48k^3+84k^2-1)$$

k	Omega polynomial: examples	*e*(*G*)	*CI*(*G*)
1	$96X^1+24X^2+12X^4$	192	36480
2	$432X^1+192X^2+96X^4$	1200	1437264
3	$1080X^1+648X^2+324X^4$	3672	13474728
4	$2112X^1+1536X^2+768X^4$	8256	68140992
	Sadhana polynomial: examples	*Sd'*(1)	
1	$96X^{191}+24X^{190}+12X^{188}$	25152	
2	$432X^{1199}+192X^{1198}+96X^{1196}$	862800	
3	$1080X^{3671}+648X^{3670}+324X^{3668}$	7531272	
4	$2112X^{8255}+1536X^{8254}+768X^{8252}$	36450240	

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

Net			co-Net	
$v_k = 24\cdot k^2(4+3(k-1)) = 24\cdot k^2(3k+1)$			$v_k = k^2(144+72(k-1)) = 72k^2(k+1)$	
k	1	2	3	4
v for net	96	672	2160	4992
v for co-net	144	864	2592	5760

CONCLUSIONS

In this paper, the design of a hypothetical carbon crystal lattice, embedded in the P-type surface, achieved by identifying two opposite open faces of a unit, of octahedral symmetry, by the aid of Nano Studio software, was presented. The topology of the net and its co-net, thus obtained, was characterized by Omega and Sadhana counting polynomials. The ops strips proved to be informative about the construction of these infinite carbon nanostructures.

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