Crystal Lattice Automata

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Abstract

A description of crystal lattices in terms of automata is presented. The words of a language represented by an automata are mapped to points in $\mathbf{R}^n$ defining lattice points and their connections. These automata descriptions of crystal lattices reveal subtle properties that are difficult to see in other descriptions.

Keywords: automata, crystallography, lattice, tiling

1 Introduction

Crystal lattices are complex three-dimensional structures. The structures are composed of arrangements of atoms, ions, or molecules. These arrangements are highly ordered. Chemists have studied crystal lattices a great deal. They have a well-developed naming and classification of crystals.

One simple example of a crystal lattice is salt (NaCl). The arrangement of the ions form a lattice called simple cubic. The ions fall into the same pattern as integer coordinates in Euclidean 3-space. The ionic bonds are formed along the lines parallel to the three axis. Another example of a crystal lattice is a diamond. The crystal, composed of carbon atoms, has a more complex arrangement than the simple cubic. Each carbon atom is connected with covalent bonds to four other carbon atoms. The local pattern is tetrahedral: one atom at the centre that is connected to four atoms that form a tetrahedron. The global pattern has these tetrahedral structures connected to each other so that each of the atoms has four connections. The four connections to each carbon has the same geometry associated with them.

The way that chemists describe the regularity of the crystals is by creating a unit tile comprised of many nodes and connections. These units, often cubic, are used to tile space. The unit tiling description of a diamond, used to describe the global pattern of the carbon atoms, is a $5 \times 5 \times 5$ grid with the opposite faces identified. Each of the eight corners of the grid and the six face centres of the grid contain nodes representing carbon atoms. As well, the following interior locations also contain nodes: (1,3,1), (3,1,1), (1,1,3), (3,3,3). The only connections between nodes are the ones between the interior and the exterior nodes where the Euclidean distance is $\sqrt{3}$.

Chemists are using the well studied field of Tiling [2] to gain insight into the structure of crystal lattices. The difficulty is that chemists must describe explicitly the insides of these units before they can use the units to tile the space of the lattice. Rather than focussing indirectly on these units that are simply a collection of the nodes and connections occupying some space, this paper focusses directly on a description of the nodes and connections.

2 Crystal Lattice Automata

The regularity of the arrangement of the nodes and their connections in a crystal lattice lend themselves to description by automata. The automata generate a language that is mapped into the space of the lattice. This idea of mapping regular languages to mathematical structures is also found in Epstein's construction of automatic groups, where he maps regular languages into groups [1].

Thus a *Crystal Lattice Automata* (*CLA*) is constructed with two components: the language and the mapping.

2.1 The Language

The automaton, M_l, defines a language with some noteworthy properties: M_l's alphabet is a set bi-directional vectors and all states are final states. Formally,

$$\begin{aligned} M_l &= (K, \Sigma, \delta, q_0) \\ K &= \text{the set finite states} \\ \Sigma &= \text{the finite alphabet, a subset of } \mathbf{R}^n \\ \delta &= K \times \Sigma \to K \\ q_0 &= \text{the start state}(q_0 \in K) \end{aligned}$$

In this formal description, bi-directional means

$$\forall a \in \Sigma\ \exists -a \in \Sigma,\ q, q' \in K \text{ such that if } \delta(q,a) = q' \text{ then } \delta(q', -a) = q$$

2.2 The Mapping

The points and the connections of the lattice are be defined by words in the language defined by M_l. The word ϵ denotes the empty word. The functions p, c, and l refer to points, connections, and lattices, respectively. The function p maps each word into the Euclidean sum of the individual vectors. The function c maps each word into an ordered pair: the base point defined by $p(w)$ and the set of all the connected points. The function l maps the language into the set connections of the lattice. Formally,

$$\begin{aligned} L_{M_l} &= \text{the language accepted by } M_l \\ w &= (a_0 a_1 a_2 \cdots a_n) \in L_{M_l}\ a_i \in \Sigma \\ p(w) &= \sum_{i=1}^{n} a_i \end{aligned}$$

$$
\begin{aligned}
c(w) &= (p(w), \{p(wa) | wa \in L_{M_l}, a \in \Sigma\}) \\
l(L_{M_l}) &= \{c(w) | w \in L_{M_l}\}
\end{aligned}
$$

The above definitions admit many structures that do not have the properties associated with crystal lattices. First, a crystal lattice should have nodes spaced relatively far apart. Second, the connections should be well-defined. These extra properties are expressed as follows:

$$
\begin{aligned}
l(L_{M_l}) \text{ is a } \textit{crystal lattice} \iff & \forall w, w' \in L_{M_l} \text{ such that } p(w) = p(w') \rightarrow c(w) = c(w') \\
\text{and } & \exists x > 0 \text{ such that for } w, w' \in L_{M_l} \\
& \quad \text{either } p(w) = p(w') \text{ or } \|p(w) - p(w')\| > x
\end{aligned}
$$

2.3 Crystal Lattice Relations

Two lattices are considered equivalent if one lattice can be rigidly moved into another. Moving rigidly refers to shape preserving transformations like rotations and translations. Formally,

$$
\begin{aligned}
\mathbf{I} &= \text{the set rigid transformations} \\
Ac(w),\, A \in \mathbf{I} &= (Ap(w), \{Ap(aw) | wa \in L_{M_l}\} \\
l(L_{N_l}) \cong l(L_{M_l}) &\iff \exists A \in I \text{ such that } \{Ac(w) | w \in L_{M_l}\} = \{c(w') | w' \in L_{N_l}\}
\end{aligned}
$$

The concept of a sub-lattice is defined as a strict subset.

$$
\begin{aligned}
l(L_{N_l}) \text{ is a sub-lattice of } l(L_{M_l}) \iff & \forall c(w) = (p, S) \in l(L_{N_l})\ \exists c(w') = (p', S') \in l(L_{N_l}) \text{ such that} \\
& p = p' \text{ and } S \subset S'
\end{aligned}
$$

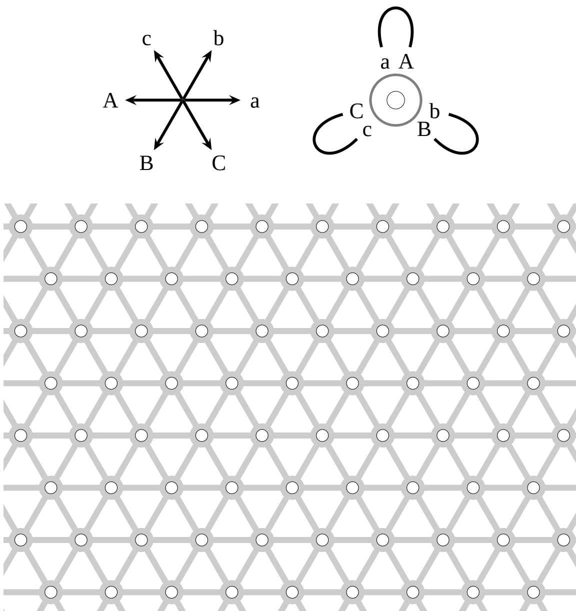
2.4 Special Crystal Lattices

Certain crystal lattices have more regularity in their arrangement than others. To help describe this regularity, a definition of similar connections is required. The node and its connections are similar if there is a rigid motion that takes one into the other.

$$
c(w') \sim c(w), w, w' \in L_{M_l} \iff \exists A \in \mathbf{I}, c(w') = Ac(w)
$$

A *regular* lattice has all of its nodes similar to each other. An *n-regular* lattice has all of its nodes similar to a set of n different nodes. A full lattice is a lattice defined by the language Σ^*. A full lattice is regular since all nodes are similar.

$$
l(L_{M_l}) \text{ is } \textit{regular} \Rightarrow c(w) \sim c(\epsilon)\ \forall w \in L_{M_l}
$$



$K = \{\bigcirc\}$
$\Sigma = \{a, b, c, A, B, C\}$ $a = (1, 0)$ $b = (cos\frac{\Pi}{3}, sin\frac{\Pi}{3})$ $c = (cos\frac{2\Pi}{3}, sin\frac{2\Pi}{3})$ $A = (-1, 0)$ $B = (-cos\frac{\Pi}{3}, -sin\frac{\Pi}{3})$ $C = (-cos\frac{2\Pi}{3}, -sin\frac{2\Pi}{3})$
$\delta(\bigcirc, a) = \bigcirc$ $\delta(\bigcirc, b) = \bigcirc$ $\delta(\bigcirc, c) = \bigcirc$
$q_0 = \bigcirc$

Figure 1: A Full Crystal Lattice

$$\begin{aligned} l(L_{M_l}) \text{ is } \textit{n-regular} \quad &\Rightarrow \quad \exists S = \{w_i | c(w_i) \not\sim c(w_j), 1 \leq i, j \geq n, w_i \in L_{M_l}\} \text{ such that} \\ &\quad\quad \forall w \in L_{M_l}\ \exists w_i \in S \text{ such that } c(w) \sim c(w_i) \\ l(L_{M_l}) \text{ is a } \textit{full} \quad &\Rightarrow \quad L_{M_l} = \Sigma^* \end{aligned}$$

Another property of lattices deals with the lengths of the connections. A lattice is called uniform if all of the connections are the same length. It is called n-uniform if there are n different lengths for the connections.

$$\begin{aligned} l(L_{M_l}) \text{ is } \textit{uniform} \quad &\Rightarrow \quad \exists x > 0, x \in \mathbf{R} \text{ such that} \\ &\quad\quad \|p(w) - p(wa)\| = x, \forall w, wa \in L_{M_l} \text{ and } a \in \Sigma \\ l(L_{M_l}) \text{ is } \textit{n-uniform} \quad &\Rightarrow \quad \exists D = \{r_i |\ \|p(w) - p(wa)\| = r_i \text{ and } r_i \neq r_j, 1 \leq i, j \geq n\} \text{ such that} \\ &\quad\quad \forall w \in L_{M_l}\ \exists r_i \in S \text{ such that } \|p(w) - p(wa)\| = r_i \end{aligned}$$

3 Exploration

The following sections explore some CLA definitions. Visualization of the CLA and the Crystal lattice are important for understand the use of CLA.

In each figure describing a CLA, the upper-left part is a visualization of the CLA: a graphical representation of the set of vectors, Σ, as well as, a graphical representation of the automaton. Three conventions are used. First, capital letters are a short form of the negative of the small letters. For instance, A is used to represent $-a$. Second, the states are

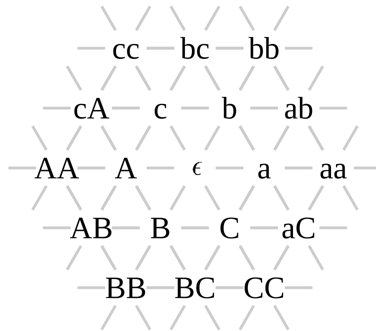


Figure 2: Points and Connections of a Few Words

labelled with graphic symbols (◯, ●, ⊙, ◉). Third, the transitions of the automaton are abbreviated. One line is used to represent the bi-directional transition. The role of letters at the endpoints of the transitions will be shown in the examples. The bottom-left part of each figure contains the crystal lattice resulting from the CLA. The connections are depicted by light grey lines and the nodes are light grey circles with the state labels inside. The right-most portion of each figure is the formal description of the CLA.

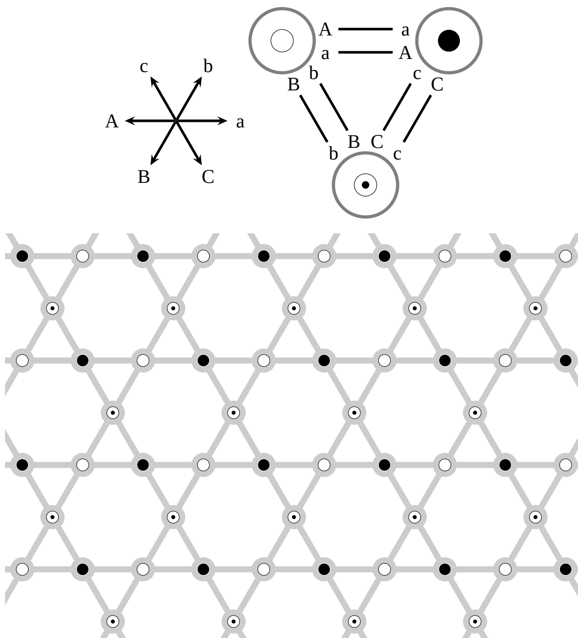
3.1 Full lattice

Figure 1 describes a full lattice. All full lattices can be represented by an automaton with one state. This particular lattice is the triangular tiling of the plane. Figure 2 shows some words accepted by the automaton in Figure 1 that map into the lattice. Infinitely many words map to each point in the lattice. For instance, AB, BA, and $AB(aA)^*$ map to the same point.

3.2 Regular Sub-lattice

In Figure 3, a CLA that has three states and six bi-directional transitions is visualized. Here, the role of the letters on the automata are more apparent. The white circle state, ◯, has four exiting transitions: a and A that go to the black circle, ●, and b and B that go to the white circle with the black dot, ⊙. Similarly, the black circle state has four exiting transitions: a and A that go to the white circle, c and C that go to the white circle with the black dot. Consider the words a^*. The empty word, ϵ, is accepted at the white state; a causes a transition to the black state; aa to the white state. In general, a^{2i} is accepted in the white state and a^{2i+1} in the black state. The positions of these words are $(2i)a$ and $(2i+1)a$ or simply $(i, 0), i \in \mathbf{Z}$ which form an infinite line. This is a regular lattice since all of the nodes look like Xs (upright or slanting). The black and white node are Xs rotated 60^o and -60^o, whereas the black dotted node is an upright X.

This lattice is a *sub-lattice* of the lattice in Figure 1 (connections at each node are a proper subset).



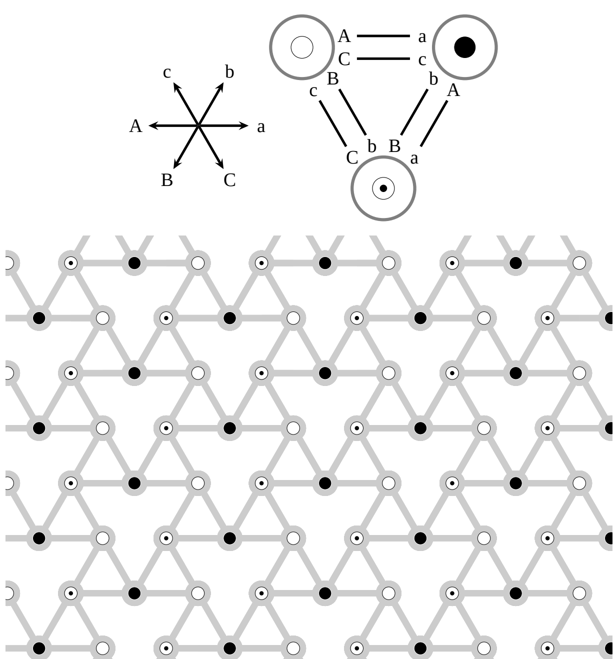
$K = \{\bigcirc, \bullet, \odot\}$

$\Sigma = \{a, b, c, A, B, C\}$
$a = (1, 0)$
$b = (cos\frac{\Pi}{3}, sin\frac{\Pi}{3})$
$c = (cos\frac{2\Pi}{3}, sin\frac{2\Pi}{3})$
$A = (-1, 0)$
$B = (-cos\frac{\Pi}{3}, -sin\frac{\Pi}{3})$
$C = (-cos\frac{2\Pi}{3}, -sin\frac{2\Pi}{3})$

$\delta(\bigcirc, a) = \bullet$
$\delta(\bigcirc, b) = \odot$
$\delta(\bullet, a) = \bigcirc$
$\delta(\bullet, c) = \odot$
$\delta(\odot, b) = \bigcirc$
$\delta(\odot, c) = \bullet$

$q_0 = \bigcirc$

Figure 3: A Regular Lattice with Three States



$K = \{\bigcirc, \bullet, \odot\}$

$\Sigma = \{a, b, c, A, B, C\}$
$a = (1, 0)$
$b = (cos\frac{\Pi}{3}, sin\frac{\Pi}{3})$
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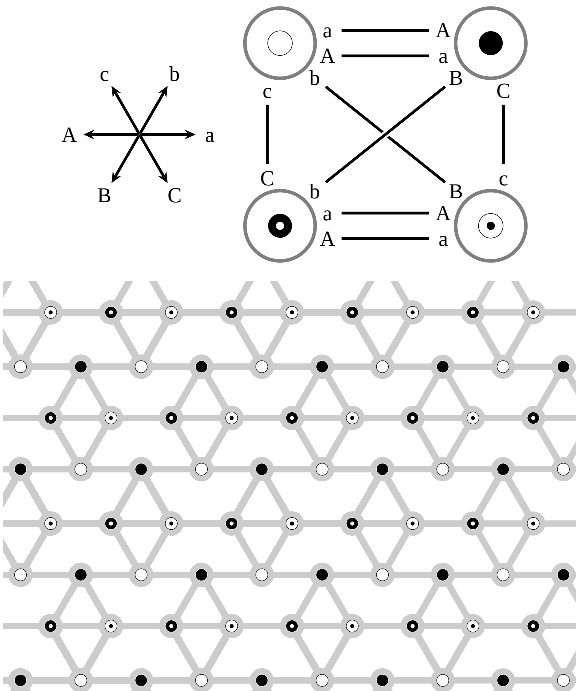
$A = (-1, 0)$
$B = (-cos\frac{\Pi}{3}, -sin\frac{\Pi}{3})$
$C = (-cos\frac{2\Pi}{3}, -sin\frac{2\Pi}{3})$

$\delta(\bigcirc, c) = \odot$
$\delta(\bullet, a) = \bigcirc$
$\delta(\bullet, b) = \odot$
$\delta(\bullet, c) = \bigcirc$
$\delta(\odot, a) = \bullet$
$\delta(\odot, b) = \bigcirc$

$q_0 = \bigcirc$

Figure 4: A Regular Lattice with no Infinite Lines



$K = \{\bigcirc, \bullet, \odot, ◉\}$

$\Sigma = \{a, b, c, A, B, C\}$
$a = (1, 0)$
$b = (cos\frac{\Pi}{3}, sin\frac{\Pi}{3})$
$c = (cos\frac{2\Pi}{3}, sin\frac{2\Pi}{3})$
$A = (-1, 0)$
$B = (-cos\frac{\Pi}{3}, -sin\frac{\Pi}{3})$
$C = (-cos\frac{2\Pi}{3}, -sin\frac{2\Pi}{3})$

$\delta(\bigcirc, a) = \bullet$
$\delta(\bigcirc, b) = \odot$
$\delta(\bigcirc, c) = ◉$
$\delta(\bullet, a) = \bigcirc$
$\delta(\odot, a) = ◉$
$\delta(\odot, c) = \bullet$
$\delta(◉, a) = \odot$
$\delta(◉, b) = \bullet$

$q_0 = \bigcirc$

Figure 5: A 2-regular Lattice

3.3 Infinite Lines

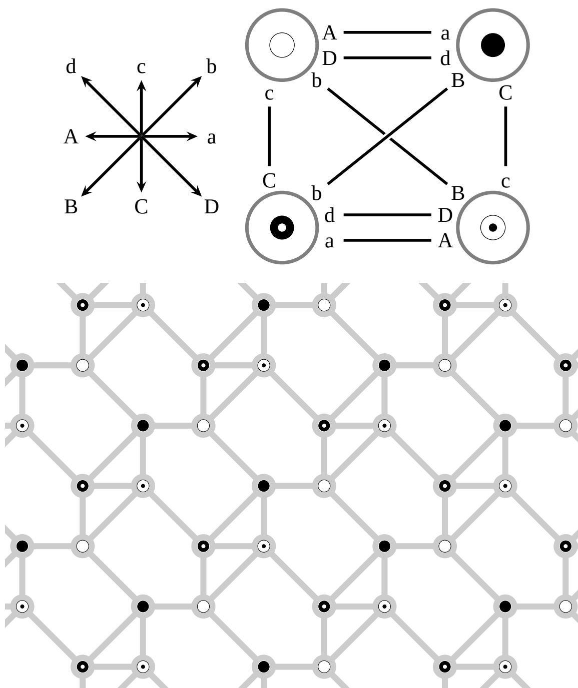
In the previous example all of the connections formed infinite lines. These lines can be described by the words $w(x)^*, x \in \Sigma, w \in L_{M_l}$. The answer to "Do all lattices have infinite lines?" is "No". Figure 4 shows an example of a lattice with line segments that contain at most three nodes. This property is reflected in the language the automaton describes. No word in the language contains the substring $xxx, x \in \Sigma$. This lattice is regular since each node connection looks like a K.

3.4 N-Regular and N-Uniform

The previous examples have all been regular and uniform. Figure 5 shows a 2-regular lattice. One of the types of nodes is the K from Figure 4 labelled with the black or white states. The other type of node looks like a peace symbol, labelled with the dotted states. The K nodes and the peace symbol nodes make rows of infinite straight lines.

The related 2-uniform lattice found in Figure 6 has the same row structure as Figure 5 but it is distorted. In Figure 6 the rows are not straight but zig-zag through the directions a and d. The automata are similar but the set of vectors are different. Figure 6 lattice's vectors are based on a square whereas the Figure 5 lattice's vectors are based on a hexagon. The vectors based on a square have two different lengths: vectors that go to the edges of the square, a, A, c,and C; and vectors that go to the corners of the square, b, B, d, and D.

The similarity in automata of Figure 6 and Figure 5 is reflected in the similarity of their resulting lattices. This suggests that automata description may capture part of the essence



$K = \{$○, ●, ⊙, ◉$\}$

$\Sigma = \{a, b, c, d, A, B, C, D\}$
$a = (1, 0)$
$b = (1, 1)$
$c = (0, 1)$
$d = (-1, 1)$
$A = (-1, 0)$
$B = (-1, -1)$
$C = (0, -1)$
$D = (1, -1)$

$\delta($○$, b) =$ ⊙
$\delta($○$, c) =$ ◉
$\delta($●$, a) =$ ○
$\delta($●$, d) =$ ○
$\delta($⊙$, c) =$ ●
$\delta($◉$, a) =$ ⊙
$\delta($◉$, b) =$ ●
$\delta($◉$, d) =$ ⊙

$q_0 =$ ○

Figure 6: a 2-regular 2-uniform lattice

of the lattices.

3.5 3D Lattices

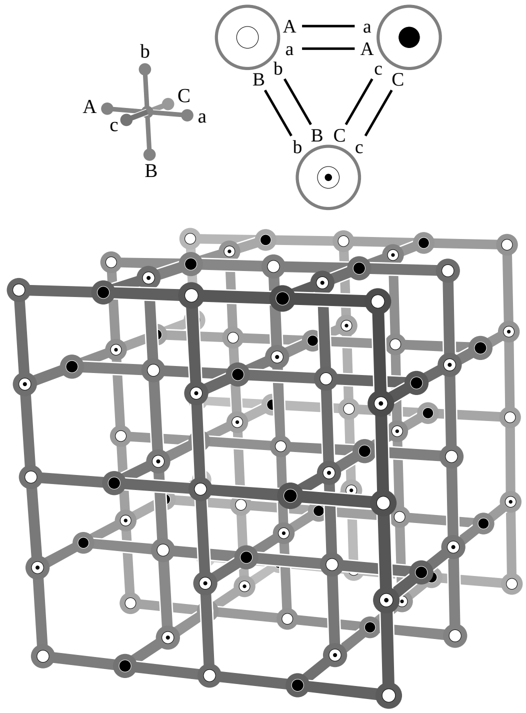
The only differences between the 2D lattices and the 3D lattices is that the vectors used are 3D instead of 2D. To illustrate this point, Figure 7 and Figure 8 are direct analogues of Figure 3 and Figure 4. In fact, the automata are identical. This means the languages that describe the lattices are identical.

The infinite lines of Figure 3 are also present in Figure 7, because the language can have arbitrarily long strings of the same letter. As well, the alternation of states while traversing straight lines is present in both.

As to Figure 8, the longest straight line is length two as with the 2D case in Figure 4. This occurs since there are no substrings of a word that have $x^3, x \in \Sigma$. One thing to note is that if this 3D lattice were to be a real chemical crystal lattice then the lattice in Figure 8 would be the unit used in the tiling description. This indicates that the automata description may be much more concise and revealing than the tiling unit description.

3.6 The Diamond Lattice

Figure 9 shows that there are 2 states in the diamond lattice. The vectors are defined by the vertices of a cube centered at the origin. This description seems easier to understand



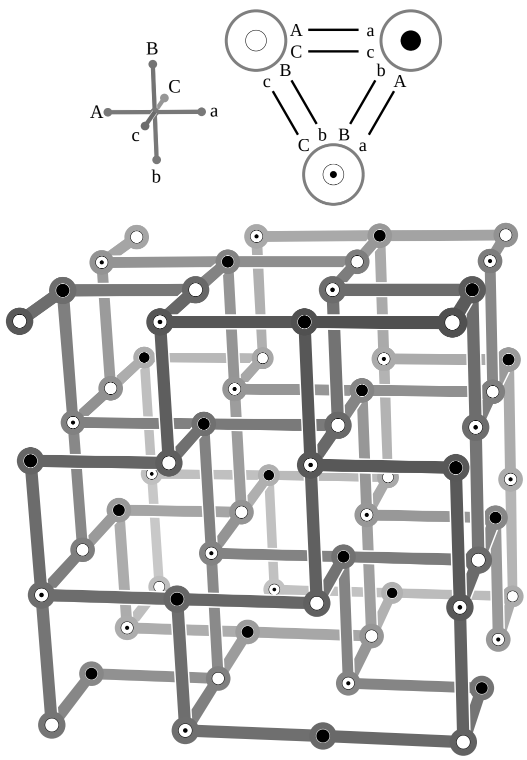
$K = \{\bigcirc, \bullet, \odot\}$

$\Sigma = \{a, b, c, A, B, C\}$
$a = (0, 1, 0)$
$b = (0, 0, 1)$
$c = (1, 0, 0)$
$A = (0, -1, 0)$
$B = (0, 0, -1)$
$C = (-1, 0, 0)$

$\delta(\bigcirc, a) = \bullet$
$\delta(\bigcirc, b) = \odot$
$\delta(\bullet, a) = \bigcirc$
$\delta(\bullet, c) = \odot$
$\delta(\odot, b) = \bigcirc$
$\delta(\odot, c) = \bullet$

$q_0 = \bigcirc$

Figure 7: a 3D regular lattice



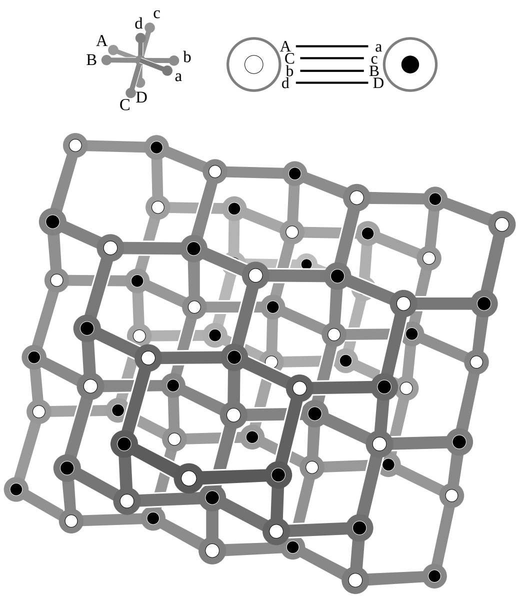
$K = \{\bigcirc, \bullet, \odot\}$

$\Sigma = \{a, b, c, A, B, C\}$
$a = (0, 1, 0)$
$b = (0, 0, 1)$
$c = (1, 0, 0)$
$A = (0, -1, 0)$
$B = (0, 0, -1)$
$C = (-1, 0, 0)$

$\delta(\bigcirc, c) = \odot$
$\delta(\bullet, a) = \bigcirc$
$\delta(\bullet, b) = \odot$
$\delta(\bullet, c) = \bigcirc$
$\delta(\odot, a) = \bullet$
$\delta(\odot, b) = \bigcirc$

$q_0 = \bigcirc$

Figure 8: a 3D regular lattice with no infinite lines.



$K = \{$○$,$●$\}$
$\Sigma = \{a, b, c, A, B, C\}$
$a = (1, 1, 1)$
$b = (-1, 1, 1)$
$c = (-1, -1, 1)$
$c = (1, -1, 1)$
$A = (-1, -1, -1)$
$B = (1, -1, -1)$
$C = (1, 1, -1)$
$D = (-1, 1, -1)$
$\delta($○$, b) =$ ●
$\delta($○$, d) =$ ●
$\delta($●$, a) =$ ○
$\delta($●$, c) =$ ○
$q_0 =$ ○

Figure 9: the diamond lattice

than the unit tiling description mentioned in the introduction.

4 Conclusions and Future Work

A method to describe crystal lattices in terms of automata has been presented. The main idea is to focus on the 1D connections rather than resort to the 2D and 3D volumes that standard tiling employs. The description seems to have potential for revealing the underlying relations between crystal lattices. To realize this potential, more complex chemical crystal lattices need to be explored. Aside from the application to crystallography, this framework seems to have geometrical merit. It has been noticed that some permutations on vectors in some of the *CLA* do not effect the resulting lattices. For instance, Figures 7 and 8, allow cyclic permutations of the vectors. A study of this property may provide a method to classify the symmetries in lattices.

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