CRYSTALS THAT NATURE MIGHT MISS CREATING

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No one should have any objections against the claim that the *diamond crystal*, the most precious gem polished usually with the brilliant cut, casts a spell on us by its stunning beauty. The beauty would be more enhanced and its emotional appeal would be raised to rational one if we would explore the microscopic structure, say the periodic arrangement of carbon atoms, which is actually responsible for the dazzling glaze caused by the effective refraction and reflection of light. Figure 1, found in many text books of solid state physics, illustrates the arrangement of atoms together with the bonding (depicted by virtual lines) of atoms provoked by atomic force. A close look at this figure (or its readymade model preferably) reveals that, as a 1-dimensional diagram in space, the diamond crystal is formed by a wed of the same hexagonal rings[1] and has a "very big" symmetry, thereby being conspicuously distinguished from other crystals by its "microscopic beauty".

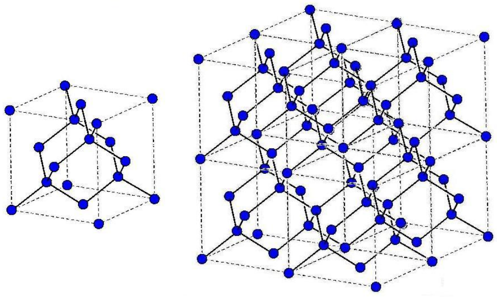

FIGURE 1. Carbon atoms in the diamond crystal

The purpose of this article is to provide a *new crystal structure*[2] having similar mathematical properties as the diamond crystal. This "crystal", which we prosaically call the K_4 *crystal* with some good reason, has valency 3, is constituted by a web of the same *decagonal rings*, and has a very big symmetry in the similar sense as the diamond crystal. A significant difference is in that the K_4 crystal has *chirality* while the diamond crystal does not. Since "*nature favors symmetry*" as is justified by plenty of examples, it makes sense to ask if this mathematical object exists in nature as a real crystal, or may be synthesized with carbon atoms (by allowing double bonds in an appropriate way).

As mentioned above, a crystal in the mathematical sense is a periodic figure of 1 dimension consisting of *vertices* (points representing positions of atoms) and *edges*

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[1] The *chair conformation* in the chemical term.

[2] This is different from the so-called diamond polytypes such as *lonsdaleite*, a rare stone of pure carbon discovered at Meteor Crater, Arizona, in 1967.

(lines representing bonding of atoms), by ignoring the physical characters of atoms and atomic forces which may be different one by one. In other words, a crystal is considered as an *infinite graph* realized periodically in space. This interpretation offers us two distinct notions of symmetry; one is *extrinsic symmetry*, the same as the classical notion bound up directly with beauty of the spatial object, which thus depends on realizations and is described in terms of congruent transformations of space; another is *intrinsic symmetry*, the notion irrelevant to realizations, solely explained in terms of automorphisms of graphs, and hence somehow denoting beauty enshrined inward. In general, intrinsic symmetry is "bigger than" extrinsic symmetry since congruent transformations leaving the crystal invariant induce automorphisms, but not vice versa.

A special feature of the diamond crystal is that intrinsic symmetry coincides with extrinsic symmetry. Furthermore the diamond crystal has a *strong isotropic property*[3] in the sense that any permutation of 4 edges with a common end point extends to a congruent transformation preserving the diamond crystal. Those observations naturally give rise to the question as to which crystal shares such noteworthy properties. The answer is, as is given in the last section, that the K_4 crystal (if leaving its mirror image out of account) is only one kinfolk of the diamond crystal in this sense (Theorem 3).

I would like to point out that the view taken up here is quite a bit different from that of classical crystallography, whose business is also the study of symmetry of crystals. Actually I came across the K_4 crystal when I was studying *discrete geometric analysis*, the field to deal with analysis on graphs by using geometric ideas cultivated in global analysis. In fact, geometric theory of random walks on crystal lattices, a topic developed recently in [1], [3], played a crucial role in its construction.

Symmetry of the diamond crystal

For a start, it is worthwhile to give a precise description of the diamond crystal. Consider a regular tetrahedron $C_1C_2C_3C_4$ together with its barycenter C. The atom at the position C is bound to atoms at C_i so that we shall draw lines joining C and C_i's. We then take the regular tetrahedron $CC_2'C_3'C_4'$ with the barycenter C_1 which is to be *point-symmetrical* with respect to the midpoint A of the segment CC_1 (see Figure 2). We do the same for other three vertices C_2, C_3, C_4, and then

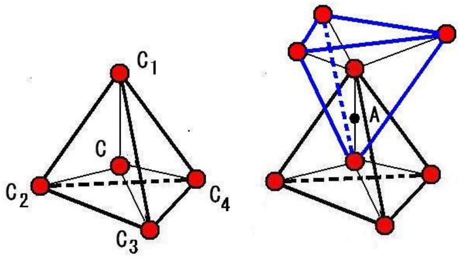

FIGURE 2. Regular tetrahedron

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[3] The term "isotropic" is used in a different context in crystallography.

continue this process. The 1-dimensional figure obtained in this manner turns out to be the diamond crystal.

There is another way to construct the diamond crystal, which allows us to see the periodicity explicitly. We again begin with the regular tetrahedron $C_1C_2C_3C_4$ and its barycenter C. Consider the parallelepiped P with the edges C_2C_1, C_2C_3, C_2C_4. Regarding P as a building block, we fill solidly space with parallelepipeds which are exactly alike (see Figure 3). Then the diamond crystal is formed by gathering up the copy, in each parallelepiped, of the above-mentioned figure inside P. From this construction, it follows that the additive group

$$L = \{n_1\overrightarrow{C_2C_1} + n_2\overrightarrow{C_2C_3} + n_3\overrightarrow{C_2C_4};\ n_1, n_2, n_3 \in \mathbb{Z}\}$$

leaves the diamond crystal invariant under translations $\mathbf{x} \mapsto \mathbf{x} + \sigma$ $(\sigma \in L)$. This is the periodicity that the diamond crystal possesses. In general, a crystal is characterized as a graph realized in space which is invariant under translations by a lattice group.

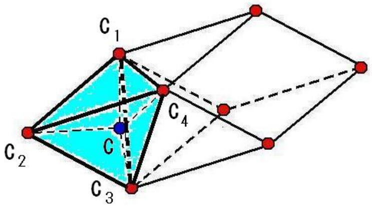

Figure 3. Parallelepiped P

The following says that the diamond crystal has not only big symmetry, but also has a *strong isotropic property*, which as well as Observation 2 below is easily checked in view of its construction.

Observation 1. *Let p and p' be vertices of the diamond crystal. Let ℓ_1, ℓ_2, ℓ_3, ℓ_4 be the edges with the end point p, and $\ell_1', \ell_2', \ell_3', \ell_4'$ be the edges with the end point p'. Then whatever order of edges may be, there exists a congruent transformation T leaving the diamond crystal invariant such that $T(p) = p'$ and $T(\ell_i) = \ell_i'$ $(i = 1, 2, 3, 4)$.*

A graph is, in general, an abstract object, having nothing to do with its realization and defined solely by an incidence relation between vertices and edges. When we think of the diamond crystal as an abstract graph, we call it the *diamond lattice*. More generally, a crystal as an abstract graph will be called a *crystal lattice*. Needless to say, there are many ways to realize a given crystal lattice periodically in space. For instance, Figure 4 gives a graphite-like realization of the diamond lattice.

A congruent transformation leaving a crystal invariant induces an automorphism of the corresponding crystal lattice in a natural manner. But every automorphism is not necessarily derived in this way. The following says that among all periodic realizations of the diamond lattice, the diamond crystal is a realization with the biggest extrinsic symmetry.

Observation 2. *Every automorphism of the diamond lattice extends to a congruent transformation leaving the diamond crystal invariant.*

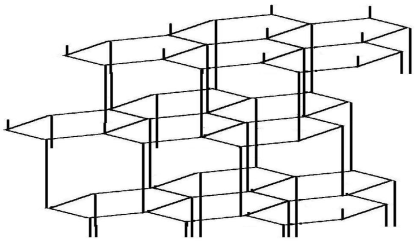

FIGURE 4. A realization of the diamond lattice of graphite type

Our concern is the existence of other crystals enjoying the properties stated in these observations.

Crystal lattices as abelian covering graphs

We need more mathematics to study crystal lattices. The discipline we step into is not classical crystallography, but an elementary part in algebraic topology applied to graphs, a realm apparently unrelated to crystals.

Recall that a crystal has periodicity with respect to the action of a lattice group in space by translations. By identifying vertices (resp. edges) when they are superposed by such translations, and by inducing the incidence relation of vertices and edges to identified objects, we obtain a finite graph[4] which we call the *fundamental finite graph.* For instance, the fundamental finite graph for the diamond crystal is the graph with 2 vertices joined by 4 multiple edges (Figure 5).

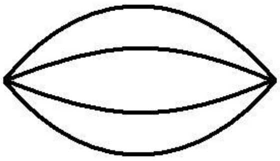

FIGURE 5. The fundamental finite graph for the diamond crystal

The canonical map from the crystal (lattice) onto the fundamental finite graph is a covering map, that is, a surjective map preserving the local incidence relations. Therefore what we have observed now amounts to the same as a crystal lattice is an *abelian covering graph* over a finite graph with covering transformation group ismorphic to $\mathbb{Z}^3$. Having this view in mind, we give an abstract definition of d-dimensional crystal lattices.

Definition *A graph is said to be a d-dimensional crystal lattice if it is an abelian covering graph over a finite graph*[5] *with a covering transformation group isomorphic to* $\mathbb{Z}^d$*, the free abelian group of rank d.*

Among all abelian covering graphs of a fixed finite graph X_0, there is a "maximal one", whose covering transformation group is $H_1(X_0, \mathbb{Z})$, the first homology group.

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[4] In other words, this is the quotient graph by the lattice group action.

[5] There are, of course, infinitely many choices of fundamental finite graphs for a fixed crystal lattice.

The diamond lattice is the maximal abelian covering graph over the graph in Figure 5. It is interesting to point out that the *hexagonal lattice* is the maximal abelian covering graph over the graph with 2 vertices joined by 3 multiple edges so that the hexagonal lattice is regarded as the 2-dimensional analogue of the diamond lattice.

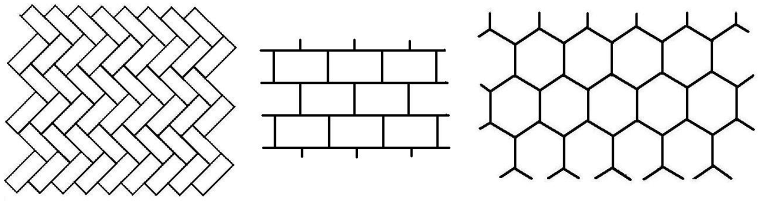

FIGURE 6. The hexagonal lattice and its various realizations

If we start from a crystal lattice X with a fundamental finite graph X_0 in the above sense, then a crystal corresponding to X should be understood as a *periodic realization* $\Phi : X \longrightarrow \mathbb{R}^d$. The periodicity of Φ is embodied by the equality $\Phi(\sigma x) = \Phi(x) + \rho(\sigma)$, where σ is a covering transformation, and ρ is an injective homomorphism of the covering transformation group into a lattice group in $\mathbb{R}^d$.

From its nature, a periodic realization is determined uniquely by the image of a finite part of the crystal lattice. To be exact, let E (resp. E_0) be the set of oriented edges in X (resp. X_0), and consider a system of vectors $\{\mathbf{v}(e)\}_{e \in E_0}$ defined by

$$\mathbf{v}(e) = \Phi\big(t(e)\big) - \Phi\big(o(e)\big) \quad (e \in E),$$

where $o(e)$ and $t(e)$ are the origin and terminus of e respectively. We should note that the function $\mathbf{v}$ on E is invariant under the action of the covering transformation group so that it is regarded as a function on E_0. It is easily observed that $\{\mathbf{v}(e)\}_{e \in E_0}$ determines the periodic realization Φ. In this sense, $\{\mathbf{v}(e)\}_{e \in E_0}$ is called a *building block*.

Energy and Standard realizations

Our mathematical experience suggests that symmetry has strong relevance to a certain *minimum principle*. Leonhard Euler, a pioneer of *calculus of variations*, said[6] "since the fabric of the Universe is most perfect and the work of a most wise creator, nothing at all takes place in the Universe in which some rule of maximum or minimum does not appear". We shall apply this "philosophy" to the problem to look for a periodic realization with biggest extrinsic symmetry[7].

We think of a crystal as a system of harmonic oscillators, that is, each edge represents a harmonic oscillator whose energy is the square of its length. We shall define the energy of a crystal "per a unit cell" in the following way[8].

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[6] The quotation in "Vector Calculus" by J. E. Marsden and A. J. Tromba.

[7] The macroscopic shape of a crystal is also characterized by a certain minimum principle (J. W. Gibbs (1878) and P. Curie (1885)).

[8] A real crystal (crystalline solid) is also physically regarded as a system of harmonic oscillators under an appropriate approximation of the equation of motion, but the shape of energy is much more complicated (see [5]).

Given a bounded domain D in $\mathbb{R}^d$, denote by $\mathcal{E}(D)$ the sum of the energy of harmonic oscillators whose end points are in D, and normalize it in such a way as

$$\mathcal{E}_0(D) = \frac{\mathcal{E}(D)}{\deg(D)^{1-2/d}\mathrm{vol}(D)^{2/d}},$$

where $\deg(D)$ is the sum of degree (valency) of vertices in D. Roughly $\mathcal{E}(D) \sim \mathrm{vol}(D)$ and $\deg(D) \sim \mathrm{vol}(D)$ as $D \uparrow \mathbb{R}^d$, so that $\mathcal{E}_0(D)$ is bounded from above. If the crystal is transformed by a homothetic transformation T, then, thanks to the term $\mathrm{vol}(D)^{2/d}$, the energy $\mathcal{E}_0(D)$ changes to $\mathcal{E}_0(T^{-1}D)$.

Take an increasing sequence of bounded domains $\{D_i\}_{i=1}^{\infty}$ with $\cup_{i=1}^{\infty} D_i = \mathbb{R}^d$ (for example, a family of concentric balls). The energy of the crystal (per a unit cell) is defined as the limit

$$E_{ner} = \lim_{i \to \infty} \mathcal{E}_0(D_i).$$

Indeed the limit exists under a mild condition on $\{D_i\}_{i=1}^{\infty}$, and E_{ner} does not depend on the choice of $\{D_i\}_{i=1}^{\infty}$. We write $E_{ner}(\Phi)$ for the energy when the crystal is given by a periodic realization Φ. It is easy to observe that $E_{ner}(T \circ \Phi) = E_{ner}(\Phi)$ for every homothetic transformation T.

For a fixed crystal lattice, there exists a unique periodic realization (up to homothetic transformations) which attains the minimum of E_{ner}. Such a realization is said to be the *standard realization*, and is characterized by two equalities

$$\sum_{e \in E_x} \mathbf{v}(e) = \mathbf{0},$$

$$\sum_{e \in E_0} \big(\mathbf{x} \cdot \mathbf{v}(e)\big)^2 = c\|\mathbf{x}\|^2 \quad (\mathbf{x} \in \mathbb{R}^d),$$

where E_x denotes the set of oriented edges whose origin is x.

The diamond crystal turns out to be the standard realization of the diamond lattice. One can also check that the honeycomb is the standard realizations of the hexagonal lattice. Thus it is not surprising that the standard realization yields a crystal with the biggest symmetry as the following theorem tells.

Theorem 1. *For the standard realization Φ, there exists a homomorphism $T : \mathrm{Aut}(X) \longrightarrow M(d)$ such that $\Phi(gx) = T(g)\Phi(x)$, where* $\mathrm{Aut}(X)$ *denotes the automorphism group and $M(d)$ is the group of congruent transformations of* $\mathbb{R}^d$.

The existence and uniqueness of standard realizations are proven along the following line. For the existence, we first fix a fundamental finite graph (in other words, fix a transformation group acting on the crystal lattice). We also fix the volume of a fundamental domain for the lattice group action in $\mathbb{R}^d$, and show that there exists a periodic realization Φ which minimizes $\sum_{e \in E_0} \|\mathbf{v}(e)\|^2$, a more manageable version of energy functional. This is easy indeed, but it is not obvious that this Φ (up to homothetic transformations) does not depend on the choice of a fundamental finite graph[9]. The independence of the choice in full generality is somehow derived from an asymptotic property of the simple random walk on X. At first sight, this might sound mysterious because of big conceptual discrepancy between "randomness" and "symmetry", or "chance" and "order" in our everyday

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[9] If we would know in advance that $\mathrm{Aut}(X)$ is isomorphic to a crystallographic group, then it is not difficult to prove this. As a matter of fact, however, $\mathrm{Aut}(X)$ is not always isomorphic to a crystallographic group.

language. However once we perceive that “laws of randomness” are solidly present in the world, it is no wonder that symmetry favored by the world is naturally connected with randomness, just like the relation between symmetry and minimum principles.

In general, a random walk on a graph X is a stochastic process on the set of vertices characterized by a transition probability, i.e., a function p on E satisfying $p(e) > 0$ and $\sum_{e\in E_x} p(e) = 1$. We think of $p(e)$ as the probability that a particle at $o(e)$ moves in a unit time to $t(e)$ along the edge e. If p is constant on E_x, i.e., $p(e) = \bigl(\deg\, o(e)\bigr)^{-1}$, the random walk is said to be *simple*.

The following theorem gives a direct relation between the standard realization and the simple random walk.

Theorem 2. ([1]) [10] *Let $p(n, x, y)$ be the n-step transition probability and let Φ be the periodic realization which minimizes $\sum_{e\in E_0} \|\mathbf{v}(e)\|^2$. There exists a positive constant C such that*

$$C\|\Phi(x) - \Phi(y)\|^2 = \lim_{n\to\infty} 2n\Bigl\{\frac{p(n,x,x)}{p(n,y,x)} + \frac{p(n,y,y)}{p(n,x,y)} - 2\Bigr\}. \tag{1}$$

This theorem is powerful enough in order to establish immediately what we have mentioned above, and eventually leads us to our claim that Φ actually minimizes E_{ner}. Crucial in the argument is the fact that the right hand side of (1) depends only on the graph structure and has nothing to do with realizations. The uniqueness and Theorem 1 are also consequences of this theorem.

Theorem 2 is a byproduct of the asymptotic expansion of $p(n, x, y)$ at $n = \infty$;

$$p(n,x,y)\bigl(\deg\, y\bigr)^{-1} \sim (4\pi n)^{-d/2} C(X)\bigl[1 + c_1(x,y)n^{-1} + c_2(x,y)n^{-2} + \cdots\bigr].$$

Having help from discrete geometric analysis, we may compute explicitly the coefficient $c_1(x, y)$ in geometric terms of graphs. Ignoring the exact shape of irrelevant terms, we find

$$c_1(x,y) = -\frac{C}{4}\|\Phi(x) - \Phi(y)\|^2 + g(x) + g(y) + c$$

with a certain function $g(x)$ and a constant c. Noting that the right hand side of (1) is equal to $c_1(x, x) + c_1(y, y) - 2c_1(x, y)$, we get Theorem 2.

As for the constant $C(X)$, we have the following relation to the energy.

$$E_{ner}(\Phi) \geq dC(X)^{-2/d},$$

where the equality holds[11] if and only if Φ is standard. The proof, available at present, of this remarkable inequality is not carried out by finding a direct link between two quantities, but is based upon a canonical expression of the standard realization, an analogue of *Albanese maps* in algebraic geometry ([1], [2], [3]).

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[10] To avoid unnecessary complication, we assume that X is non-bipartite so that $p(n, x, y) > 0$ for sufficiently large n, where a graph is said to be *bipartite* if one can paint vertices by two colors in such a way that any adjacent vertices have different colors. We need a minor modification for the bipartite case.

[11] This inequality is for non-bipartite crystal lattices. In bipartite case, the right hand side should be replaced by $d\Bigl(\dfrac{C(X)}{2}\Bigr)^{-2/d}$.

We conclude this section with the case of maximal abelian covering graphs. Let $P : C_1(X_0, \mathbb{R}) \longrightarrow H_1(X_0, \mathbb{R})(\subset C_1(X_0, \mathbb{R}))$ be the orthogonal projection with respect to the inner product on $C_1(X_0, \mathbb{R})$, the group of 1-chains on X_0, defined by

$$\langle e, e' \rangle = \begin{cases} 1 & (e = e') \\ -1 & (e = \overline{e'}) \qquad (e, e' \in E_0) \\ 0 & (\text{otherwise}). \end{cases} \tag{2}$$

Identify $H_1(X_0, \mathbb{R})$ with $\mathbb{R}^d$ ($d = \dim H_1(X_0, \mathbb{R})$) by choosing an orthonormal basis for the inner product on $H_1(X_0, \mathbb{R})$ induced from (2). Fixing a reference point $x_0 \in V$, and taking a path $c = (e_1, \cdots, e_n)$ in X with $o(e_1) = x_0, t(e_n) = x$, we put

$$\Phi(x) = P(\pi(e_1)) + \cdots + P(\pi(e_n)),$$

where π is the covering map. The map Φ, in which the reader may feel a fravor of Albanese maps, is well-defined and turns out to be the standard realization.

The $\mathbf{K_4}$ crystal

We mentioned that the diamond crystal have the strong isotropic property. This property leads us to the following general definition in terms of crystal lattices.

Definition *A crystal lattice X (or a general graph) of degree n is said to be strongly isotropic if, for any $x, y \in V$ and for any permutation σ of $\{1, 2, \cdots, n\}$, there exists $g \in \mathrm{Aut}(X)$ such that $gx = y$ and $ge_i = f_{\sigma(i)}$ where $E_x = \{e_1, \cdots, e_n\}$, $E_y = \{f_1, \cdots, f_n\}$.*

In veiw of Theorem 1, the standard realization of a crystal lattice with this property is strongly isotropic as a crystal.

We wish to list all crystal lattices[12] with the strong isotropic property in dimension two and three. We thus follow the Greek tradition in geometry that beautiful objects must be classified. Actually the classification of regular polyhedra[13] turns out to have a close connection with our goal

It is straightforward to check that the hexagonal lattice is a unique 2-dimensional crystal lattice with the strong isotropic property (look at the standard realization). In the 3-dimensional case, we have another crystal lattice with this property besides the diamond lattice. It is the maximal abelian covering graph over the complete graph K_4 with 4 vertices[14], which we call the K_4 *lattice* in plain words.

Since the graph K_4 has the strong isotropic property, so does its maximal abel cover. The K_4 *crystal* is then defined to be the standard realization of the K_4 lattice. The definition as such is quite simple. But its concrete construction is a bit involved, and put in practice by following the recipe at the end of the previous section. Consider three closed paths $c_1 = (e_2, f_1, \overline{e_3})$, $c_2 = (e_3, f_2, \overline{e_1})$, $c_3 = (e_1, f_3, \overline{e_2})$ in Figure 7. The cycles c_1, c_2, c_3 constitute a $\mathbb{Z}$-basis of $H_1(K_4, \mathbb{Z})$, and satisfy $\|c_1\|^2 = \|c_2\|^2 = \|c_3\|^2 = 3$, $\langle c_i, c_j \rangle = -1 \ \ (i \neq j)$ as vectors in $H_1(K_4, \mathbb{R}) = \mathbb{R}^3$ (note that, if $c_i = \overrightarrow{OP_i}$, then P_i's are three vertices of the regular tetrahedron with

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[12] We restrict ourselves to the class of crystal lattices whose standard realizations are injective on the set vertices.

[13] Legend has it that the origin is in their curiosity to the shapes of various crystals.

[14] In general, K_n stands for the complete graph with n vertices, that is, the graph such that any two vertices are joined by a single edge.

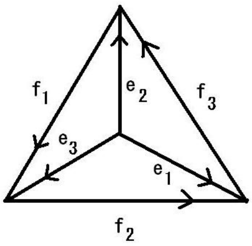

Figure 7. K_4

the barycenter O). Looking at the projections of 1-chains $e_1, e_2, e_3, f_1, f_2, f_3$ onto $H_1(K_4, \mathbb{R})$, and expressing them as linear combinations of c_1, c_2, c_3, we obtain

$$\begin{aligned}
&\mathbf{v}(e_1) = -\frac{1}{4}c_2 + \frac{1}{4}c_3, \quad \mathbf{v}(e_2) = \frac{1}{4}c_1 - \frac{1}{4}c_3, \quad \mathbf{v}(e_3) = -\frac{1}{4}c_1 + \frac{1}{4}c_2,\\
&\mathbf{v}(f_1) = \frac{1}{2}c_1 + \frac{1}{4}c_2 + \frac{1}{4}c_3, \quad \mathbf{v}(f_2) = \frac{1}{4}c_1 + \frac{1}{2}c_2 + \frac{1}{4}c_3,\\
&\mathbf{v}(f_3) = \frac{1}{4}c_1 + \frac{1}{4}c_2 + \frac{1}{2}c_3.
\end{aligned}$$

Since the vectors $\pm\mathbf{v}(e_1), \pm\mathbf{v}(e_2), \pm\mathbf{v}(e_3)$, $\pm\mathbf{v}(f_1), \pm\mathbf{v}(f_2), \pm\mathbf{v}(f_3)$ give a building block, we get a complete description of the K_4 crystal.

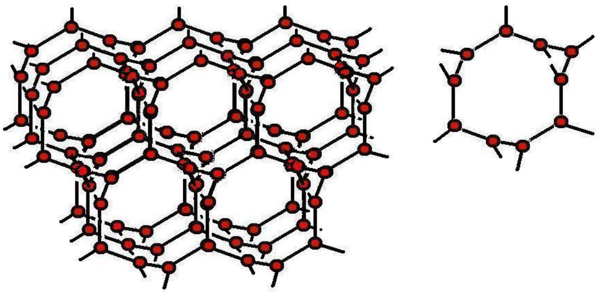

Figure 8. K_4 crystal

More useful to see how edges are joined mutually is the following observation. In the K_4 crystal, the terminuses p_1, p_2, p_3 of three edges with a common origin p form an equilateral triangle with the barycenter p; thus being contained in a plane, say α. If β is the plane containing the equilateral triangle for the origin p_3 (see Figure 9), then the dihedral angle θ between α and β satisfies $\cos\theta = 1/3$; that is, θ is the dihedral angle of the regular tetrahedron.

The K_4 crystal looks no less beautiful than the diamond crystal. Its artistic structure has intrigued me for sometime. The reader may agree on my sentiments if he would produce a model by himself by using a chemical kit[15]. An interesting feature observed in this model is that non-planar decagons all of which

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[15] As a matter of fact, there are no readymade models of the K_4 crystal so that one must put existing pieces in a kit together by oneself.

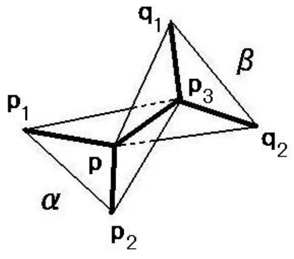

FIGURE 9. Configuration of edges in the K_4 crystal

are congruent form together the K_4 crystal. Figure 10 exhibits a decagonal ring projected onto two particular planes[16] which is obtained from the closed path[17] $(e_1, f_3, \overline{e_2}, e_3, f_2, \overline{e_1}, e_2, \overline{f_3}, \overline{f_2}, \overline{e_3})$ of length 10. More interestingly, the K_4 crystal has *chirality*; namely, its mirror image can not be superposed on the original one by a rigid motion. This is quickly checked by taking a look at a decagonal ring which itself has chirality. In contrast, the diamond crystal has no chirality.

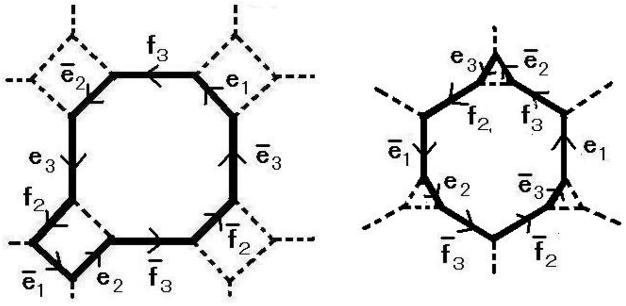

FIGURE 10. Decagonal ring projected onto planes

At present, the K_4 crystal is purely a mathematical object. Because of its beauty, however, we are tempted to ask if the K_4 crystal exists in nature, or possibility to synthesize the K_4 crystal. More specifically, one may ask whether it is possible to synthesize it by using only carbon atom. In connection with this question, it should be pointed out that, just like the *Fullerene* C_{60}, a compound of carbon atoms[18], whose model is (the 1-skeleton of) the *truncated icosahedron* with suitably arranged double bonds[19], we may arrange double bonds, at least theoretically, in such a way that every atom has valency 4. Indeed the lifting of double bonds in K_4 as in Figure 11 yields such an arrangement in the K_4 crystal.

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[16] These projections give covering maps of the K_4 lattice onto the 2-dimensional lattices in Figure 10.

[17] This closed path is homologous to zero, so that its lifting to the K_4 lattice is also closed. There are 6 decagonal rings such that every decagonal ring is a translation of one of them.

[18] Its existence was confirmed in 1990.

[19] A double bond should be thought of representing a chemical characteristic of bonding, and hence does not mean a multiple edge.

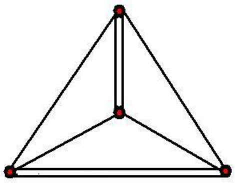

FIGURE 11. K_4 with double bonds

Strongly isotropic crystals

Leaving the non-mathematical question aside, we go back to our primary problem. The following theorem states that there are no other 3-dimensional crystal lattices with the strong isotropic property than the diamond and K_4 lattices.

Theorem 3. *The degree of a* 3*-dimensional crystal lattice with the strong isotropic property is three or four. The one with degree four is the diamond lattice, and the one with degree three is the* K_4 *lattice.*

The proof runs roughly as follows. For a d-dimensional crystal lattice X with the strong isotropic property, one can easily show that its degree n is less than or equal to $d+1$ (use the standard realization). In particular, for $d=3$, we conclude that $n=3$ or 4 (the case $n=2$ is excluded since a crystal lattice of degree two is the 1-dimensional standard lattice).

First take a look at the case $n=4$. Let Φ be the standard realization of X, and $T : \mathrm{Aut}(X) \longrightarrow M(3)$ be the injective homomorphism induced from Φ (Theorem 1). Put $O = \Phi(x)$, and let P_1, P_2, P_3, P_4 be the points determined by $\overrightarrow{OP_i} = \mathbf{v}(e_i)$ ($E_x = \{e_1, e_2, e_3, e_4\}$). Then $K = P_1P_2P_3P_4$ is a regular tetrahedron with the barycenter O. The strong isotropic property leads us to the following alternatives:

(1) the point symmetry S_i with respect to the midpoint of OP_i ($i = 1, 2, 3, 4$) belongs to $T\big(\mathrm{Aut}(X)\big)$, or

(2) the reflection R_i with respect to the plane going vertically through the midpoint of OP_i ($i = 1, 2, 3, 4$) belongs to $T\big(\mathrm{Aut}(X)\big)$.

If the case (2) occurs, then, say R_1R_2 is the rotation whose angle is twice the dihedral angle θ of the regular tetrahedron so that the crystallographic group $T\big(\mathrm{Aut}(X)\big)$ must contain a rotation of infinite order since θ/π is irrational, thereby leading to a contradiction. We thus have (1), which implies that the standard realization of X is the diamond crystal. Therefore X is the diamond lattice.

The proof for the claim that X with $n=3$ is the K_4 lattice is also elementary, although demanding more care in chasing down the cases of the relation between $\Phi(E_x)$ and $\Phi(E_y)$ for adjacent vertices x, y. The key is to verify that the factor group K of $\mathrm{Aut}(X)$ by the maximal abelian subgroup is a finite subgroup of the rotation group $SO(3)$ which is reflected in the chilarity of the K_4 crystal, and allows us to employ the classification of finite subgroups of $SO(3)$. On the other hand, the group K acts transitively on V_0 in a natural manner. In view of the fact that the possible order of elements in K is $1, 2, 3, 4$ or 6, we may prove that K is isomorphic to the octahedral group[20], from which it follows that $|V_0| = 4$, and hence $X_0 = K_4$. An easy argument leads to the conclusion that X is the maximal abel cover of K_4.

We are now on the final stage. It is checked that a realization of the diamond lattice with maximal symmetry is the diamond crystal. We can also demonstrate, again in an ad-hoc manner, that a realization of the K_4 lattice with maximal symmetry is the K_4 crystal or its mirror image[21]. To sum up, we have found out that *there are only three kinds of crystal structures in space with maximal symmetry and the strong isotropic property, that is, the diamond crystal, the* K_4 *crystal, and its mirror image*. This is what we primarily aimed to observe in this article.

It is a challenging problem to list all crystal lattices with the strong isotropic property in general dimension. A typical example is the d-dimensional diamond lattice, a generalization of the hexagonal and diamond lattices, defined as the maximal abelian covering graph over the finite graph with two vertices and $d + 1$ multiple edges joining them. The maximal abelian covering graph over the complete graph K_n also gives an example, whose dimension is $(n - 1)(n - 2)/2$.

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[20] Note that the octahedral group is isomorphic to the symmetry group S_4, which is also identified with the automorphism group of K_4.

[21] In general, a realization with maximal symmetry is not necessarily standard.