Diamond Twin Revisited

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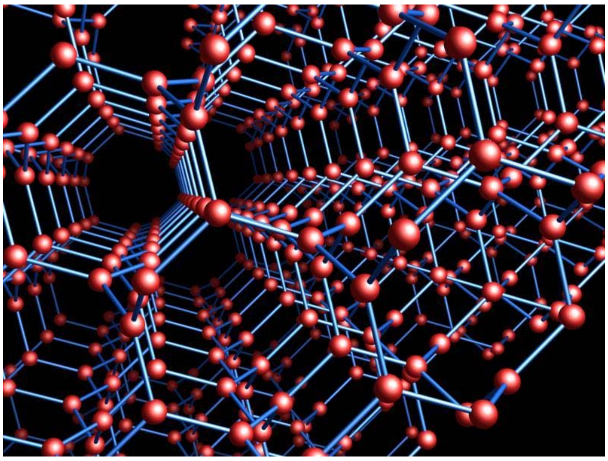

Figure 1: Diamond twin (CG-image created by Kayo Sunada)

1. Introduction

In 2006, I noticed that the hypothetical crystal—described for the first time by crystallographer F. Laves (1932) and designated "Laves' graph of girth ten" by geometer H. S. M. Coxeter (1955)—is a unique crystal net sharing a remarkable symmetric property with the diamond crystal, thus deserving to be called the *diamond twin* although their shapes look quite a bit different at first sight. This short note provides an interesting mutual relationship between them, expressed in terms of "building blocks" and "period lattices." This may give further justification to employ the word "twin." What is more, our discussion brings us to the notion of "orthogonally symmetric lattice," a generalization of *irreducible root lattices*, which makes the diamond and its twin very distinct among all crystal structures.

For the convenience of the reader, we shall first enumerate a few remarkable properties of Laves' graph:

1. It is mathematically defined as the *standard realization* of the maximal abelian covering graph of the complete graph K_4 with 4 vertices (see [8], [10], [16] for the terminology).

2. It has *maximal symmetry* in the sense that every automorphism of Laves' graph as an abstract graph extends to a congruent transformation of space (note that any congruent transformation fixing a crystal net induces an automorphism).

3. It has the *strongly isotropic property*; meaning that for any two vertices x and y of the crystal net, and for any ordering of the directed edges with the origin x and any ordering of the directed edges with the origin y, there is a net-preserving congruence taking x to y and each x-edge to the similarly ordered y-edge ([17]). Here we should not confuse the strongly isotropic property with the *edge-transitivity*

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or the notion of *symmetric graphs* (for instance, the lattice $\mathbb{Z}^3$ with the standard network structure is symmetric, but not strongly isotropic).

4. It is a web of congruent *decagonal rings* (minimal circuits of length 10 in the graph-theoretical sense). There are 15 decagonal rings passing through each vertex (Fig. 2).

5. It is characterized by the *minimizing property* for a certain energy functional.[1]

6. There exists a Cartesian coordinate system such that each vertex has an integral coordinate.

7. It has *chirality*; that is, it is non-superposable on its mirror image.

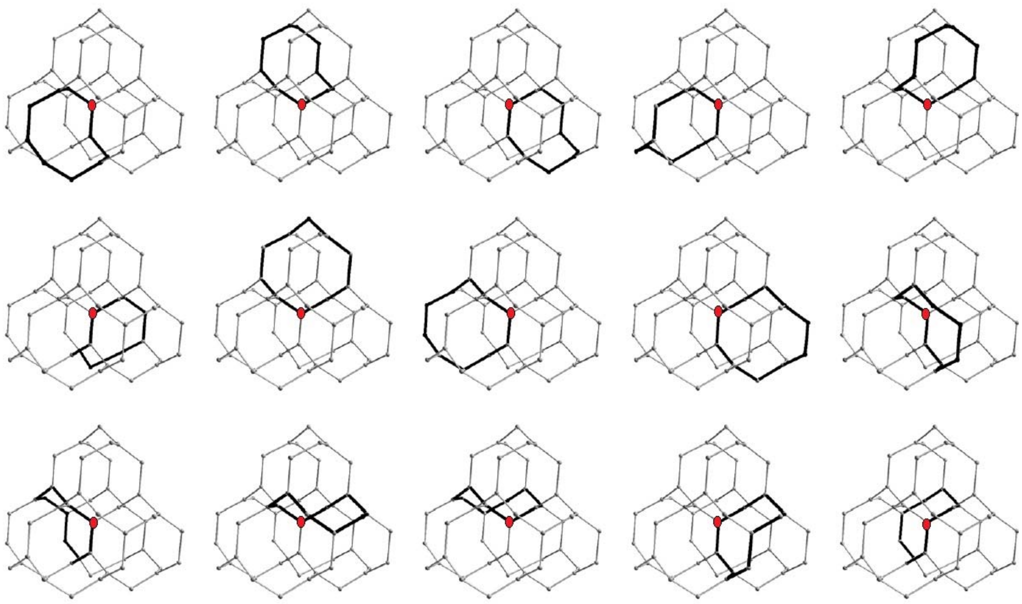


Figure 2: 15 decagonal rings (CG-image created by Hisashi Naito)

To justify the name "diamond twin" for Laves' graph, we look at the structure of the (cubic) diamond, a real crystal with very big microscopic symmetry.[2] The diamond structure is the standard realization of the maximal abelian covering graph of the *dipole graph* with two vertices joined by 4 parallel edges, and is a web of congruent hexagonal rings (called *chair conformation*). Moreover, it has Properties 2, 3, 5, 6. The number of hexagonal rings passing through each vertex is 12, which is less than 15 but still a big number.

What is more, a crystal having Properties 2, 3, 4 must be either diamond or Laves' graph (or its mirror image because of chirality) ([17]). In this sense, Laves' graph and the diamond structure are very kinfolk as mathematical objects (a difference is that the diamond structure has no chirality).

[1] Regarding a crystal as a system of harmonic oscillators, we may define "energy per unit cell". See [8], [10], [19] for the detail.

[2] By abuse of language, the term "diamond" is used to express its network structure throughout, not to stand for the diamond as an actual crystal.

Here is one remark in order. The diamond twin does not belong to the family of crystal structures of the so-called *diamond polytypes* (or *diamond cousins* in plain language) such as *Lonsdaleite* (named in honor of Kathleen Lonsdale and also called *Hexagonal diamond*, a rare stone of pure carbon discovered at Meteor Crater, Arizona, in 1967). Incidentally, the network structure of Lonsdaleite—having much less symmetry than the diamond—is a web of two types of congruent hexagonal rings; one being in the chair conformation, and another being in the *boat conformation*. A shape-similarity between the structures of diamond and Lonsdaleite is brought out when looking at the graphite-like realizations of those structures (see the lower figures in Fig. 3), therefore if we stick to the apparent shape, not to symmetry enshrined inward, it might be appropriate to call Lonsdaleite the twin of diamond, but we do not adopt this view.

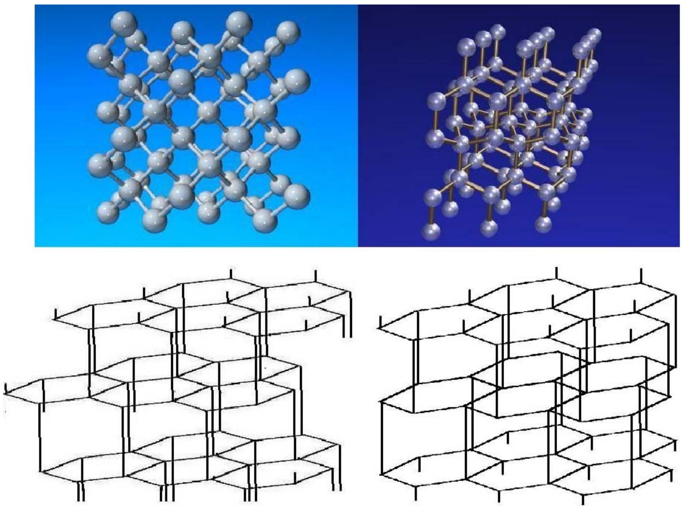


Figure 3: Diamond and Lonsdaleit. From https://www.webelements.com

In a nutshell, what we attempt to do in this note is to provide a specific example that concretizes Kepler's famous statement "At ubi materia, ibi Geometria" (where there is matter, there is geometry).[3]

2. Preparation

We shall very briefly review some materials in graph theory and elementary algebraic topology to explain the notion of building blocks associated with crystal nets. Although the objects of our concern is 3-dimensional crystals, we deal here with crystals of general dimension. See [18], [19] for the details.

A *graph* is represented by an ordered pair $X = (V, E)$ of the set of *vertices* V and the set of all *directed edges* E. For a directed edge e, we denote by $o(e)$ the *origin*, and by $t(e)$ the *terminus*. The inversed edge of e is denoted by $\overline{e}$. The set of directed edges with origin $x \in V$ is denoted by E_x; i.e., $E_x = \{e \in E |\, o(e) = x\}$.

The net associated with a d-dimensional crystal is not just an infinite graph realized in $\mathbb{R}^d$, but a graph with a translational action of a *lattice* (called "period lattice")[4] which

[3] J. Kepler, *De Fundamentis Astrologiae Certioribus* (Concerning the More Certain Fundamentals of Astrology), 1601. In this regard, it is worth recalling that geometry in ancient Greece—especially the classification of regular polyhedra that is regarded as the culmination of Euclid's *Elements*—had its source in the curiosity to the shapes of crystals, as it is often said.

[4] A lattice is a discrete subgroup of the additive group $\mathbb{R}^d$ of maximal rank. More specifically, $L \subset \mathbb{R}^d$

becomes a finite graph when factored out.[5] The finite graph obtained by factoring out is called the *quotient graph*.

We let $X = (V, E)$ be the abstract graph associated with a d-dimensional crystal net with a period lattice L, and let $X_0 = (V_0, E_0)$ be the quotient graph. We assign a vector $\mathbf{v}(e)$ to each directed edge e in X_0 as follows. Choose a direct edge e' in X which corresponds to e. In the crystal net, e' is a directed line segment, so e' yields a vector $\mathbf{v}(e) \in \mathbb{R}^d$, which, as easily checked, does not depend upon the choice of e'. Obviously $\mathbf{v}(\overline{e}) = -\mathbf{v}(e)$.

Put $\mathbf{E}_x = \mathbf{v}(E_{0x})$. The system of vectors $\{\mathbf{E}_x\}_{x\in V_0}$ completely determines the original crystal net and its period lattice. In fact, we obtain the original crystal net by summing up vectors $\mathbf{v}(e_i)$ for all paths $(e_1, \ldots, e_n)$ $(e_i \in E_0)$ on X_0 which start from a reference vertex.[6] The period lattice L turns out to be the image $\widehat{\mathbf{v}}(H_1(X_0, \mathbb{Z}))$ of the homomorphism $\widehat{\mathbf{v}} : H_1(X_0, \mathbb{Z}) \longrightarrow \mathbb{R}^d$ defined by $\widehat{\mathbf{v}}\big(\sum_{e\in E_0} a_e e\big) = \sum_{e\in E_0} a_e \mathbf{v}(e)$, where $H_1(X_0, \mathbb{Z})$ is the 1st homology group of X_0. Thus, the system $\{\mathbf{E}_x\}_{x\in V_0}$ deserves to be called the *building block* of the crystal.

For later purposes, we make a small remark: In the case that X is the maximal abelian covering graph of X_0 (thus $d = \operatorname{rank} H_1(X_0, \mathbb{Z})$), one may take closed paths $c_1, \ldots, c_d$ in X_0 such that $\widehat{\mathbf{v}}([c_1]), \ldots, \widehat{\mathbf{v}}([c_d])$ comprise a basis of the period lattice, where $[c_i]$ is the homology class represented by c_i.

3. Building blocks of the diamond and its twin

We shall now describe explicitly the building blocks for the diamond and its twin in the coordinate space $\mathbb{R}^3$. To facilitate understanding of the configurations of vectors in the building blocks, we employ the cube Q as an auxiliary figure whose vertices are $(1,1,1), (1,-1,1)$, $(-1,1,1)$, $(-1,-1,1)$, $(1,1,-1)$, $(1,-1,-1)$, $(-1,1,-1)$, $(-1,-1,-1)$.

(I) The building block for the diamond twin

Let X_0 be the complete graph K_4 with vertices A, B, C, D (see the lower figure in Fig. 4), and put

$$\begin{aligned}
\mathbf{E}_A &= \{{}^t(0,1,1), {}^t(-1,-1,0), {}^t(1,0,-1)\},\\
\mathbf{E}_B &= \{{}^t(1,0,1), {}^t(-1,1,0), {}^t(0,-1,-1)\},\\
\mathbf{E}_C &= \{{}^t(-1,0,1), {}^t(0,1,-1), {}^t(1,-1,0)\},\\
\mathbf{E}_D &= \{{}^t(0,-1,1), {}^t(-1,0,-1), {}^t(1,1,0)\},
\end{aligned}$$

where vectors in $\mathbb{R}^3$ are represented by column vectors. The system $\{\mathbf{E}_A, \mathbf{E}_B, \mathbf{E}_C, \mathbf{E}_D\}$ forms the building block for the diamond twin (see the upper diagrams of Fig. 4). Note that each of $\mathbf{E}_A$, $\mathbf{E}_B$, $\mathbf{E}_C, \mathbf{E}_D$ comprises an equilateral triangle in a plane with barycenter $\mathbf{o} = (0,0,0)$. More specifically, the planes containing $\mathbf{E}_A, \mathbf{E}_B, \mathbf{E}_C, \mathbf{E}_D$ are orthogonal to the vectors $\mathbf{a} = {}^t(1,-1,1), \mathbf{b} = {}^t(1,1,-1), \mathbf{c} = {}^t(-1,-1,\ -1), \mathbf{d} = {}^t(-1,1,1)$, respectively, from which we see that the dihedral angle of any two planes is $\arccos 1/3 \fallingdotseq 70.53°$.

is a lattice if there exists a basis $\{\mathbf{a}_1, \ldots, \mathbf{a}_d\}$ of $\mathbb{R}^d$ such that $L = \{k_1\mathbf{a}_1 + \cdots + k_d\mathbf{a}_d |\, k_i \in \mathbb{Z}\ (i = 1, \ldots, d)\}$. $\{\mathbf{a}_1, \ldots, \mathbf{a}_d\}$ is called a $\mathbb{Z}$-basis of L.

[5] This fact was pointed out by crystallographers. Mathematically, a crystal net as an abstract graph is an infinite-fold abelian covering graph of a finite graph.

[6] A path means a sequence of edges $(e_1, \ldots, e_n)$ with $t(e_i) = o(e_{i+1})$ $(i = 1, \ldots, n-1)$.

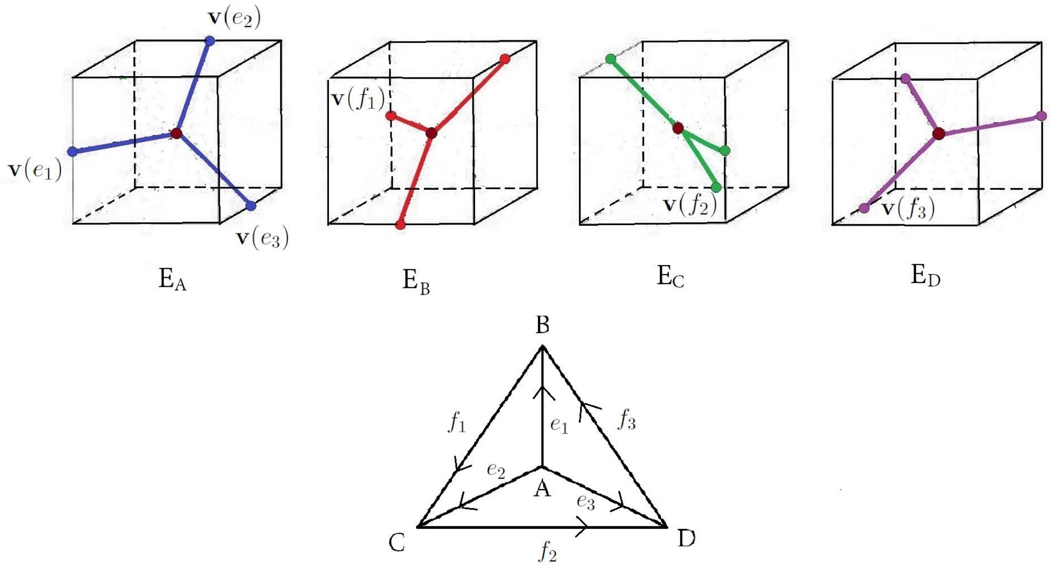


Figure 4: The building block and the quotient graph for the diamond twin

In view of Fig. 4, we have $\mathbf{v}(e_1) = {}^t(-1,-1,0), \mathbf{v}(e_2) = {}^t(0,1,1), \mathbf{v}(e_3) = {}^t(1,0,-1)$ and $\mathbf{v}(f_1) = {}^t(-1,1,0), \mathbf{v}(f_2) = {}^t(0,1,-1), \mathbf{v}(f_3) = {}^t(-1,0,-1)$. As a $\mathbb{Z}$-basis of $H_1(X_0,\mathbb{Z})$, one can take $[c_1],[c_2],[c_3]$ where $c_1 = (e_2, f_1, \overline{e}_3),\quad c_2 = (e_3, f_2, \overline{e}_1),\quad c_3 = (e_1, f_3, \overline{e}_2)$. We then have

$$\begin{aligned}
\widehat{\mathbf{v}}([c_1]) &= {}^t(0,1,1) + {}^t(-1,1,0) + {}^t(-1,0,1) = 2\cdot {}^t(-1,1,1),\\
\widehat{\mathbf{v}}([c_2]) &= {}^t(1,0,-1) + {}^t(0,1,-1) + {}^t(1,1,0) = 2\cdot {}^t(1,1,-1),\\
\widehat{\mathbf{v}}([c_3]) &= {}^t(-1,-1,0) + {}^t(-1,0,-1) + {}^t(0,-1,-1) = 2\cdot {}^t(-1,-1,-1),
\end{aligned}$$

which comprise a $\mathbb{Z}$-basis of the period lattice of the diamond twin.

We let $L_{\mathcal{DT}}$ be the lattice with $\mathbb{Z}$-basis ${}^t(-1,1,1)$, ${}^t(1,1,-1)$, ${}^t(-1,-1,-1)$ (hence $2L_{\mathcal{DT}}$ is the period lattice of the diamond twin). It is checked that

$$L_{\mathcal{DT}} = \{(x_1,x_2,x_3) \in \mathbb{Z}^3 |\, x_1+x_2,\ x_2+x_3,\ x_3+x_1 \text{ are even}\}.$$

Indeed, if we write $(x_1,x_2,x_3) = k_1(-1,1,1) + k_2(1,1,-1) + k_3(-1,-1,-1)$, then $x_1+x_2 = 2(k_2-k_3)$, $x_2+x_3 = -2k_3$, $x_3+x_1 = 2(-k_1-k_3)$, and $k_1 = \frac{1}{2}(x_1+x_2) - x_1$, $k_2 = \frac{1}{2}(x_1+x_3) - x_3$, $k_3 = -\frac{1}{2}(x_2+x_3)$.

The lattice $L_{\mathcal{DT}}$ is what is called the *body-centered cubic lattice* in crystallography (look at the cube in Fig. 5 depicted by the bold lines).

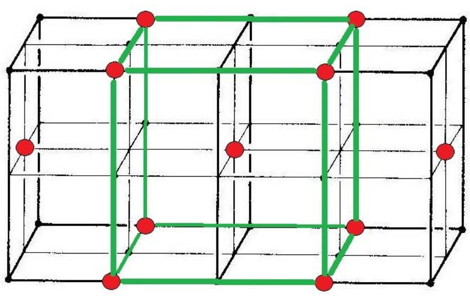


Figure 5: Body-centered cubic lattice

(II) The building block for the diamond

Let X_0 be the graph with two vertices A, B joined by 4 parallel edges e_1, e_2, e_3, e_4 (see the lower figure in Fig. 6), and put

$$\mathbf{E}_A = \{{}^t(-1,1,1), {}^t(1,-1,1), {}^t(-1,-1,-1), {}^t(1,1,-1)\},$$
$$\mathbf{E}_B = \{{}^t(1,1,1), {}^t(-1,-1,1), {}^t(-1,1,-1), {}^t(1,-1,-1)\} = -\mathbf{E}_A.$$

The system $\{\mathbf{E}_A, \mathbf{E}_B\}$ forms the building block for the diamond (see the upper diagrams of Fig. 6). Note that each of $\mathbf{E}_A$ and $\mathbf{E}_B$ comprises a regular tetrahedron with barycenter $\mathbf{o}$.

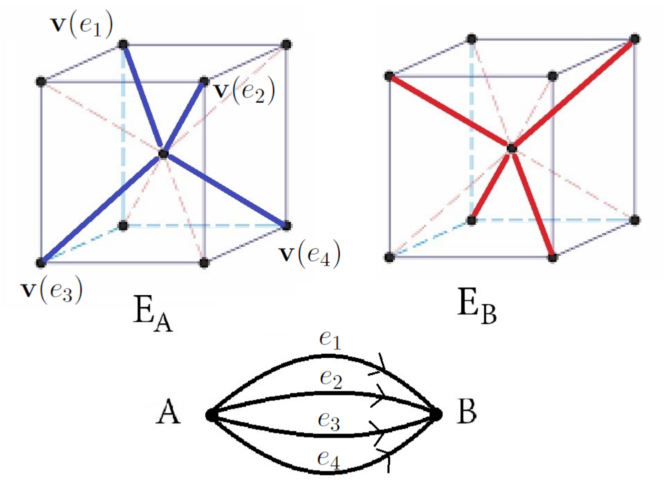


Figure 6: The building block and the quotient graph for the diamond

As shown in Fig. 6, we put $\mathbf{v}(e_1) = {}^t(-1,1,1)$, $\mathbf{v}(e_2) = {}^t(1,-1,1)$, $\mathbf{v}(e_3) = {}^t(-1,-1,-1)$, $\mathbf{v}(e_4) = {}^t(1,1,-1)$. As a $\mathbb{Z}$-basis of $H_1(X_0,\mathbb{Z})$, one can take $[c_1]$, $[c_2]$, $[c_3]$ where $c_1 = (e_1, \overline{e}_2)$, $c_2 = (e_2, \overline{e}_3)$, $c_3 = (e_3, \overline{e}_4)$. We then have

$$\widehat{\mathbf{v}}([c_1]) = {}^t(-1,1,1) + {}^t(-1,1,-1) = 2\cdot{}^t(-1,1,0),$$
$$\widehat{\mathbf{v}}([c_2]) = {}^t(1,-1,1) + {}^t(1,1,1)) = 2\cdot{}^t(1,0,1),$$
$$\widehat{\mathbf{v}}([c_3]) = {}^t(-1,-1,-1) + {}^t(-1,-1,1) = 2\cdot{}^t(-1,-1,0),$$

which comprise a $\mathbb{Z}$-basis of the period lattice of the diamond.

We let $L_{\mathcal{D}}$ be the lattice with $\mathbb{Z}$-basis ${}^t(-1,1,0)$, ${}^t(1,0,1)$, ${}^t(-1,-1,0)$ (hence $2L_{\mathcal{D}}$ is the period lattice of diamond). By the same method as described in (I), it is checked that

$$L_{\mathcal{D}} = \{(x_1,x_2,x_3) \in \mathbb{Z}^3 | \, x_1 + x_2 + x_3 \text{ is even}\}.$$

This is what is called the *face-centered cubic lattice* in crystallography (look at the cube in Fig. 7 depicted by the bold lines).

So far, no relationship can be found between the diamond and its twin. A mutual relation between them, though not a big deal, is observed only after considering the union $\mathbf{E}_{\mathcal{DT}} = \mathbf{E}_A \cup \mathbf{E}_B \cup \mathbf{E}_C \cup \mathbf{E}_D$ for the diamond twin and the union $\mathbf{E}_{\mathcal{D}} = \mathbf{E}_A \cup \mathbf{E}_B$ for the diamond (Fig. 8). Perhaps both systems of vectors may be familiar to the reader. For instance, $\mathbf{E}_{\mathcal{DT}}$ is nothing but the irreducible root system A_3 (see the next section).

The system $\mathbf{E}_{\mathcal{DT}}$ for the diamond twin generates the lattice $L_{\mathcal{D}}$ since $\mathbf{E}_{\mathcal{DT}} \subset L_{\mathcal{D}}$ and contains a basis of $L_{\mathcal{D}}$. (Remember that $2L_{\mathcal{D}}$ is the period lattice for the diamond, not

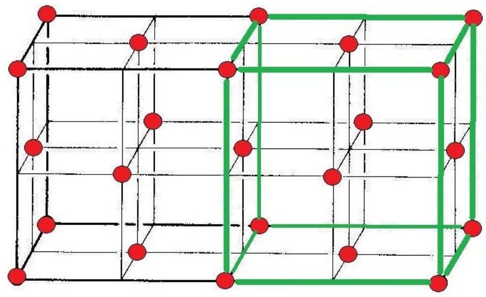


Figure 7: Face-centered cubic lattice

for the diamond twin!). On the other hand, the system $\mathbf{E}_{\mathcal{D}}$ for the diamond generates the lattice $L_{\mathcal{DT}}$ since $\mathbf{E}_{\mathcal{D}} \subset L_{\mathcal{DT}}$ and contains a basis of $L_{\mathcal{DT}}$. Hence, passing from the building blocks to the period lattices, the role exchange between the diamond and its twin takes place.

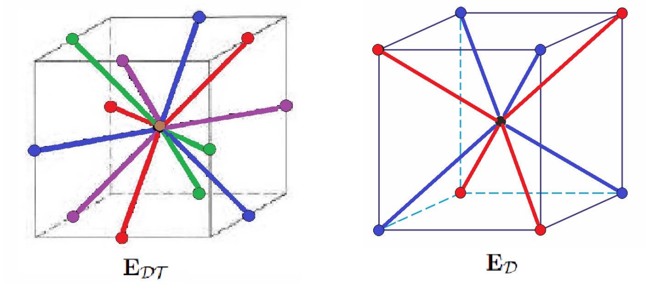


Figure 8: $\mathbf{E}_{\mathcal{DT}}$ and $\mathbf{E}_{\mathcal{D}}$

Furthermore, if we denote by L^* the dual (reciprocal) lattice of a lattice $L \subset \mathbb{R}^d$ in general,[7] we have

$$L_{\mathcal{DT}}{}^* = \frac{1}{2} L_{\mathcal{D}}, \quad L_{\mathcal{D}}{}^* = \frac{1}{2} L_{\mathcal{DT}}$$

since the dual of the $\mathbb{Z}$-basis $\{{}^t(-1,1,1), {}^t(1,1,-1), {}^t(-1,-1,-1)\}$ of $L_{\mathcal{DT}}$ is $\{{}^t(-1/2, 1/2, 0),\ {}^t(0, 1/2,\ -1/2), {}^t(-1/2, 0,\ -1/2)\}$. Here we should note that $\{{}^t(-1,1,0), {}^t(0,1,-1), {}^t(-1,0,-1)\}$ is a $\mathbb{Z}$-basis of $L_{\mathcal{D}}$.

4. Orthogonally symmetric lattices

What is more peculiar than the facts obtained by the simple observations above is that $L_{\mathcal{D}}$ and $L_{\mathcal{DT}}$ are *orthogonally symmetric lattices*, the notion that distinguishes the diamond and its twin from all other crystal structures (with one exception).

Before embarking on this topic, we need some preparation.

We denote by $S_r(\mathbf{a})$ the sphere in $\mathbb{R}^d$ of radius r, centered at $\mathbf{a} \in \mathbb{R}^d$. Given a general lattice L in $\mathbb{R}^d$, we put $\alpha(L) := \min_{\mathbf{y} \neq \mathbf{0} \in L} \|\mathbf{y}\|$, and

$$K(L) := \{\mathbf{x} \in L |\, \|\mathbf{x}\| = \alpha(L)\},$$
$$G(L) := \{g \in \mathrm{O}(d) |\, g(L) = L\}$$

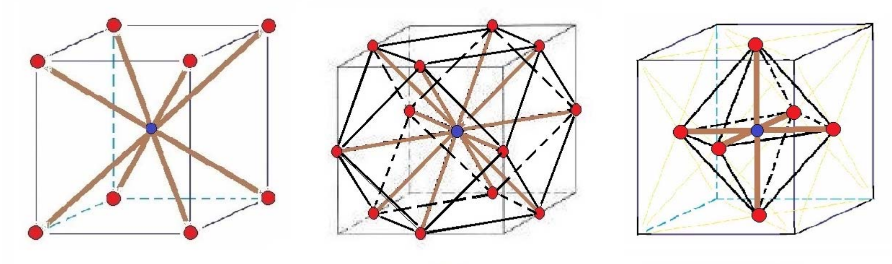
Since $\|\mathbf{x} - \mathbf{y}\| \geq \alpha(L)$ for $\mathbf{x}, \mathbf{y} \in L$ with $\mathbf{x} \neq \mathbf{y}$, we observe that $\{S_{\alpha(L)/2}(\mathbf{a})\}_{\mathbf{a} \in K(L)}$ is a family of non-overlapping spheres touching the common sphere $S_{\alpha(L)/2}(\mathbf{o})$. Therefore

[7] $L^* = \{\mathbf{x} \in \mathbb{R}^d |\, \langle \mathbf{x}, \mathbf{y} \rangle \in \mathbb{Z}$ for every $\mathbf{y} \in L\}$.

$|K(L)|$ is less than or equal to the maximum possible *kissing number* $k(d)$. It is known that $k(3) = 12$,[8] and hence $|K(L)| \le 12$ for a 3-dimensional lattice L. For example,

$$\begin{aligned}
&\alpha(\mathbb{Z}^3) = 1, \quad K(\mathbb{Z}^3) = \{\pm{}^t(1,0,0), \pm{}^t(0,1,0), \pm{}^t(0,0,1)\}, \quad |K(\mathbb{Z}^3)| = 6,\\
&\alpha(L_{\mathcal{DT}}) = \sqrt{3}, \quad K(L_{\mathcal{DT}}) = \mathbf{E}_{\mathcal{D}}, \quad |K(L_{\mathcal{DT}})| = 8\\
&\alpha(L_{\mathcal{D}}) = \sqrt{2}, \quad K(L_{\mathcal{D}}) = \mathbf{E}_{\mathcal{DT}} \quad |K(L_{\mathcal{D}})| = 12.
\end{aligned}$$

What we should notice is that $G(\mathbb{Z}^3) = G(L_{\mathcal{DT}}) = G(L_{\mathcal{D}})$. Indeed, these groups coincide with the symmetry group $\mathrm{Iso}(Q)$ of the cube Q introduced in the previous section, which acts transitively on the set of vertices not only of Q, but also of *cuboctahedron* and of the octahedron depicted in Fig. 9.[9] Actually, $\mathrm{Iso}(Q)$ is identified with the full octahedral group $\mathrm{O_h}$, which acts irreducibly on $\mathbb{R}^3$.



(1) (2) (3)

Figure 9:

Now, keeping in mind the three examples of lattices $\mathbb{Z}^3$, $L_{\mathcal{DT}}$, $L_{\mathcal{D}}$, we make the following definition.

Definition 1. A lattice L in $\mathbb{R}^d$ is said to be *orthogonally symmetric* if

(i) $K(L)$ generates L,

(ii) $G(L)$ acts transitively on $K(L)$, and

(iii) the $G(L)$-action on $\mathbb{R}^d$ is irreducible.

Notice that $G(L) = \{g \in \mathrm{O}(d) |\, g(K(L)) = K(L)\}$ because of Condition (i), and that $G(L)$ contains the *central reflection* $\sigma_0 : (x, y, z) \mapsto (-x, -y, -z)$.

As observed above, the three lattices $\mathbb{Z}^3$, $L_{\mathcal{DT}}$, and $L_{\mathcal{D}}$ are orthogonally symmetric.

Typical examples of orthogonally symmetric lattices of general dimension are *irreducible root lattices* whose properties actually motivate the definition above. For the convenience of the reader, let us recall the definition of root lattices.

For an *even lattice* L, i.e., $\|\mathbf{x}\|^2 \in 2\mathbb{Z}$ for all $\mathbf{x} \in L$, we let $R(L) = \{\mathbf{x} \in L |\, \|\mathbf{x}\|^2 = 2\}$. An element $\mathbf{x} \in R(L)$ is called a *root*. Clearly $\alpha(L) = \sqrt{2}$ and $R(L) = K(L)$.

Definition 2. An even lattice L is called a *root lattice* if the root system $R(L)$ generates L. A root lattice L is said to be *irreducible* if L is not a direct sum of two non-trivial lattices.

[8] This fact was conjectured correctly by Newton in a famous controversy between him and David Gregory (1694), and was proved by Schütte and van der Waerden in 1953.

[9] The cuboctahedron (also called the *heptaparallelohedron* or *dymaxion*) is one of thirteen *Archimedean solids*.

Representatives of irreducible root lattices are A_d and D_d ($A_3 = D_3$) in the usual notations for root systems.[10] Here A_d is the lattice in the orthogonal complement $(\underbrace{1,\ldots,1}_{d+1})^{\perp}$ in $\mathbb{R}^{d+1}$ defined by

$$A_d = \{(x_1,\ldots,x_{d+1}) \in \mathbb{Z}^{d+1} | \, x_1 + \cdots + x_{d+1} = 0\}.$$

The root system $R(A_4)$ consists of vectors such that all but two coordinates equal to 0, one coordinate equal to 1, and one equal to -1. As for D_d, it is defined as

$$D_d = \{(x_1,\ldots,x_d) \in \mathbb{Z}^d | \, x_1 + \cdots + x_d \text{ even}\}.$$

The root system $R(D_d)$ consists of all integer vectors in $\mathbb{R}^d$ of length $\sqrt{2}$.

Note that the root lattice A_3 $(= D_3)$ coincides with $L_{\mathcal{D}}$.[11]

The following is the statement referred to in the previous section.

Proposition 1. *The three lattices $\mathbb{Z}^3$, $L_{\mathcal{DT}}$ and $L_{\mathcal{D}}$ (up to similarity) are the only examples of orthogonally symmetric lattices of 3-dimension.*

Let L be an orthogonally symmetric lattice. It suffices to show that $K(L)$ is one of $K(\mathbb{Z}^3)$, $K(L_{\mathcal{DT}})$. $K(L_{\mathcal{D}})$ (up to similarity).

The idea of proof is as follows.

(1) Recall the classification of finite subgroups of O(3) containing the central reflection $(x,y,z) \mapsto (-x,-y,-z)$. Possible cases are:

$$G(L) = \begin{cases} S_4 \times \mathbb{Z}_2 \\ A_4 \times \mathbb{Z}_2 \\ A_5 \times \mathbb{Z}_2 \end{cases}$$

(2) Use the crystallographic restriction, from which it follows that the last case is excluded because $G(L)$ contains no element of order 5. It is also concluded that $|K(L)| = 6, 8, \text{or } 12$.

(3) Determine the configuration of vectors in $K(L)$ in each case. This will be done by brute-force, rather than a systematic method.

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