Exact Formula Computing the Wiener Index on Rows of Unit Cells of the Diamond Cubic Grid Connected in a Row *

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Abstract.

The Wiener Index, the sum of distances between all pairs of vertices in a connected graph, is a graph invariant much studied in both mathematical and chemical literature.Topological graph indices are introduced as mathematical tools for molecule descriptions. Recently, they were computed not only for graphs representing molecules, but for other regular structured graphs including some 2 and 3 dimensional structures. The Carbon atoms in the diamond are arranged in a well defined structure. In this paper, the graph of this structure is analysed, especially, the connected part of a sequence of unit cells. The Wiener index, as the sum of the distances for every pair of atoms is computed, a closed formula depending only on the number of unit cells is proven.

Keywords: Wiener Index, Body-Centered Cubic Grid, Face-Centered Cubic, Diamond Grid, Shortest Paths, Non-Traditional Grids.

إيجاد صيغ رياضية لحساب مؤشر وينر لبنية الألماس المكعبة عن طريق حساب مجموع اقصر المسافات التي تربط الرؤوس داخل الرسم البياني الكيميائي

ملخص:

هدفت هذه الورقة العلمية إلى إيجاد وحساب مؤشر وينر Wiener Index في نظرية الرسم البياني الكيميائي Chemical Graph for Diamond Grid. ويعرف مؤشر وينر على أنه مؤشر طوبولوجي هام لتحديد بعض الصفات للعناصر. ومؤشر وينر للرسم البياني G يساوي مجموع المسافات بين جميع الرؤوس داخل الرسم البياني الكيميائي. في هذه الورقة تم إيجاد صيغ رياضية لحساب مؤشر وينر لـ Diamond Grid. حيث نقوم بحساب أقصر المسافات بين جميع الرؤوس في الشكل الذي تم اعتماده في هذه الورقة العلمية وإيجاد مجموع اقصر المسافات التي تربط هذه الرؤوس ومن ثم حساب مؤشر وينر لهذه الشبكة.

الكلمات المفتاحية: مؤشر وينر، مكعب مركزي الجسم، مكعب مركزي الوجه، أقصر المسافات، شبكات غير تقليدية.

Introduction

A molecular graph is a collection of vertices representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry [12].To identify molecular structures of chemical compound, the molecular graph invariants, called topological indices could be used too [2]. There has been extensive progress in the study of topological indices in the recent years with the result that formulas for the Wiener index W of many types of graphs have been determined. Wiener first introduced the Wiener index for approximating the boiling points of alkanes [12]. In computer science, Weiner index is considered one of the basic descriptors of fixed interconnection networks because it provides the average distance between any two nodes in the network. Chemical problems have greatly influenced the development of the theory of the Wiener index [8]. It has received considerable attention since its introduction in 1947 [21].Wiener index of various 2 and 3 dimensional structures has been considered in [4][8][12].

In digital geometry, spaces are digital, i.e. they consist of discrete sets of points. Neighborhood relation is essential between the points. Usually, digital spaces are described by vectors with integer coordinate values. The square and cubic grids are well-known and frequently used in applications, since they use a Cartesian coordinate system [16]. In digital spaces, and thus, in image processing path-based (also called digital) distances are useful [10]; distances based on neighborhood sequences are widely used [18]. Some recent directions of research deal with descriptions, coordinate systems, computing distances, relations and applications of non-traditional grids [17][15][18][20]. The most known non-traditional grids come from solid-state physics and crystallography.

In crystallography, there are various crystal systems and crystal lattices to describe various solid-state materials. One of the seven crystal lattice systems is the cubic, and it includes three well-known Bravais lattices: the simple cubic, the body-centered cubic (bcc) and the face-centered cubic (fcc) lattices. The diamond cubic grid, which is actually, the structure of the diamond, the silicon and also the germanium, are based on the face-centered cubic grid [5]. In the diamond grid, every carbon atom is connected to four neighbor atoms by covalent bonds, and these neighbors form the vertices of a tetrahedron, the simplest regular three-dimensional object. This structure makes diamond the hardest material in the world and this is one of the reasons why its structure has substantial importance both in theory and applications. Various coordinate systems and descriptions are developed to describe the diamond grid [6][5][16][17]. In addition, digital geometry with path-based distances has been considered [9][15][19][18]. Opposite to the cubic, fcc, bcc and honeycomb lattices, the diamond grid does not form a point-lattice, i.e., in the diamond grid there are grid vectors that do not map the grid into itself. There is a software implementation for a geometrical model of the morphology of various types' growth of crystals in cubic crystal system [1]. Diamond growth is still a hot topic of research [7][11][22].

In our previous work, the Wiener index for lines of unit cells of the body-centered cubic and face-centered cubic lattices were computed [13][14]. In this paper, the diamond grid is considered and the graph of this structure is analysed, especially, the connected part of a sequence of unit cells. The Wiener index, as the sum of the distances for every pair of atoms is computed, uses a proven closed formula that depends only on the number of unit cells.

Preliminaries

Wiener Index

A graph is a pair G = (V, E) of sets satisfying that the elements of E are 2-element subsets of V. To avoid notational ambiguities, we shall always assume that V and E are disjoint, i.e., $V \cap E = \phi$. The elements of V are the vertices (nodes, or points) of the graph G, the elements of E are its edges (connections or lines) [3]. Under distance dG(u,v) between vertices u,v$\in$V we mean the usual distance in graph G, i.e., the number of edges on a shortest path connecting these vertices in G. The distance of a vertex v $\in$V, dG(v), can be defined as the sum of distances between v and all other vertices of G [8]. Summing up this value for the whole graph, the sum of distances is obtained(1).

In [21], Wiener introduced the notion of, as he called it, the path number of a graph. Actually, it was the sum of distances between any two carbon atoms in the molecules in terms of carbon-carbon covalent bonds. Subsequently, the index named after Wiener, is generalised to any graph G as

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v) \qquad (1)$$

The sum of the distances for each pair of vertices of the graph G is computed; the sum runs over all ordered pairs of vertices, and dG(u,v) denote the length of a shortest path in G between vertices u and v.

2.2 The Diamond Cubic Grid

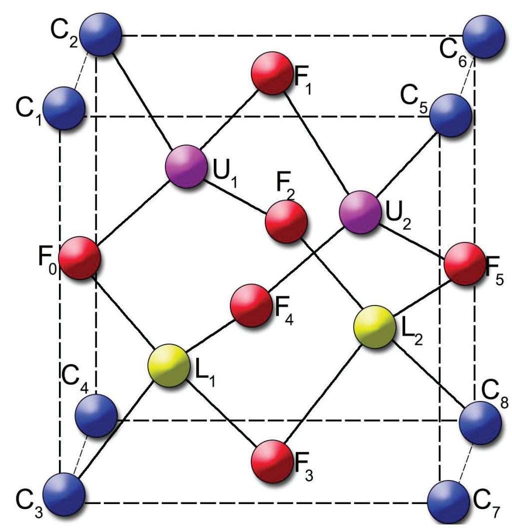

Figure 1:
A diamond unit cell

The diamond cubic grid is the grid of carbon atoms in the diamond crystal. The diamond cubic crystal structure (shortly, the diamond grid) can be seen as two interpenetrating face-centered cubic lattices, displaced along the body diagonal of the cubic cell by a quarter length of the diagonal. The diamond grid is a repeating pattern of 8 atoms. Silicon and certain other materials adopt the same structure. In the following, we will give some formal details about the diamond grid. We use

(1) The value should be divided by 2 to ensure that he distance between each pair of nodes is counted only once.

unit cells as it can be observed in Figure 1. We repeat the structure by putting the unit cells next to each other, so they share the carbon atoms on their face, e.g., C5 and F5.

Basic Results and Notations

We start this section by some easy computations respecting graphs formed by unit cells arranged in a row.

Lemma 1. Let n be the number of diamond unit cells connected in a row, the number of all points/vertices |V all| (cube points, intermediate points (upper and lower) and face center points) in this graph is given by

$$\left|V_{all}\right| = (13n + 5). \tag{2}$$

However, the number of connected points is

$$\left|V'_{all}\right| = (13n + 1). \tag{3}$$

The number of cube points |Vc| for n diamond unit cells connected in a row is calculated using the formula

$$\left|V_{C}\right| = (4n + 4). \tag{4}$$

Notice that in the end of the rows there are unit cells with two of their corners (e.g., C1 and C4) not connected to the row. They become connected only by adding another unit cell. Thus, the number of cube points that are connected to the remaining part of the grid is

$$\left|V'_{C}\right| = 4n. \tag{5}$$

The number of face center points $\left|V_f\right|$ for n diamond connected in a row is given by the following formula

$$\left|V_{f}\right| = (5n + 1). \tag{6}$$

Further, the number of intermediate (upper and lower) points $\left|V_{u,l}\right|$ for n diamond connected in a row is given by the following formula

$$\left|V_{u,l}\right| = 4n. \tag{7}$$

In our research, we will use the following names, labels and terminology for vertices/points (see Figure 2):

- ♦ The cube points are those that are located at the corners of the unit cells, e.g, C1, C2… C4n+4 (including the ones that are not connected to the grid, shown by empty circles in Figure 2; however in the computation they are dismissed.)
- ♦ Face center points are those that are located at the center of a face of a unit cell, for example,F0, F1, F2.We differentiate side center points and shared center points as follows:
- - Shared center points are the face center points that are on the centerline of the row of the unit cells, e.g., F0, F5, F10.
- - By side centers, we mean all other face centers: they are not shared between two neighbor unit cells in the row, the row length is not important here.
- ♦ Intermediate points: the points that do not belong to the face centered cubic grid described earlier. We differentiate upper and lower intermediate points:
- - Upper intermediate points are intermediate points above the midlevel of the row of the unit cells, e.g, U1, U2,...,U2n.
- - Lower intermediate points are under the midlevel of the unit cells, e.g. L1, L2, …, L2n.

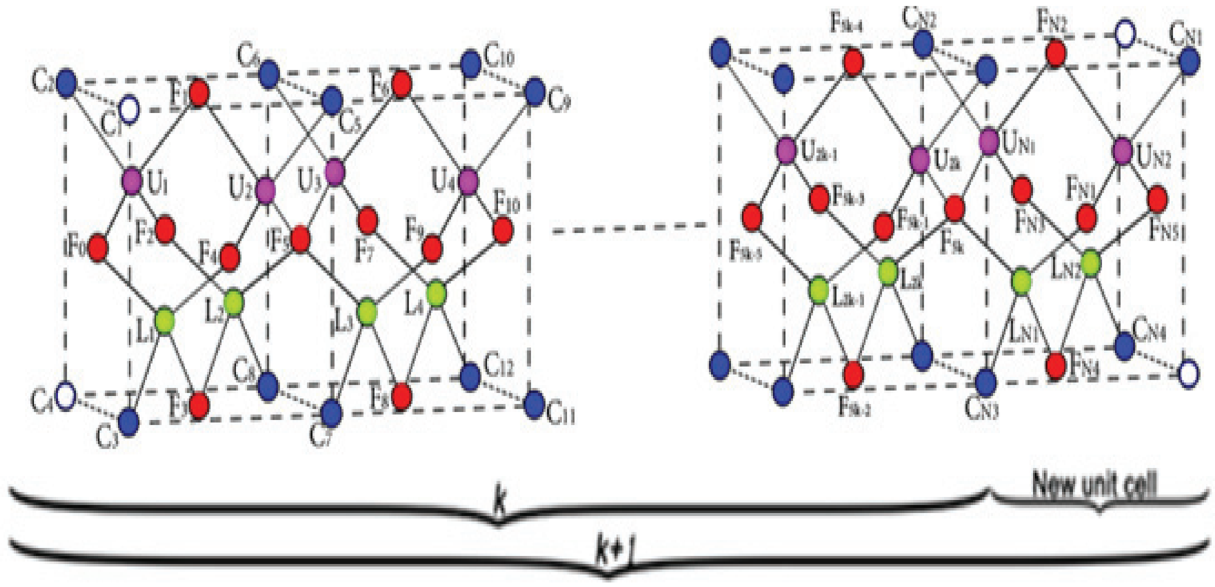

Figure 2: k diamond unit cells are connected in a row with a new unit cell attached to the end of the row.

Detailed Computation

Sum of distances between (side and shared) face center points

Lemma 2. Let k diamond unit cells be connected in a row. A new unit cell is connected to the end of the row to form a graph that represents k+1 unit cells in a row. Then the sum of all distances between the pairs of new face center points (shared and side center points) and between new face center points and old center points (shared and side center points) is

$$50k^2 + 70k + 36 \quad (8)$$

Proof:

In our proof, we will calculate the sum of total distance as follows:

- First of all, and according to Figure 2, the sum of total distance between the pairs built up from the new face center points (shared and side center points) is 24.
- The distance between first shared center i.e.F0 and new face center points is

$$4(5k+3) = 20k + 12$$

It is 32 when k=1, 52 when k= 2, etc...

Next, we will calculate the distance between new face center points with old face center points:

The sum of total distance between new face center points and all old center points is

$$100 + 200 + 300 + 400 + \cdots + 100k = 100(1+2+3+\cdots+k) = \frac{100k(k+1)}{2} = 50k^2 + 50k$$

The final formula to calculate the sum of total distance between new face center points and between new face center points and old center points, when we add a new diamond unit cell to the k diamond unit cells connected in a row, is given by:

$$24 + 20k + 12 + 50k^2 + 50k = 50k^2 + 70k + 36$$

Lemma 3. Let n diamond unit cells be connected in a row. Then the sum of all distances between face center points (side and shared points) in this (segment of the) diamond grid graph is given by

$$\frac{50n^3 + 30n^2 + 28n}{3} \quad (9)$$

Proof: The proof goes by induction on the number of unit cells.

The base of the induction is the case n = 1. In this case, there is only 6 face centers (side and shared center points), and the sum of distances between these center points equals to 36 and the formula (9) holds.

Now, let us assume that the formula is satisfied if n = k.

Let us prove that it also holds for the value n = k + 1. Through Lemma 2, we know the sum of the distances obtained by the new face center points and old centers. Applying this, along with the induction hypothesis, we must prove that the left side equals to the right side, so we have:

$$\frac{50k^3+30k^2+28k}{3}+(50k^2+70k+36)=\frac{50(k+1)^3+30(k+1)^2+28(k+1)}{3}.$$

$$\frac{50k^3+30k^2+28k}{3}+\frac{(150k^2+210k+108)}{3}=\frac{50(k+1)^3+30(k+1)^2+28(k+1)}{3}$$

$$\frac{50k^3+180k^2+238k+108}{3}=\frac{50k^3+180k^2+238k+108}{3}.$$

Therefore, the left side equals the right side, and the proof of the induction is complete. By the induction, formula 9 is true for all (non-negative integer value of) n.

Sum of distances between (side and shared) face center points and cube points

Lemma 4. Let k diamond unit cells be connected in a row and let a new (k + 1)st diamond unit cell be connected to the end of this row (see Figure 2). Then the sum of the distances between

- new face center points and new cube points plus the sum of the distances between
- old face center points and new cube points plus the sum of the distances between
- the new face center points and old cube points

is

$$80k^2+136k+72 \qquad (10)$$

Proof:

In our proof, we have to calculate the sum of the total distance as follows.

♦ First of all, the sum of distances between the new points:

- The sum of total distances between cube pointsCN1,CN4 (in the k-th diamond unit cell) and the new face center points is 28.
- The sum between cube points CN2,CN3 and the new face center points is 32.

♦ Now, for the sum of old face centers and new cube points:

- The distance between F0 and new cube points is 4k + 2 to each of the points CN2,CN3 and it is 4k + 4 to each of CN1,CN4. Thus, it is
- 16k + 12.
- Next, we will calculate the distance between other old shared centers, i.e, F5,…, F5k, with the new cube points: to F5k it is 2 for each of the points CN2,CN3 and 4 for each of the other two new cube points. For shared face centers farther, these distances are growing by 4 with the growing distance of the unit cells. Thus, we have

$$12+28+44+\ldots+4(4k-1))=4(3+7+11+\ldots+(4k-1))=\frac{4k(3+4k-1)}{2}=8k^2+4k$$

- The sum of total distance between the four new cube points and the old side face center points is

$$(8\cdot 6+8\cdot 10+8\cdot 14+\cdots+8\cdot 2(2k+1))+(8\cdot 4+8\cdot 8+8\cdot 12+\cdots+32k)=32k^2+48k$$

Now, let us continue with this sum:

- The sum of distances between C2,C3 and the five new face center points: for the new side face centers is 4k + 2, for each of these 8 distances; and 4k + 4 for the new shared center FN5 for each given cube points, thus it is $8(4k+2)+2(4k+4)=40k+24$.
- The sum of total distance between the last shared center, i.e.,FN5, and old cube points except C2,C3 is computed now (since we have already computed the distance from these two cube point in the previous point). It is: $2\cdot(6+8+10+\cdots+4k+4k+2)=8k^2+12k-8.$
- The sum of total distance between new side face centers (FN1, …, FN4) points and old cube points except C2 and C3 is $4\cdot(2\cdot 4+2\cdot 6+2\cdot 8+\cdots+2\cdot 4k)=32k^2+16k-16$

Finally, the final formula to calculate the total sum of the distances between old face center points and new cube points plus the sum of the distances between the new face center points and old cube points plus the sum of distances between new cube and center points is the sum of all previous distances, i.e.,

$$28+32+16k+12+32k^2+48k+40k+24+8k^2+12k-8+32k^2+16k-16+8k^2+4k=$$
$$80k^2+136k+72.$$

Lemma 5. Let n diamond unit cells be connected in a row. Then the sum of all distances between face center points and cube points in this diamond grid graph is given by

$$\frac{80n^3+84n^2+52n}{3}. \quad (11)$$

Proof: The proof goes by induction on n.

The base of the induction is the case n = 1. In this case, there is only 6 face centers, and only 4 of the 8 corners of the cube are connected. For each face center there are 2 cube points with distance 2 and 2 of them with distance 4. Thus, the sum of total distance is 6×(2×2+2×4) =72. Formula 11 also gives this value.

Let us assume that the formula satisfies if n = k. Let us prove that it also satisfies if n = k + 1. Through Lemma 4, we know the sum of the new distances obtained between face center points and cube points when the (k + 1)st unit cell is attached to the end of the line. Applying this with the induction hypothesis, we get the following statement that is needed to be proven.

We have to prove that the left side equals the right side:

$$\frac{80k^3+84k^2+52k}{3}+(80k^2+136k+72)=\frac{80(k+1)^3+84(k+1)^2+52(k+1)}{3}$$

$$\frac{80k^3+84k^2+52k}{3}+\frac{(240k^2+408k+216)}{3}=\frac{80(k+1)^3+84(k+1)^2+52(k+1)}{3}$$

$$\frac{80k^3+324k^2+460k+216}{3}=\frac{80k^3+324k^2+460k+216}{3}$$

So the left side equals the right side and the proof of the induction is complete.

Sum of distances between (side and shared) face center points and upper intermediate points

Lemma 6. Let k diamond unit cells be connected in a row and let a new diamond unit cell be connected to the end of this row. Then the sum of the distances between old face center points and new upper intermediate points, plus the sum of the distances between the old upper intermediate points and new face center points, and the sum of total distance between pairs of new face center points and upper intermediate is

$$40k^2+48k+24. \quad (12)$$

Proof:

- The sum of the total distance between new upper intermediate and new face center points is 20.
- Next, the sum of total distance between old upper intermediate points and new side face center points except FN5 is:

$$4(8+16+24+\cdots+8k)=32(1+2+3+\cdots+k)=\frac{32k(k+1)}{2}=16k^2+16k$$

Next, the sum of the total distance between new upper intermediate points and old side face center points is:

$$4(8+16+24+\cdots+8k)=32(1+2+3+\cdots+k)=\frac{32k(k+1)}{2}=16k^2+16k$$

- The sum of total distance between old shared center (i.e.F0, F5, F10…etc.) with new upper intermediate points is given by

$$(4+12+20+28+\cdots+4(2k+1))=4(1+3+5+7+\cdots+(2k+1))=4(k+1)^2=4k^2+8k+4$$

- The sum of total distance between new shared centerFN5 with old upper intermediate points:

$$12+20+28+\cdots+4(2k+1)=4(3+5+7+\cdots+(2k+1))=4k^2+8k$$

The final formula to calculate the sum of total distance between face center points (new and old) and between upper intermediate points (new and old) is given by:

$$20+16k^2+16k+16k^2+16k+4k^2+8k+4+4k^2+8k=40k^2+48k+24$$

Lemma 7. Let n diamond unit cells be connected in a row. Then the sum of all distances between face center points and upper intermediate points in this diamond grid graph is given by

$$\frac{40n^3+12n^2+20n}{3}. \quad (13)$$

Proof: The proof goes by induction on n.

The base of the induction is the case n = 1. In this case, there is only 6 centers, and 2 upper intermediate points, so the sum of total distance is 24, formula 13 also gives this value.

Let us assume that the formula satisfies if n = k. Let us prove that it also satisfies if n = k + 1. Through Lemma 6, we know the sum of the new distances obtained between old face center points and new upper intermediate points (of the (k + 1)st unit cell), between the centers of the new, (k + 1)st unit cell and upper intermediate points (of the previous k unit cells), and between the new face center and the new upper intermediate points (of the (k + 1)st unit cell). Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

In this proof, we have to prove that the left side equals the right side:

$$\frac{40k^3+12k^2+20k}{3}+(40k^2+48k+24)=\frac{40(k+1)^3+12(k+1)^2+20(k+1)}{3}$$

$$\frac{40k^3+12k^2+20k}{3}+\frac{(120k^2+144k+72)}{3}=\frac{40(k+1)^3+12(k+1)^2+20(k+1)}{3}$$

$$\frac{40k^3+132k^2+164k+72}{3}=\frac{40k^3+132k^2+164k+72}{3}$$

So the left side equals the right side, and the proof of the induction is complete.

Sum of distances between (side and shared) face center points and lower intermediate points

The same formula holds as in the case of face centers and upper intermediate points, because of symmetry.

Lemma 8. Let n diamond unit cells be connected in a row. Then the sum of all distances between face center points and lower intermediate points in this diamond grid graph is given by

$$\frac{40n^3+12n^2+20n}{3}. \tag{14}$$

Sum of distances between intermediate points

In this subsection, we count the distances between upper and lower intermediate points, between pairs of lower intermediate points and between pairs of upper intermediate points.

Lemma 9. Let k diamond unit cells be connected in a row and let a new diamond unit cell be connected to the end of this row. Then the sum of the distances between old (upper and lower) intermediate points and new(upper and lower) intermediate points plus the sum of the distances between new (upper and lower) intermediate points is

$$32k^2+32k+12. \tag{15}$$

Proof:

- ♦ The sum of total distance between new upper/lower intermediate points is 12, since there are 4 such points and the distance is 2 between any two of them.
- ♦ Next, the sum of total distance between new upper/lower intermediate points with old upper/lower intermediate points is counted:
- - The distance between new lower points and old upper points:

$$(2+4+\ldots+4k)+(4+6+\ldots+(4k+2))$$

$$=16\cdot(1+2+3+\cdots+k)=16\cdot\sum_{i=1}^{k} i=8k^2+8k.$$

- - Similarly, the distance between new lower points and old lower points:

$$16\cdot(1+2+3+\cdots+k)=16\cdot\sum_{i=1}^{k} i=8k^2+8k.$$

The distance between new upper points and old lower points is also:

$$16\cdot\sum_{i=1}^{k} i=8k^2+8k.$$

The final formula used to calculate the sum of total distance between upper/lower intermediate points when we add a new diamond unit cell to k diamond connected in a row is $12+4(8k^2+8k)=32k^2+32k+12$.

The proof is finished.

Lemma 10. Let n diamond unit cells be connected in a row. Then the sum of all distances between (upper/lower) intermediate points in this diamond grid graph is given by

$$\frac{32n^3+4n}{3} \quad (16)$$

Proof: The proof goes by induction on n.

The base of the induction is the case n = 1. In this case, there is only 2 upper intermediate and 2 lower intermediate points, and the sum of total distance is 12, also, formula 16 gives this value.

Let us assume that the formula satisfies if n = k. Let us prove its inheritance, i.e., that it also satisfies if n = k + 1. By Lemma 9, we know the sum of the new distances obtained between intermediate points adding the (k + 1)st unit cell is $32k^2+32k+12$. Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

In this proof, we have to show that the left hand side equals to the right hand side:

$$\frac{32k^3+4k}{3}+(32k^2+32k+12)=\frac{32(k+1)^3+4(k+1)}{3}$$

$$\frac{32k^3+4k}{3}+\frac{(96k^2+96k+36)}{3}=\frac{32(k+1)^3+4(k+1)}{3}$$

$$\frac{32k^3+96k^2+100k+36}{3}=\frac{32k^3+96k^2+100k+36}{3}$$

Thus, the proof of the induction is complete.

Sum of distances between cube points

Lemma 11. Let k diamond unit cells be connected in a row and let a new diamond unit cell be connected to the end of this row. Then the sum of the total distances between old cube points and new cube points plus the sum of the distances between the pairs of new cube points is

$$32k^2+64k+24 \quad (17)$$

Proof:

- First of all, the sum of total distance between the pairs of new cube points is 24, since there are 4 new cube points and the distance of any pair of them is 4.
- The sum of total distance between C2,C3 (see Figure 2) and the new cube points is:

$$2\cdot 2((2+4k)+(4+4k))=8(4k+3)=32k+24.$$

- Next, the sum of total distance between new cube points and old cube points (without C2 and C3) is calculated as follows. The distance of CN1 with the old cube points is 6, 8, …,4k+2. Similarly, for CN4 the distances are less by 2, respectively when they are measured from CN2 and CN3. Thus,

$$4(6+8+\cdots+(4k+2))+4(4+6+\cdots+(4k))=$$
$$=16k^2+24k-16+16k^2+8k-8=32k^2+32k-24$$

The final formula to calculate the sum of total distance between cube points when we add a new diamond unit cell to k diamond connected in a row is:

$$24+32k^2+32k-24+32k+24=32k^2+64k+24$$

Lemma 12. Let n diamond unit cells be connected in a row. Then the sum of all distances between cube points in this diamond grid graph is given by

$$\frac{32n^3+48n^2-8n}{3} \quad (18)$$

Proof: The proof goes by induction on n.

The base of the induction is the case n= 1. In this case, there are 8 corners cube, but actually only 4 cube points are connected to the other points. The distance between each pair is 4 and there are 6 pairs. Therefore, the sum is 24, formula 18 also gives this value.

Let us assume that the formula satisfies if n = k. Let us prove that it also satisfies if n = k + 1. By Lemma 11, we know the sum of the new distances obtained between old cube points and new cube points (of the (k + 1)st unit cell), between the new cube points of the new, (k + 1)st unit cell.

Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

In this proof, we have to prove that the left side equals the right side:

$$\frac{32k^3+48k^2-8k}{3}+(32k^2+64k+24)=\frac{32(k+1)^3+48(k+1)^2-8(k+1)}{3},$$

expanding both sides,

$$\frac{32k^3+48k^2-8k}{3}+\frac{96k^2+192k+72}{3}=\frac{32k^3+96k^2+96k+32+48k^2+96k+48-8k-8}{3}$$

$$\frac{32k^3+144k^2+184k+72}{3}=\frac{32k^3+144k^2+184k+72}{3}$$

So the left side equals the right side, and the proof of the induction is complete.

Sum of distances between upper intermediate points and cube points

Lemma 13. Let k diamond unit cells be connected in a row and let a new diamond unit cell be connected to the end of this row. Then the sum of the distances between old upper intermediate points and new cube points plus the sum of the distances between the new upper intermediate points and (old and new) cube points is

$$32k^2+48k+20. \tag{19}$$

Proof:

In our proof, we will calculate the sum of total distance as follows:

- ♦ First of all, and according to Figure 2, the sum of total distance between the pairs built up from the 2 new upper intermediate points and the 4 new cube points is: twice 1, and six times 3, resulting sum is 20.
- ♦ Next, the sum of total distance between old upper intermediate points and new cube points is, two times 3 plus two times 5 for U_{2k} and each distance is two more from U_{2k-1}, etc., resulting sum is 40 for the upper intermediate points of the k-th cell, etc. Summing up these values for the first k cells, we have

$$40+72+104+\dots+8(4k+1)=8(5+9+13+\dots+(4k+1))=16k^2+24k.$$

- ♦ The sum of total distance between new upper intermediate points and old cube points is computed as follows. The four cube points belonging to the k-th cell have distances 3,3 and 5,5 from UN1 and distances 5,5 and 7,7 from UN2, meaning 40 for this unit cell. Summing up the previously mentioned with the sums of other unit cells, we have,

$$40+\dots+8(4k+1)=16k^2+24k.$$

The final formula to calculate the sum of the new distance between cube points and upper intermediate points when we add a new diamond unit cell to k diamond connected in a row is:

$$32k^2+48k+20.$$

Lemma 14. Let n diamond unit cells be connected in a row. Then the sum of all distances between cube points and upper intermediate points in this diamond grid graph is given by

$$\frac{32n^3+24n^2+4n}{3}. \tag{20}$$

Proof: The proof goes by induction on n.

The base of the induction is the case n = 1. In this case, there is only 4 cube points and 2 upper intermediate points, and the sum of total distance between each pairs is 20 (similarly as in the part a) of the proof of Lemma 13) and also, formula 20 gives this value.

Let us assume that the formula satisfies if n = k. Let us prove that it also satisfies if n = k + 1. Through Lemma 13, we know the sum of the new distances when the (k + 1)st unit cell is added. Applying this, with the induction hypothesis gives the following statement that is needed to be proven:

$$\frac{32k^3+24k^2+4k}{3}+(32k^2+48k+20)=\frac{32(k+1)^3+24(k+1)^2+4(k+1)}{3},$$

multiplying both sides by 3, we get

$$32k^3+24k^2+4k+96k^2+144k+60=32k^3+96k^2+96k+32+24k^2+48k+24+4k+4$$

which is clearly, the same:

$$32k^3 + 120k^2 + 148k + 60 = 32k^3 + 120k^2 + 148k + 60 .$$

The proof is complete.

1.1. Sum of distances between upper intermediate points and cube points

Because of symmetry, the same formula and proof work as in the case of cube points and upper intermediate points. Stating the result formally.

Lemma 15. Let n diamond unit cells be connected in a row. Then the sum of the distances between cube points and lower intermediate points in this fragment of the diamond grid graph is given by

$$WI(n) = \frac{338n^3 + 234n^2 + 124n}{3} . \quad (21)$$

Main result

Now, based on Table 1 (in which, because of symmetry, only the upper triangular part is used), we state the main result. In table 1 we see that if we need for example to compute the sum of total distances between face centers vertices we have to use lemma 3 and equation 9 for that type of computation.

Table 1.

Sum of distances between various types of points are computed.

	F	C	U	L
F	Lemma3, equation 9	Lemma5, equation 11	Lemma7, equation 13	Lemma 8, equation 14
C		Lemma12, equation 18	Lemma14,equation 20	Lemma15, equation 21
U			Lemma10, equation 16	Lemma10, equation 16
L				Lemma10, equation 16

Theorem 1. Let n be the number of diamond unit cells that are connected in a row. Then the formula to find the Wiener-index for the graph of the unit cells is:

$$\frac{32n^3 + 24n^2 + 4n}{3} . \quad (22)$$

Proof: The formula is the sum of equations (9), (11), (13), (14), (16), (18), (20) and (21). Table 2 shows some of first elements of Wiener index for some small value of n. in table 2, we can see the total sum of the distances between center vertices (C-C), if we have just one diamond cube (i.e. n=1), which is 24. In addition, the total sum of distances between face and center vertices (F-C) if we have 2 diamond cube connected in a row (i.e. n=2) is 360.

Table 2.

Some values of the subsums and WI for a few diamond grid cells connected in a row.

n	1	2	3	4	5	6	7	8	9	10	Equation Number
C-C	24	144	424	928	1720	2864	4424	6464	9048	12240	18
F-C	72	360	1024	2224	4120	6872	10640	15584	21864	29640	11
F-F	36	192	568	1264	2380	4016	6272	9248	13044	17760	9
C-U/C-L	20	120	364	816	1540	2600	4060	5984	8436	11480	21/20
F-U	24	136	416	944	1800	3064	4816	7136	10104	13800	13
F-L	24	136	416	944	1800	3064	4816	7136	10104	13800	14
U-L+L-L+U-U	12	88	292	688	1340	2312	3668	5472	7788	10680	16
WI	232	1296	3868	8624	16240	27392	42756	63008	88824	120880	22

Conclusions and future work

In this section we deduct the following observations, the study of mathematical and chemical significance of Wiener index and its limitations is still an ongoing area of research. Topological descriptors and graph indices are widely used in chemistry. These indices can also be computed for some finite fragments of various crystals. In this paper, the structure of the diamond is analyzed from this point of view.

There are several ways to further this research, of which:

1. One can compute the longest distances between vertices (i.e. Detour Index) for this type of graph.
2. One can compute other topological indices, e.g., Szeged index for these graphs.
3. One can extend the results to two and three dimensional rectangles and blocks.

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