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OMEGA POLYNOMIAL IN CRYSTAL-LIKE NETWORKS

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ABSTRACT. Omega polynomial $\Omega(G,x)$, defined by Diudea in *Carpath. J. Math*., 2006, *22*, 43-47, counts topologically parallel edges eventually forming a strip of adjacent faces/rings, in a graph *G*=*G*(*V*,*E*). The first and second derivatives, in *x*=1, of Omega polynomial enables the evaluation of the Cluj-Ilmenau *CI* index. Analytical close formulas for the calculation of this polynomial in two hypothetical crystal-like lattices are derived.

Keywords: *Omega polynomial, crystal networks*

INTRODUCTION

Design of polyhedral units, forming crystal-like lattices, is of interest in crystallography as many metallic oxides or more complex salts have found application in chemical catalysis. Various applied mathematical studies have been performed, in an effort to give new, more appropriate characterization of the world of crystals. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures.[1-8] They present data on real but also hypothetical lattices designed by computer.

The geometry and polyhedral tiling is function of the experimental conditions and can be designed by dedicated software programs. Such a program, called Cage Versatile CV-NET, was developed at TOPO Group Cluj, Romania. It works by net operations, as a theoretical support.

Three basic net/map operations Leapfrog *Le*, Quadrupling *Q* and Capra *Ca*, associated or not with the more simple Medial *Med* operation, are most often used to transform small polyhedral objects (basically, the Platonic solids) into more complex units. These transforms preserve the symmetry of the parent net.[9-11]

The article is devoted to the study of two new double periodic crystal-like network, by using a topological description in terms of the Omega counting polynomial.

OMEGA POLYNOMIAL

A counting polynomial 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*.

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

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[12]

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

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 $H \subseteq G$ 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[13]) and Θ (Winkler[14]) relations.[15]

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.

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[16,17] $\Omega(x)$ 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

$$\Omega(x) = \sum_s m \cdot x^s \quad (3)$$

The first derivative (in x=1) can be taken as a graph invariant or a topological index:

$$\Omega'(1) = \sum_{s} m \cdot s = \left|E(G)\right| \qquad (4)$$

An index, called Cluj-Ilmenau,[12] $CI(G)$, was defined on $\Omega(x)$:

$$CI(G) = \left\{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\right\} \qquad (5)$$

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

Main Results

The nets herein discussed were built up by combinations of map operations.

Net A. The unit of this net is an isomer of cuboctahedron (which is the medial of Cube and Octahedron). The net is constructed by identifying some squares so that the net appears as "translated" on the Z-axis, each time one row (Figure 1)

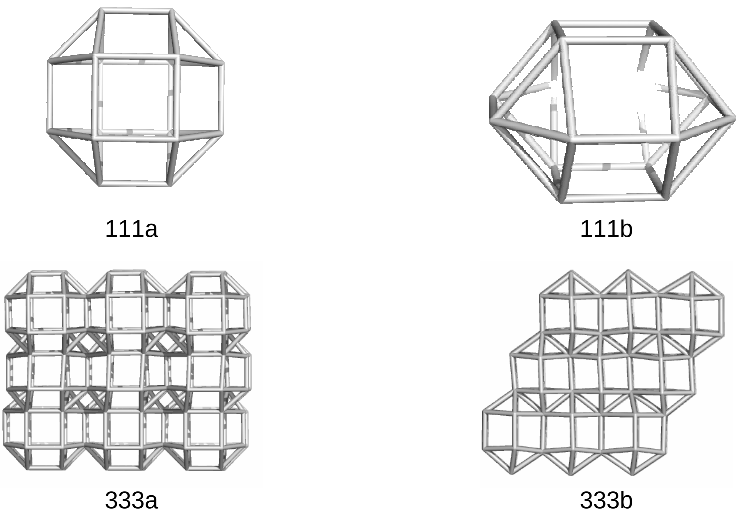

Figure 1. Net A; unit 111 (top) and 333 (bottom)

The computed data for the Omega polynomial of this net were rationalized as in the formulas presented below and Table 1.

$$a = 1 \quad \Rightarrow \quad \Omega(G,x) = 4x^1 + 8x^2 + 2x^6$$

$$\Omega(G,x) = 4a(2a-1)x^1 + (2a^3 + 7a^2 + 3a - 4)\,x^2 + ax^{2a(a+2)} + ax^{3a(a+1)} + (a-1)x^{4(a-1)(3a+2)} \qquad (6)$$

$$|E(G)| = \Omega'(G,1) = 21a^3 + 13a^2 - 2a \qquad (7)$$

$$CI\ (G) = 441a^6 + 389a^5 + 291a^4 - 5a^3 - 272a^2 - 8a + 80 \qquad (8)$$

Table 1. Omega polynomial and CI index of the Net A: Examples

a	Omega Polynomial	CI
1	$4x^1+8x^2+2x^6$	916
2	$24x^1+46x^2+2x^{16}+2x^{18}+1x^{32}$	44264
3	$60x^1+122x^2+3x^{30}+3x^{36}+2x^{88}$	437060
4	$112x^1+248x^2+4x^{48}+4x^{60}+3x^{168}$	2274544
5	$180x^1+436x^2+5x^{70}+5x^{90}+4x^{272}$	8280740
6	$264x^1+698x^2+6x^{96}+6x^{126}+5x^{400}$	23966456
7	$364x^1+1046x^2+7x^{126}+7x^{168}+6x^{552}$	59104804
8	$480x^1+1492x^2+8x^{160}+8x^{216}+7x^{728}$	129524240

Net B. The unit of this net is as for the case A but the edges sharing triangles were deleted. Moreover, the net is constructed not translated (Figure 2). Note, these networks and only double periodic, as can be seen from bottom rows of figures.

The computed data for the Omega polynomial of this net were rationalized as in the formulas presented below and Table 2.

$$a=1 \quad \Rightarrow \quad \Omega(G,x)=2x^6+2x^8$$

$$\Omega\,(G,x)=4\sum_{i=1}^{a-1}x^{(10+4(a-2))\;i}+2x^{2a(2a+1)}+1x^{16a^3} \tag{9}$$

$$|\,E(G)\,|=\Omega'\,(G,1)=24a^3+4a^2=4a^2(6a+1) \tag{10}$$

$$|\,V(G)\,|=8a^2(a+1) \tag{11}$$

$$\Omega''\,(G,1)=256a^6+\frac{64}{3}a^5+\frac{64}{3}a^4-8a^3+\frac{20}{3}a^2+\frac{8}{3}a \tag{12}$$

$$CI\ (G)=320a^6+\frac{512}{3}a^5-\frac{16}{3}a^4-16a^3+\frac{32}{3}a^2-\frac{8}{3}a= 8a\left(40a^5+\frac{64}{3}a^4-\frac{2}{3}a^3-2a^2-\frac{4}{3}a-\frac{1}{3}\right) \tag{13}$$

Table 2. Omega polynomial and CI index of the Net B: Examples

a	Omega Polynomial	CI
1	$2x^6+2x^8$	584
2	$4x^{10}+2x^{20}+1x^{128}$	25680
3	$4x^{14}+4x^{28}+2x^{42}+1x^{432}$	273784
4	$4x^{18}+4x^{36}+4x^{54}+2x^{72}+1x^{1024}$	1482912
5	$4x^{22}+4x^{44}+4x^{66}+4x^{88}+2x^{110}+1x^{2000}$	5527720
6	$4x^{26}+4x^{52}+4x^{78}+4x^{104}+4x^{130}+2x^{156}+1x^{3456}$	16246256
7	$4x^{30}+4x^{60}+4x^{90}+4x^{120}+4x^{150}+4x^{180}+2x^{210}+1x^{5488}$	40497240
8	$4x^{34}+4x^{68}+4x^{102}+4x^{136}+4x^{170}+4x^{204}+4x^{238}+2x^{272}+1x^{8192}$	89447744

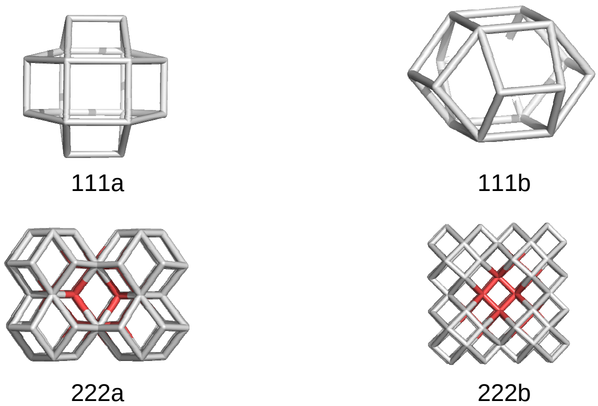

Figure 2. Net B; unit 111 (top) and 222 (bottom)

CONCLUSIONS

Omega polynomial can be used in topological description of polyhedral crystal networks.

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REFERENCES

1. L. Carlucci, G. Ciani and D. Proserpio, *Coord. Chem. Rev*., **2003**, *246*, 247.
2. L. Carlucci, G. Ciani and D. Proserpio, *Cryst. Eng. Comm*., **2003**, *5*, 269.
3. V.A. Blatov, L. Carlucci, G. Ciani and D. Proserpio, *Cryst. Eng. Comm*., **2004**, *6*, 377.
4. I. Baburin, V.A. Blatov, L. Carlucci, G. Ciani and D. Proserpio, *J. Solid State Chem*., 2005, 178, 2452.
5. O. Delgado-Friedrichs and M. O'Keeffe, *J. Solid State Chem*., **2005**, *178*, 2480.
6. V.A. Blatov, O. Delgado-Friedrichs, M. O'Keeffe, and D. Proserpio, *Acta Cryst*., **2007**, A63, 418.
7. M.V. Diudea and A. Ilić, *MATCH, Commun. Math. Comput. Chem.,* **2011**, *65*, 153.
8. A.E. Vizitiu and M.V. Diudea, *Studia Univ. Babes-Bolyai Chemia*, **2009**, *54* (1), 173.
9. M.V. Diudea and P.E. John, *Commun. Math. Comput. Chem.* (*MATCH*), **2001**, *44*, 103.

10. M.V. Diudea, P.E. John, A. Graovac, M. Primorac, and T. Pisanski, *Croat. Chem. Acta*, **2003**, *76*, 153.
11. M.V. Diudea, *J. Chem. Inf. Model.,* **2005**, *45,* 1002.
12. P.E. John, A.E. Vizitiu, S. Cigher, and M.V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 479.
13. D.Ž. Djoković, *J. Combin. Theory Ser. B*, **1973**, *14*, 263.
14. P.M. Winkler, *Discrete Appl. Math*.,**1984**, *8*, 209.
15. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008**, *59*, 217.
16. M.V. Diudea, *Carpath. J. Math*., **2006**, *22*, 43.
17. M.V. Diudea, *Nanomolecules and Nanostructures - Polynomials and Indices*, MCM, No. 10, Univ. Kragujevac, Serbia, **2010**.