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OMEGA POLYNOMIAL IN CUBE MED_MED_AII CRYSTAL-LIKE NETWORK

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ABSTRACT. Omega polynomial $\Omega(G,x)$ is defined on opposite edge strips *ops* which are quasi orthogonal cuts *qoc* in a graph *G*=*G*(*V*,*E*), with the meaning the transitivity relation is not necessarily obeyed. The first and second derivatives, in *x*=1, of Omega polynomial provide the Cluj-Ilmenau *CI* index. The polynomial provides an appropriate topological description of infinite crystal-like networks. Close formulas for the number of atoms, Omega polynomial and *CI* index are derived for a lattice designed by using operations on maps/networks.

Keywords: graphene, CorSu network, Omega polynomial.

INTRODUCTION

The rigorous architecture of crystal networks attracted the interest of scientists in a broad area, from crystallographers, to chemists and mathematicians [1-9]. The studies on classification were followed by studies on the usefulness, in chemical reactions or in physical devices, and more recently by applied mathematical studies, in an effort to give new, more appropriate characterization of the world of crystals. Thus, recent articles in crystallography promoted the idea of topological description and classification of crystal structures [1-6]. They present data on real but also hypothetical lattices designed by computer.

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya [10,11]: *Z*(*G*,*X*) counts independent edge sets while *H*(*G*,*X*) (initially called Wiener and later Hosoya [12,13]) refers to distances in the graph. Hosoya also proposed the sextet polynomial [14-17] for counting the resonant rings in a benzenoid molecule. More about polynomials the reader can find in ref [18].

Some distance-related properties can be expressed in polynomial form, with coefficients calculable from the layer and shell matrices [19-22].

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These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package [23]. The most important, in this respect, is the evaluation of the coefficients of Hosoya $H(G,X)$ polynomial from the layer of counting LC matrix.

The present work describes the design and topology (in terms of Omega polynomial) of a crystal-like lattice, derived from the cube by applying map/net operations. The article is organized as follows: The second section illustrates the construction of the lattice while the third section provides definitions of Omega polynomial and *CI* derived index, and derives close formulas for their calculation in this network. Conclusions and references will close the article.

DESIGN OF NETWORK

A map *M* is a combinatorial representation of a (closed) surface. Some geometrical-topological transformations, called operations on maps, are used to relate parents and transformed associate graphs of fullerenes (in general, nanostructures). In this respect, operations such as: dualization *Du*, medial *Me*, truncation *Tr*, polygonal P_r capping or Snub Sn, are well known [24-28]. Our original software CageVersatile (CVNET), enables such operations and proved to be a useful tool [29].

Medial *Med* is an operation which can be achieved by putting a new vertex in the middle of each original edge and next by joining two such vertices if the parent edges spanned an angle. The *Med* transform is always a 4-valent graph, as can be seen in Figure 1. The medial operation rotates parent *s*-gonal faces by π/s. Points in the medial map represent original edges.

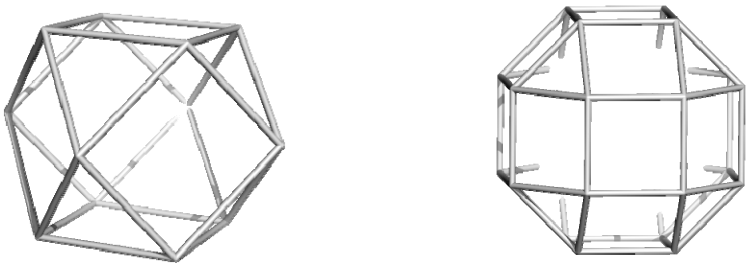

Figure 1. Transforms of the cube by Med (left) and Med(Med) (right) operations.

The objects in the above figure can be used as repeat units in building infinite networks. Figure 2 illustrates the crystal-like network built up by identifying the square faces of the *Med*(*Med*(*C*)) unit, in the three directions of coordinates. The same lattice can be obtained by performing the double medial *Med_Med_all* operation on all the hard rings which form the square 3D network [30].

Any lattice has its co-lattice, thus we focused on the *Med_Med_all* transform and assign it to be the main lattice (Figure 2, left column). Consequently, its co-lattice is that which includes the interstices and borders of the main net (Figure 2, right column).

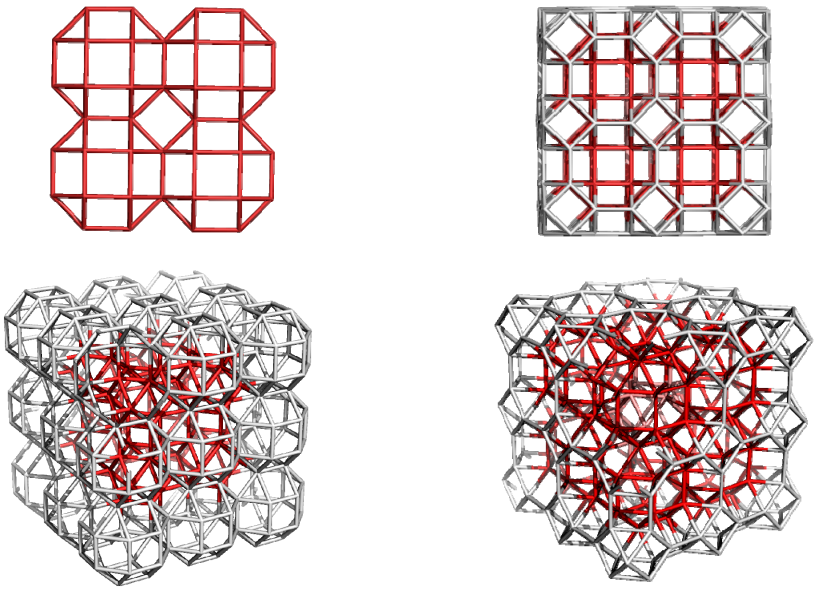

Figure 2. Lattice (333; *v*=432; left) and co-lattice (222; v=324; right) designed by Med(Med(C))_all operation, in plane projection (top) and 3D (bottom)

OMEGA POLYNOMIAL IN MED_MED_All CRYSTAL NETWORK

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

$$d(x,v) = d(x,u) + 1 = d(y,v) + 1 = d(y,u) \tag{1}$$

Let $C(e) \coloneqq \{f \in E(G);\ f\ co\ e\}$ denote the set of edges in *G*, codistant to the edge $e \in E(G)$. If relation *co* is an equivalence relation, then *G* is called a *co-graph*. The set *C*(*e*) is called an *orthogonal cut (oc* for short*)* of *G*, with respect to edge *e*. If *G* is a *co-graph* then its orthogonal cuts $C_1, C_2, ..., C_k$ form a partition of *E*(*G*): $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \varnothing, i \neq j$. Observe *co* is a Θ relation, (*Djoković-Winkler* [31-33]).

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* of length *s* and define the Omega polynomial as [34-36]:

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s \tag{2}$$

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

$$\Omega'(G,1) = \sum_s m(G,s) \cdot s = e = \left|E(G)\right| \tag{3}$$

On Omega polynomial, the Cluj-Ilmenau index [37], *CI*=*CI*(*G*), was defined:

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

Within this paper, the main results (see Table) refer to $R_{max}(4)$. If faces instead rings are considered, the polynomial complicates both in much more terms and their structural interpretation. Other rings tested were $R_{max}(6)$ and $R_{max}(8)$. In the first case, the inclusion of hexagons consisting the cubeoctahedral units of the co-lattice brings complications in that the number of structural units, clearly envisaged in case of $R_{max}(4)$ (see below), will be lowered in the expense of longer, but more obscure *ops*. In the last case, there is a single strip and the polynomial is written as: $\Omega(G,x) = 1 \times x^s$. Consequently, the index $CI(G) = s^2 - (s + s(s-1)) = s^2 - s^2 = 0$. In this case, the strip is a "Hamiltonian strip" and its length gives just the total number of edges in *G*.

Resuming to our case $R_{max}(4)$, the Omega polynomial has only three terms (see Table). The term at *s*=2 refers to the squares visited from directions where odd rings are limiting the strip length. The term at *s*=4 counts the cubes filling the space (i.e., the interstices) left free from lattice (cube double medial) and co-lattice (cube single medial) main objects, visited from two isolated directions. Finally, the term at maximum exponent counts the main domains of the 3D structure, visited from the coordinate axe directions. We consider that this description is the most informative with respect to the infinite triple periodic crystal-like network herein studied.

The data on the co-lattice are similar to those for the main lattice (in fact is the same structure), the differences reflecting the different borders (as topology and number of atoms) of the cube domain taken into account. Formulas for counting the *CI* values (examples are given) and the number of atoms lying in the two delimitations of the structure are also included in the table.

Table. Formulas for Omega polynomial in *MedMed_all* transform of the Cube (*k*,*k*,*k*) net.

	Formulas
1	$\Omega(x) = a_2 x^2 + a_4 x^4 + a_{\max} x^{e_{\max}}$
2	$\Omega(MedMed\_all(C), x) = 12k(2k-1)x^2 + 6k(k-1)^2 x^4 + 3kx^{4k(k+1)}$
	$\Omega'(MedMed\_all(C), 1) = 12k^2(3k+1)$
	$\Omega''(MedMed\_all(C), 1) = 12k(4k^4 + 8k^3 + 9k^2 - 9k + 4)$
	$CI(MedMed\_all(C)) = 48k(27k^5 + 17k^4 + k^3 - 3k^2 + 2k - 1)$
3	Examples: (2,2,2): $72x^2+12x^4+6x^{24}$; *CI* = 108960 (4,4,4): $336x^2+216x^4+12x^{80}$; *CI* = 6148416 (7,7,7): $1092x^2+1512x^4+21x^{224}$: *CI* = 166257840
4	$\Omega(co-net, x) = 12(k+1)^2 x^2 + 6k(k+1)^2 x^4 + 3kx^{4(k+1)^2}$
	$\Omega'(co-net, 1) = 12(3k+2)(k+1)^2$
	$\Omega''(co-net, 1) = 12(k+1)^2(4k^3 + 8k^2 + 9k + 2)$
	$CI(co-net) = 48(k+1)^2(27k^4 + 89k^3 + 109k^2 + 57k + 11)$
5	Examples: (2,2,2): $108x^2+108x^4+6x^{36}$; *CI* = 736560 (3,3,3): $192x^2+288x^4+9x^{64}$; *CI* = 4418304 (4,4,4): $300x^2+600x^4+12x^{100}$; *CI* = 17509200
6	$v(MedMed\_all(C)) = 12k^2(k+1)$
	$v(co-net) = 12(k+1)^3$

Data were calculated by the original software Nano-Studio [38], developed at TOPO Group Cluj, Romania.

CONCLUSIONS

Omega polynomial $\Omega(G,x)$, defined on opposite edge strips *ops* which are quasi orthogonal cuts *qoc* in a graph, was aimed to be a simple tool in description of the topology of polyhedral molecules and crystal networks. Indeed, the first and second derivatives, in *x*=1, of Omega polynomial provide the Cluj-Ilmenau *CI* index but also an appropriate topological description of the mentioned structures. Close formulas for the Omega polynomial, *CI* index and the number of atoms, are derived for a lattice designed by using operations on maps/networks.

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