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OMEGA POLYNOMIAL IN *AST*-CRYSTAL STRUCTURE

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ABSTRACT. Graphs associated to crystal networks can be designed by operations on maps. A repeating unit, made by such an operation, is used to build up the translational network. The topology of the *ast* crystal network is described here in terms of Omega counting polynomial. Close formulas for calculating the polynomial and the Cluj-Ilmenau index derived from it are given for two embeddings of this network.

Keywords: *Omega polynomial, CI index, ast-crystal lattice.*

INTRODUCTION

Several new carbon allotropes have been discovered and studied for applications in nano-technology, in the last twenty years, which can be assigned as the "Nano-era". The impact of the Nano-Science resulted in reduction of dimensions of electronic devices and increasing their performances, al a lower cost of energy and money. Among the carbon new structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) are the most studied [1,2]. The attention of scientists was also focused to inorganic compounds, a realm where almost any metal atom can form clusters, tubules or crystal networks, very ordered structures at the nano-level. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [3-8]. They present data on real, but also hypothetical lattices, designed by computer.

The present study deals with the design and topological description, in terms of Omega polynomial, of the ast/octadecasil crystal network, presented here in two embeddings.

OMEGA POLYNOMIAL

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 [9]:

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

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; 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: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \emptyset, i \neq j$. Klavžar [10] has shown that relation *co* is a theta Djoković-Winkler relation [11,12].

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*. The Omega polynomial [13-15] is defined as:

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

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

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

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

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

LATTICE BUILDING

The crystal network named ast/octadecasil/sqc3869 is a 2-nodal net that belongs to the group Fm-3m [16]. It has the point symbol for net $(4^3.6^3)4(6^6)$ and stoichio-metry (4-c)4(4-c). Figure 1, left presents the unit CQ_32, designed by the quadrupling Q-map operation performed on the cube C and having 32 atoms; in the right part of this figure the unit cell of the net is illustrated.

The net is constructed by identifying the hexagonal faces of the units and is denoted CQ6. Figure 2 presents two different embeddings of this crystal network, on which we performed the calculations.

Figure 1. Repeating unit of ast/sqc3869 network:
CQ_32; $(4.6^2)(6^3)$ (left) and CQ6_unit cell (right)

Figure 2. Two embeddings of ast network:
CQ6_DP-series ((3,3,3)_492, left) and CQ6_TP-series ((3,3,3)_484, right)

MAIN RESULTS

Within this paper, the Omega polynomial and derived Cluj-Ilmenau CI index refer to $F_{max}(6)$. Data were calculated by software program Nano Studio [17], developed at the TOPO Group Cluj. Formulas for the infinite networks of the two series were derived by numerical analysis, function of *k* that is the number of repeating units in a row of a cubic domain (*k*,*k*,*k*), and are listed in Tables 1 and 2; examples are given at the bottom of these tables. Formulas for the number of vertices and number of various rings are given in Tables 3 and 4, respectively.

Table 1. Omega polynomials in **CQ6_DP**

Formulas
$\Omega(G,x)=2\left[\sum_{i=1}^{k-1}x^{(2k-2)+(4k+4)i}+\sum_{i=1}^{k}x^{2i^2+6i}+2\sum_{i=1}^{k-1}x^{2k+(2k+2)i}+\sum_{i=1}^{\frac{2k-7-(-1)^k}{4}}x^{(2k^2+6k)+4(k-1-i)i}\right]$ $+(2k+2)\,x^{2k(k+2)}+k\,x^{4k(k+1)}+\frac{3+(-1)^k}{2}\,x^{(3k^2+4k+\frac{1-(-1)^k}{2})}+1\,x^{4k^2+6k-2}$
$CI(G)=400k^6+\frac{7756}{5}k^5+\frac{2648}{3}k^4-\frac{3532}{3}k^3+\frac{2384}{6}k^2-\frac{1408}{15}k+8$
$\lvert E(G)\rvert=20k^3+40k^2-14k+2$

k	Omega polynomial: examples	e(G)	CI(G)
2	$2x^8+4x^{10}+2x^{14}+6x^{16}+2x^{20}+2x^{24}+1x^{26}$	294	81352
3	$2x^8+4x^{14}+4x^{20}+4x^{22}+8x^{30}+4x^{36}+1x^{40}+3x^{48}+1x^{52}$	860	711552
4	$2x^8+4x^{18}+2x^{20}+2x^{26}+4x^{28}+2x^{36}+4x^{38}+2x^{46}+10x^{48}+2x^{56}+2x^{64}+2x^{66}+4x^{80}+1x^{86}$	1866	3383432
5	$2x^8+2x^{20}+4x^{22}+2x^{32}+4x^{34}+2x^{36}+4x^{46}+4x^{56}+4x^{58}+12x^{70}+4x^{80}+2x^{92}+1x^{96}+2x^{104}+5x^{120}+1x^{128}$	3432	11511472
6	$2x^8+2x^{20}+4x^{26}+2x^{36}+2x^{38}+4x^{40}+4x^{54}+2x^{56}+2x^{66}+4x^{68}+2x^{80}+4x^{82}+2x^{94}+14x^{96}+2x^{108}+2x^{122}+2x^{124}+2x^{132}+2x^{150}+6x^{168}+1x^{178}$	5678	31627912

Table 2. Omega polynomials in **CQ6_TP**

Formulas

$$\Omega(G,x)=2\left[\sum_{i=1}^{k}x^{i^2+4i+1}+3\sum_{i=1}^{k-1}x^{2k+(4k+2)i}+\sum_{i=1}^{\frac{2k-7-(-1)^k}{4}}x^{k^2+4k+1+2(k-1)i-2i^2}\right]$$

$$+\frac{3+(-1)^k}{2}\,x^{\frac{6k^2+12k+5-(-1)^k}{4}}+3k\,x^{2k(k+2)}+3\,x^{4k(k+1)}$$

$$CI(G)=400k^6+\frac{6969}{5}k^5+917k^4-650k^3-116k^2+\frac{86}{5}k+6$$

$$\left|E(G)\right|=20k^3+36k^2-6k-2$$

k	Omega polynomial: examples	e(G)	CI(G)
2	$2x^6+2x^{13}+6x^{14}+6x^{16}+3x^{24}$	290	79250
3	$2x^6+2x^{13}+6x^{20}+2x^{22}+1x^{24}+9x^{30}+6x^{34}+3x^{48}$	844	686034
4	$2x^6+2x^{13}+2x^{22}+6x^{26}+2x^{33}+2x^{37}+6x^{44}+12x^{48}+6x^{62}+3x^{80}$	1830	3257022
5	$2x^6+2x^{13}+2x^{22}+6x^{32}+2x^{33}+2x^{46}+2x^{52}+7x^{54}+15x^{70}+6x^{76}+6x^{98}+3x^{120}$	3368	11094692
6	$2x^6+2x^{13}+2x^{22}+2x^{33}+6x^{38}+2x^{46}+2x^{61}+6x^{64}+2x^{69}+2x^{73}+6x^{90}+18x^{96}+6x^{116}+6x^{142}+3x^{168}$	5578	30544554

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

$$|\mathrm{V(CQ6\_DP)}| = 10\mathrm{k}^3 + 26k^2 - 4k,$$
$$|\mathrm{V(CQ6\_TP)}| = 10\mathrm{k}^3 + 24k^2 - 2$$

k	CQ6_DP	CQ6_TP
2	176	174
3	492	484
4	1040	1022
5	1880	1848
6	3072	3022

Table 4. Number of rings

$$\mathrm{CQ6\_DP} \Rightarrow |\mathrm{R[4]}| = 6\mathrm{k}^3 + 20k^2 + 18k + 6, \quad |R[6]| = 10\mathrm{k}^3 + 36k^2 + 33k + 12$$
$$\mathrm{CQ6\_TP} \Rightarrow |\mathrm{R[4]}| = 6\mathrm{k}^3, \quad R[6]| = 10\mathrm{k}^3 + 3k^2 - 3k + 2$$

	CQ6_DP		CQ6_TP	
k	R[4]	R[6]	R[4]	R[6]
2	50	91	48	88
3	170	302	162	290
4	402	705	384	678
5	782	1360	750	1312
6	1346	2327	1296	2252

CONCLUSIONS

Crystal networks can be represented by graphs of which design can be performed by operations on maps. The repeating unit, made by Quadrupling operation applied on the cube, was used to build up the *ast*-network. The topology of this crystal network was described in terms of Omega counting polynomial. Close formulas for calculating the polynomial and the Cluj-Ilmenau index were given for two embeddings of the net.

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REFERENCES

1. M.V. Diudea, Ed., “Nanostructures, novel architecture”, NOVA, **2005**.
2. M.V. Diudea and Cs.L. Nagy, “Periodic Nanostructures”, Springer, **2007**.
3. L. Carlucci, G. Ciani and D. Proserpio, *Coord. Chem. Rev.*, **2003**, *246*, 247.
4. L. Carlucci, G. Ciani and D. Proserpio, *Cryst. Eng. Comm.*, **2003**, *5*, 269.
5. V.A. Blatov, L. Carlucci, G. Ciani and D. Proserpio, *Acta Cryst. Eng. Comm.*, **2004**, *6*, 377.
6. I.A. Baburin, V.A. Blatov, L. Carlucci, G. Ciani and D. Proserpio*, J. Solid State Chem.*, **2005**, *178*, 2452.
7. O. Delgado-Friedrichs and M. O’Keeffe, *J. Solid State Chem.*, **2005**, *178*, 2480.
8. V.A. Blatov, O. Delgado-Friedrichs, M. O’Keeffe, and D. Proserpio, *Acta Cryst. Eng. Comm.*, **2007**, A63, 418.
9. P.E. John, A.E., Vizitiu, S. Cigher, M.V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 479.
10. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008**, *59*, 217.
11. D.Ž. Djoković, *J. Combin. Theory Ser. B*, **1973**, *14*, 263.
12. P.M. Winkler, *Discrete Appl. Math.,***1984**, *8*, 209.
13. M.V. Diudea, *Carpath. J. Math.*, **2006**, *22*, 43.
14. M.V. Diudea, S. Cigher and P.E. John, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 237.
15. M.V. Diudea, S. Cigher, A.E. Vizitiu, M.S. Florescu and P.E. John, *J. Math. Chem.*, **2009**, *45*, 316.
16. http://www.topos.ssu.samara.ru/index.html
17. Cs.L. Nagy, M.V. Diudea, “Nano Studio software“, Babes-Bolyai Univ., **2009**.