Space groups and crystallography

Elisabet Edvardsson

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1 Introduction

Crystals are solids that possess long range order. In order to understand and describe the properties of solids, one needs to know more about what this long range order is. To do this one studies the crystal structure. A crystal structure can be described as a repeating pattern that can be extended indefinitely in space. One usually talks about the unit cell, the smallest unit that when repeated makes up the pattern without leaving any holes. The theory behind the crystal structures is not limited to the study of solids, it describes all repeated patterns that can be obtained in this way, in any dimension.

An interesting question is how many of these structures there are. In this report a way to classify and count n-dimensional crystal structures will be examined. Section 2 and section 3 will give a mathematical definition of a crystal structure along with some basic properties of isometries, i.e. distance preserving maps, which are essential in the description of crystal structures. In section 4 the concept of space groups will be introduced and it will be shown that instead of classifying and counting crystal structures, one can classify and count space groups. A way to determine equivalence between space groups will be given. In section 5, the concept of crystal classes will be defined. Section 6 gives a brief introduction to cohomology of groups and shows a way to prove the *Main Theorem of Mathematical Crystallography*, a theorem that is used to count the number of possible n-dimensional crystal structures. Finally, section 7 shows how this theorem can be used in the 2-dimensional case.

2 Crystals structures and the Euclidean space

Let $\mathbb{R}^n$ denote the n-dimensional real space. A point in $\mathbb{R}^n$ is specified by n real ordered numbers, $(x_1, x_2, ..., x_n)$. Points are added component-wise and can be multiplied by a scalar. Naturally, to describe crystal structures, one has to be able to talk about lengths and angles and thus the inner product on $\mathbb{R}^n$ is needed.[1]

Definition 2.1. Let $x = (x_1, x_2, ..., x_n)$ and $y = (y_1, y_2, ..., y_n)$ be vectors in $\mathbb{R}^n$. The inner product of x and y is the sum

$$\langle x, y\rangle = \sum_{i=1}^{n} x_i y_i$$

Definition 2.2. The length of a vector, x, is defined as

$$\|x\| = \sqrt{\langle x, x\rangle}$$

Definition 2.3. The angle, θ, between two vectors, x and y, is defined as

$$\cos\theta = \frac{\langle x, y\rangle}{\|x\|\,\|y\|}$$

Definition 2.4. The distance between two vectors, x and y, is defined as $\|x - y\|$.

The real space, $\mathbb{R}^n$, together with the inner product described above defines an n-dimensional Euclidean space and is denoted by $\mathbb{E}^n$.

Definition 2.5. [1, 2] An isometry, or rigid motion, of the Euclidean space is a map $f : \mathbb{E}^n \to \mathbb{E}^n$ that preserves distances. That is, $\|f(x) - f(y)\| = \|x - y\|$ for all $x, y \in \mathbb{E}^n$.

Remark. It is clear that all translations are isometries [4].

Having defined these concepts, it is possible to give a precise mathematical definition of a crystal structure.

Definition 2.6. [1, 2] Let $C \subset \mathbb{E}^n$ and let R be the set of isometries that preserve C. Then C is a n-dimensional crystal structure if:

- R contains n linearly independent translations.
- There exists a $D > 0$ such that any translation in R has a magnitude greater than D.

The n linearly independent translations with a smallest magnitude in a crystal structure correspond to the repetition of the unit cell described in section 1.

3 Isometries on the Euclidean space

The set of all isometries will be denoted by $\text{Isom}(\mathbb{E}^n)$.

As mentioned in section 2 all translations are isometries. Further, this is also true for all orthogonal transformations. The orthogonal transformations form a group, $O(n)$, under composition of maps. Let t_v denote a translation by v and let $V = \{t_v : v \in \mathbb{E}^n\}$ denote the set of all translations on $\mathbb{E}^n$. V forms a group under composition of maps given by $t_v \circ t_w = t_{v+w}$. It turns out that these kinds of isometries are sufficient to describe all rigid motions as can be seen by the following theorem:

Theorem 3.1. [4] *An isometry of $\mathbb{E}^n$ can be written uniquely as $t_v \circ \phi$, where t_v is a translation by a vector v and $\phi \in O(n)$*

Proof. Let $f : \mathbb{E}^n \to \mathbb{E}^n$ be an isometry. If $f = t_v \circ \phi$, then for all vectors $x \in \mathbb{E}^n$ one has that $f(x) = t_v(\phi(x)) = \phi(x) + v$. Setting $x = 0$ one has that $f(0) = \phi(0) + v = v$. Thus v is determined by f. Substituting $f(0)$ for v one gets that $\phi(x) = f(x) - f(0)$, which means that also ϕ is determined by f. To see that also the converse is true, define $g_1(x) = x + f(0)$ and $g_2(x) = f(x) - f(0)$. Then g_1 is a translation and g_2 an orthogonal transformation. The last equality gives $f(x) = g_2(x) + f(0) = g_1 \circ g_2(x) = t_v \circ \phi(x)$ for $v = f(0)$. Thus f is uniquely determined.[4] ∎

It turns out that it is desirable to rewrite this in terms of abstract algebra. To simplify notation, let (v, ϕ) denote the element $t_v \circ \phi$ in $\text{Isom}(\mathbb{E}^n)$.

Theorem 3.2. [1] *Isom$(\mathbb{E}^n)$ forms a group under composition of maps.*

Proof. : Let $(v, \phi), (v_1, \phi_1), (v_2, \phi_2) \in \text{Isom}(\mathbb{E}^n)$. Consider the product of two elements, (v_1, ϕ_1) and (v_2, ϕ_2), of $\text{Isom}(\mathbb{E}^n)$ acting on some vector $x \in \mathbb{E}^n$.

$$\begin{aligned}(v_1, \phi_1)(v_2, \phi_2)(x) &= (v_1, \phi_1)(v_2 + \phi_2(x)) = v_1 + \phi_1(v_2 + \phi_2(x)) = \\ &= v_1 + \phi_1(v_2) + \phi_1\phi_2(x) = (v_1 + \phi_1(v_2), \phi_1\phi_2)(x)\end{aligned}$$

It is clear that $(v_1, \phi_1)(v_2, \phi_2) = (v_1 + \phi_1(v_2), \phi_1\phi_2)$ is again an element of $\mathrm{Isom}(\mathbb{E}^n)$, thus $\mathrm{Isom}(\mathbb{E}^n)$ is closed under composition of maps.

One also sees that $(0,1)(v,\phi) = (0 + 1(v), 1\phi) = (v,\phi) = (v + \phi(0), \phi 1) = (v,\phi)(0,1)$, and thus $(0,1)$ is the unit element of $\mathrm{Isom}(\mathbb{E}^n)$.

As mentioned, V forms a group under composition of maps and it is clear that $t_v^{-1} = t_{-v}$. Also, since $O(n)$ is a group, every ϕ has an inverse, ϕ^{-1}. From the formula for multiplication of two elements, it is easy to see that an inverse of (v,ϕ) must be $(v,\phi)^{-1} = (-\phi^{-1}(v), \phi^{-1})$

Since composition of maps is associative, $\mathrm{Isom}(\mathbb{E}^n)$ forms a group under composition of maps. ■

This group is called the Euclidean group or the group of isometries. A closer examination of the product of two isometries given in theorem 3.2 immediately brings the thought to the semi-direct product of two groups:

Definition 3.1. Let H and G be two groups, and define an action of H on G by $\rho : H \to \mathrm{Aut}(G)$. The semi-direct product, $H \rtimes_\rho G$ is defined as the set $H \times G$ together with a product:

$$(h_1, g_1)(h_2, g_2) = (h_1\rho(g_1)(h_2), g_1g_2)$$

Thus $\mathrm{Isom}(\mathbb{E}^n)$ can be written as [1]

$$\mathrm{Isom}(\mathbb{E}^n) = V \rtimes O(n)$$

There are several important subgroups of $\mathrm{Isom}(\mathbb{E}^n)$, two of which will be described in the following propositions.

Proposition 3.3. [1] *V is a normal subgroup of Isom($\mathbb{E}^n$).*

Proof. Let $t_v = (v,1) \in V$ and let $f = (w,\phi) \in \mathrm{Isom}(\mathbb{E}^n)$. Now consider conjugation of t_v by f:

$$\begin{aligned} f^{-1} \circ t_v \circ f &= (w,\phi)^{-1}(v,1)(w,\phi) = (-\phi^{-1}(w), \phi^{-1})(v,1)(w,\phi) = \\ &= (-\phi^{-1}(w) + \phi^{-1}(v), \phi^{-1})(w,\phi) = (-\phi^{-1}(w) + \phi^{-1}(v) + \phi^{-1}(w), \phi^{-1}\phi) = \\ &= (\phi^{-1}(v), 1) \end{aligned}$$

Since $(\phi^{-1}(v), 1) \in V$, V is a normal subgroup of $\mathrm{Isom}(\mathbb{E}^n)$ ■

Proposition 3.4. [2] *The set of isometries R, that preserve a crystal structure, $C \subset \mathbb{E}^n$, is a subgroup of Isom($\mathbb{E}^n$).*

Proof. It is clear that the identity transformation preserves C. Let $r \in R$ and $c \in C$. Every isometry has an inverse and if $r(c) = c' \in C$ it is clear that $r^{-1}(r(c)) = r^{-1}(c') = c \in C$. Thus, $r^{-1} \in R$. Further, if $r_1, r_2 \in R$, then $r_2(r_1(c)) \in C$ and $r_2 \circ r_1 \in R$. Thus $R < \mathrm{Isom}(\mathbb{E}^n)$ ■

That the group of translations is a normal subgroup, is a fact that turns out to be essential in the description of crystal structures, and will be of use later in the report.

Proposition 3.4 means that instead of directly describing the crystal structure, one can look at the associated group, R, and describe the properties of the group. As will be seen in the next section, R is a so called space group and the classification of crystal structures can be done by classifying the space groups.

4 Space groups

To understand the concept of space groups one needs some knowledge of topology, in particular the following basic definitions are useful:

Definition 4.1. [6, 7] A topology on a set X is a collection of subsets, τ, including X itself and the empty set, such that any union of sets in τ is in τ and any finite intersection of sets in τ is in τ.

Remark. The sets in τ are called open.

Definition 4.2. [6, 7] A topological space is a set X together with a topology, τ.

Definition 4.3. [6] Let Y be a subset of X. If, for any collection of open sets $\{U_\alpha : \alpha \in A\}$ such that X is contained in the union of the U_α, there is a finite subset $\{\alpha_1, ..., \alpha_m\}$ of A so that Y is contained in the union $U_{\alpha_1} \cup ... \cup U_{\alpha_1}$, Y is called compact.

Remark. In particular, in $\mathbb{R}^n$, a compact subspace is a subspace that is closed and bounded.

Definition 4.4. [1] Let G be a group, let X be a subset of $\mathbb{R}^n$ and define an action of G on X. A fundamental domain of the action of G on X is an open subset D that satisfies the following two properties:

1. $\bigcup_{g \in G} g.D = X$

2. $D \cap g.D = \emptyset$ for $g \neq 1$

Proposition 4.1. [1] *The action of G on X is an equivalence relation $\sim$, by $x \sim y$ if there exists a $g \in G$ such that $x = g.y$*

Proof. Since the identity element is in G, $x \sim x$. Every element in G has an inverse, therefore, if $x = g.y$, then $y = g^{-1}.x$ and $x \sim y \Rightarrow y \sim x$. Finally, if $x \sim y \Leftrightarrow x = g_1.y$ and $y \sim z \Leftrightarrow y = g_2.z$,then $x = g_1 g_2.z \Leftrightarrow x \sim z$. Thus $\sim$ is an equivalence relation. ∎

This is a useful fact due to the following defintions.

Definition 4.5. [7] Let X be a topological space and let $\sim$ be an equivalence relation on X. The quotient space $Y = X/\sim$ is defined as $Y = \{[x] \,|x \in X\}$, where $[x]$ is the equivalence class that contains x.

What one does when dividing a topological space into quotient spaces is basically to identify subsets and say that their elements are one and the same. A slightly different way to think of quotient spaces, is therefore to think of them as gluing subsets together [7]. For example, consider a straight line with end points p_1 and p_2 and an equivalence relation $x \sim y \Leftrightarrow x = y$ or $x = p_1, y = p_2$. This can be thought of as saying that p_1 and p_2 are the same point and thus as gluing the end points of the circle together. Therefore the quotient space of the straight line in this case is topologically a circle.

Definition 4.6. [1] A discrete subgroup G of Isom($\mathbb{E}^n$) is a space group if the quotient space $\mathbb{E}^n/G$ is compact.

Using the argument above about gluing, it is not difficult to see that compactness of the quotient space is equivalent to compactness of the closure of the fundamental domain of the action of G on $\mathbb{E}^n$. This means that instead of determining the quotient space, one can calculate the orbits of the action of G on $\mathbb{E}^n$, something that might be simpler.

It is not immediately obvious how the definition of a space group relates to the definition of crystal structures, but the following two theorems show the connection and allows to identify every space group, G, with a crystal structure preserving group, R.

Theorem 4.2. [1] Bieberbach's first theorem
A discrete subgroup G of Isom($\mathbb{E}^n$) is a space group if and only if G contains n linearly independent translations.

Theorem 4.3. *A group G is a space group if and only if it preserves a crystal structure $C \subset \mathbb{E}^n$*

The proof is an altered version of the proof given in [2].

Proof. Definition 2.6 says that every group R that preserves a crystal structure is discrete and contains n linearly independent translations. Thus, by definition 4.6 and theorem 4.2 every such group R is a space group.

To see that the converse is true, one must show that given a space group G, it is possible to construct a crystal structure that is preserved under the action of G. First of all, consider the action of G on $\mathbb{E}^n$. By definition of the space group, the fundamental domain, D, of this action is bounded. Choose an asymmetric subset $P \subset D$ (i.e. choose P such that the only isometry that preserves P is the identity transformation). This means that $P \cap g.P = \emptyset$ for all $g \in G$. Let C be the orbit of P under the action of G. Let R be the set of transformations that preserve C. Since the pattern of P is asymmetric, any $r \in R$ must send P into the same place as some $g \in G$. Thus $R = G$ and since G is discrete and contains n linearly independent translations, C is a crystal structure. Thus the statement is true. ■

Theorem 4.3 shows that instead of classifying and counting crystal structures one can classify and count space groups. To be able to do this, one needs to know when two space groups are considered equivalent. There are two generally accepted definitions of this, that turn out to be equivalent.

Definition 4.7. [1] Two space groups are equivalent if they are isomorphic as groups.

This definition is certainly nice from a group theoretic point of view, but it is not immediately obvious that it is equally nice from a crystallographic point of view. However, it turns out that the above mentioned equivalent definition solves this problem, but to see this one first needs to define what an affine transformation is.

Definition 4.8. [3] An affine transformation is a transformation that preserves collineratity (i.e. points lying on a straight line will still lie on a straight line after the transformation) and ratios of distances.

Remark. In contrast to isometries, affine transformations need not preserve distances.

Just as in the case of isometries, the affine transformations form a group under composition of maps.

Definition 4.9. The affine group on $\mathbb{E}^n$, $\mathrm{Aff}(\mathbb{E}^n)$, is the group of all invertible affine transformations on $\mathbb{E}^n$.

The affine group of the affine space, A, on a vector space V can be realized as the semi-direct product of all translations on V and the general linear group on V. That is, $\mathrm{Aff}(A) = V \rtimes \mathrm{GL}(V)$, with the action of $\mathrm{GL}(V)$ on V being the natural one, i.e. linear transformations [1].

Theorem 4.4. [1] Bieberbach's second theorem
Any abstract isomorphism of space groups can be realized by conjugation by an affine motion of $\mathbb{E}^n$.

This means that two space groups are isomorphic if and only if they are conjugate by an element of $\mathrm{Aff}(\mathbb{E}^n)$. This shows that definition 4.7 is nice also when considering the crystal structure, since conjugation in the affine group means that one does not distinguish between crystal structures that differ in e.g. size [2].

5 Crystal classes

A more abstract version of theorem 4.2 is the following:

Theorem 5.1. [1] *An abstract group G is isomorphic to an n-dimensional space group if and only if G contains a finite index, normal, free abelian subgroup of rank n, that is also maximal abelian.*

No complete proof will be given here. However, a discrete group of translations must be free abelian. Therefore, by theorem 4.2 and proposition 3.3 one sees that a space group contains a free abelian normal subgroup of rank n.

The maximal abelian subgroup of rank n described in the theorem corresponds to the n linearly independent translations in theorem 4.2. This subgroup is denoted by M. Since M is free abelian one has that $M \cong \mathbb{Z}^n$ and therefore it is called the lattice [1].

M is a normal subgroup of G, and therefore the quotient group $H = G/M$, called the point group, can be constructed [1]. It turns out that H is isomorphic to a finite subgroup of $O(n)$. That this is true can be seen by rewriting the expression for H in the following way [2].

$$H = G/M = G/G \cap V \cong V.G/V \hookrightarrow \mathrm{Isom}(\mathbb{E}^n)/V = O(n)$$

Definition 5.1. [1] A sequence of groups, G_1, G_2, G_3, with connecting homomorphisms $f_1 : G_1 \to G_2$ and $f_2 : G_2 \to G_3$, usually written as

$$G_1 \stackrel{f_1}{\to} G_2 \stackrel{f_2}{\to} G_3$$

is a short exact sequence if f_1 is a monomorphism, f_2 an epimorphism and $\mathrm{im}(f_1) = \ker(f_2)$.

Remark. A short exact sequence can also be written as an exact sequence with five elements: $1 \to G_1 \stackrel{f_1}{\to} G_2 \stackrel{f_2}{\to} G_3 \to 1$. This appears to be more common, but in this report the notation used in [1] has been chosen.

It is straightforward to check that G, H and M fit info a short exact sequence

$$M \stackrel{i}{\to} G \stackrel{p}{\to} H$$

By this there is an induced action of H on M. Let $h \in H$ and $m \in M$, then $h.m = h'mh'^{-1}$ with $h' \in G$ such that $p(h') = h$.

The fact that M, G and H fit into a short exact sequence, gives a way to classify crystal structures and divide them into so called crystal classes: The lattice M, together with the point group H and the action of H on M determine a crystal class, denoted by (H, M) [1].

Since M is free abelian, it is possible to choose an integral basis for M. The action of H on M is then an injective homomorphism, $f : H \to \mathrm{Aut}(M) \cong \mathrm{GL}(n, \mathbb{Z})$. Therefore, after choosing this basis for M, H is embedded as a subgroup $f(H)$ of $\mathrm{GL}(n, \mathbb{Z})$ [1].

Again, to be able to classify crystal structures, one needs to know when they are considered equivalent. This is also the case for crystal classes. In fact there are two different notions of equivalence, there are the arithmetic- and the geometric crystal classes.

Definition 5.2. [1] Let (H, M) and (H, M') be two crystal classes with actions f and f' respectively. If there exists an isomorphism $\alpha : M \to M'$ such that

$$\alpha f(h) = f'(h)\alpha$$

for all $h \in H$, then (H, M) and (H, M') are said to be arithmetically equivalent.

Rewriting the relation in the definition gives $\alpha \circ f \circ \alpha^{-1} = f'$, which says that the subgroups $f(H)$ and $f'(H)$ are conjugate in $\mathrm{GL}(n, \mathbb{Z})$. If one allows the subgroups to be conjugate in $\mathrm{GL}(n, \mathbb{Q})$, the crystal classes are instead called geometrically equivalent [1].

In the rest of this report only the arithmetic equivalence will be considered.

6 Cohomology of groups

To further count and classify the crystal structures, the concept of cohomology of groups is needed.

Definition 6.1. [8] Let $..., A^{-2}, A^{-1}, A^0, A^1, A^2, ...$ be a sequence of abelian groups connected by homomorphisms, $d^n : A^n \to A^{n+1}$, such that $d^{n+1} \circ d^n = 0$. The sequence together with the homomorphisms form a cochain complex.

Definition 6.2. [6, 8] An element of the kernel of d^n is called a n-cocycle and an element of the image of d^{n-1} is called a n-coboundary. The group of n-cocycles is denoted by Z^n and the group of n-coboundaries is denoted by B^n.

Since all A^n are abelian, all their subgroups are normal. Further, since $d^{n+1} \circ d^n = 0$, $\text{im}(d^{n-1})$ must be a normal subgroup also of $\ker(d^n)$. Thus the quotient group of these can be formed.

Definition 6.3. [6, 8] Let $H^n = Z^n/B^n$. This is called the nth cohomology group of the cochain.

As will be seen later, in the case of crystal structures, one is interested in certain types of maps between groups of maps. This motivates the following definitions:

Definition 6.4. [6, 8] Let $C^n(G, M)$ be the group of all functions from G^n (the Cartesian product of n copies of G) to M. The elements of this group are called n-cochains.

Definition 6.5. [8] A n-coboundary is a homomorphism $d^n : C^n(G, M) \to C^{n+1}(G, M)$ that for any $f \in C^n(G, M)$ satisfies

$$d^n f(g_1, g_2, ..., g_n) = g_1 f(g_2, ..., g_{n+1}) + \sum_{i=1}^{n} (-1)^i f(g_1, ..., g_{i-1}, g_i g_{i+1}, g_{i+2}, ..., g_{n+1}) + \\ + (-1)^{n+1} f(g_1, ..., g_n)$$

In particular, for $n = 0$ and $n = 1$, one has that

- $d^0 m(g) = gm - m$ (This is a special case. Since a 0-cochain has no arguments it is a constant $m \in M$.)
- $d^1 f(g_1, g_2) = g_1 f(g_2) - f(g_1 g_2) + f(g_2)$

Proposition 6.1. [8] *For all n-coboundaries, $d^{n+1} \circ d^n = 0$.*

The proof of this proposition involves long calculations and is therefore left out.

This proposition shows that the groups $C^n(G, M)$ form a cochain complex and thus it is possible to define the coboundary-, cocycle- and cohomology groups. For the discussion of crystal structures, only the 1-cocycles and 1-coboundaries are needed.

- A 1-cocycle is obtained by letting the expression for $d^1 f(g_1, g_2)$ equal zero. Therefore, the group of 1-cocycles, $Z^1(G, M)$, must consist of all functions, $f : G \to M$ that satisfy $f(g_1 g_2) = f(g_1) + g_1.f(g_2)$.

- The group of all 1-coboundaries, $B^1(G,M)$, are simply all functions, $f_m : G \to M$, that satisfy $f_m(g) = d^0m(g) = m - g.m$.

Combining these, one gets the first cohomology group:[8]

$$H^1(G,M) = Z^1(G,M)/B^1(G,M)$$

Before one can appreciate the necessity of cohomology of groups, a few more observations are needed. Returning to the description of the space group in terms of a short exact sequence,

$$M \xrightarrow{i} G \xrightarrow{p} H$$

together with the induced action of H on M, it is natural to wonder if G is the semidirect product of M and H. As the following result will tell, this is not always the case.

Proposition 6.2. [5] *Let $M \xrightarrow{\alpha} G \xrightarrow{\beta} H$ be a short exact sequence. Then G is isomorphic to a semidirect product of the two groups M and H, $M \rtimes_\gamma H$ if and only if there exists a homomorphism $\phi : H \to G$ such that $\beta \circ \phi = id_H$. In this case $\gamma : H \to Aut(M)$ is given by*

$$\alpha(\gamma(h)(m)) = \phi(h)\alpha(n)\phi(h^{-1})$$

The proof of this is long and will be left out, it can however be found in [5], page 5.

Also, given M and H, they do not uniquely determine a G. This is because non-isomorphic groups can have isomorphic normal subgroups with isomorphic quotient groups. For example there are the groups

$$D_4 = \langle r, m | r^4, m^2, (rm)^2 \rangle$$

and

$$Q_8 = \langle -1, i, j, k | (-1)^2 = 1, i^2 = j^2 = k^2 = ijk = -1 \rangle$$

Clearly D_4 is not isomorphic to Q_8. However, $\langle r^2 \rangle \triangleleft D_4$ and $\{\pm 1\} \triangleleft Q_8$. One also has that $\langle r^2 \rangle \cong \{\pm 1\} \cong \mathbb{Z}_2$ and $D_4 / \langle r^2 \rangle \cong Q_8 / \{\pm 1\} \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ [5]

By proposition 3.4, $G < \text{Isom}(\mathbb{E}^n)$, which is the same thing as saying that $G < V \rtimes O(n)$, and thus every element of G can be written as (v, h) where $v \in V$ and $h \in O(n)$. As mentioned earlier, H is isomorphic to a finite subgroup of $O(n)$. Since this report is only concerned with the number of unique space groups, and not with what the elements of G are, one can choose G such that H is a subgroup of $O(n)$ (since counting the number of unique space groups is the same thing as determining the number of non-isomorphic space groups). Therefore, since p is a map from G to H, one can let p be a projection onto $h \in O(n)$.

Let $\tau : H \to G$ be a map such that $p(\tau(h)) = h$ for all $h \in H$. Since p is a projection onto $O(n)$, $\tau(h) = (\sigma(h), h)$ for some map $\sigma : H \to V$. The map σ is called the section of the exact sequence [1].

The choise of σ is not unique, since every h allows for $\sigma(h)$ to one be of many elements of V. However, by composing σ with the natural projection, $\pi : V \to V/M$, such that $v \in V$ is mapped to the coset of M containing v, one gets a new map $s = \pi \circ \sigma : H \to V/M$ [1].

Proposition 6.3. [1] *The map $s : H \to V/M$ is well defined.*

Proof. Let σ and σ' be two sections of the exact map and let $\pi : V \to V/M$ be the natural projection. Let $s = \pi \circ \sigma$ and $s' = \pi \circ \sigma'$. Assume that $s(h) \neq s'(h)$. Then consider the following product: $(\sigma(h), h)(\sigma'(h), h)^{-1} = (\sigma(h), h)(-h^{-1}\sigma'(h), h^{-1}) = (\sigma(h) - \sigma'(h), 1)$. For this to make sense, $\sigma(h) - \sigma'(h)$ must be in M. Composing this with the natural projection, one has that $\pi(\sigma(h) - \sigma'(h)) = 0$ and since π is a homomorphism, this gives $\pi(\sigma(h)) = \pi(\sigma'(h))$. However, the assumption was that $s(h) \neq s'(h)$, thus this is a contradiction. Therefore $s'(h) = s(h)$ and s is well defined. [1] ■

The map s turns out to be important. By proposition 6.4, s is determined by G. Further, also G is determined by s, as can be realized by observing that [1]

$$G = \{(v, h) \in \mathrm{Isom}(\mathbb{E}^n) : h \in H, v = s(h)\}$$

Therefore, instead of classifying space groups one can classify the maps s. To do this, a closer study of s is required.

Proposition 6.4. [1] *The map s satisfies the following two properties:*

1. $s(1) = 0$
2. $s(h_1 h_2) = s(h_1) + h_1 s(h_2)$

Proof. Consider the product $(s(x), x)(s(y), y)$. M is invariant under the action of H, therefore there is also an action of H on V/M and multiplication can be carried out in the same way as earlier. One gets that $(s(x), x)(s(y), y) = (s(x) + x.s(y), xy)$. For this to make sense, one needs to identify $s(xy)$ and $s(x)+x.s(y)$ and thus 2. is proven [1].

1. follows from 2. in the following way: $s(1) = s(1 \cdot 1) = s(1) + 1.s(1) = s(1) + s(1) \Leftrightarrow s(1) = 0$. ■

A closer look at the expression for $s(xy)$, shows that s must be a 1-cocycle and the set of all such $s : H \to V/M$ therefore form the group $Z^1(H, V/M)$.

Bieberbach's second theorem, theorem 4.4, says that two space groups are equivalent if they are conjugate in the Affine group. Therefore, to classify the elements of $Z^1(H, V/M)$, one needs to examine what happens to the 1-cocycles under this kind of conjugation and determine which 1-cocycles give the same space group. As mentioned earlier, the affine group on $\mathbb{E}^n$ is given by $\mathrm{Aff}(\mathbb{E}^n) = V \rtimes \mathrm{GL}(V)$. Let (a, g) be an element of $\mathrm{Aff}(\mathbb{E}^n)$. It is clear that $(a, g) = (0, g)(a, 1)$. Hence every element of $\mathrm{Aff}(\mathbb{E}^n)$ can be written as a composition of a translation and an element of $GL(V)$ and it suffices to check the conjugacy of a space group with each of these two elements seperately. [1]

Let $a \in V$ and let $s : H \to V/M$ be a 1-cocycle. Then one has

$$(a, 1)(s(h), h)(a, 1)^{-1} = (a, 1)(s(h), h)(-a, 1) = (a + s(h) - h(a), h)$$

One sees that conjugating by $(a, 1)$ is the same as adding the expression $B_\alpha = \alpha - h(\alpha)$, where $\alpha = a \mod M$, to s. Comparing this to the expression for a 1-coboundary mentioned above, one sees that the set of all B_α forms the group $B^1(H, V/M)$ [1].

Thus all space groups corresponding to maps s plus an arbitrary 1-coboundary are isomporphic, and thus equivalent. To get rid of these isomorphisms, one can consider the quotient group of $Z^1(H, V/M)$ and $B^1(H, V/M)$, but as defined above, this is exactly the first cohomology group, $H^1(H, V/M)$ [1].

Now consider the effect of conjugation with an element of $GL(V)$. Let $(0, g) \in \mathrm{GL}(V)$. Then

$$(0, g)(s(h), h)(0, g)^{-1} = (0, g)(s(h), h)(0, g^{-1}) = (g(s(h)), ghg^{-1})$$

To see where this leads, one needs to define an action of g on the set of 1-cocycles. A convenient choice is:

$$(g.s)(h) = gs(g^{-1}hg)$$

Then one has that

$$(0, g)(s(h), h)(0, g)^{-1} = (gs(g^{-1}hg), ghg^{-1})$$

If g is in the normalizer, $N(H, M) = \{g \in \mathrm{Aut}(M) : gH = Hg\}$, of H in $\mathrm{Aut}(M)$, then the space groups are isomorphic, and the 1-cocycles should be identified. This also shows that conjugating a space group by $(0, g)$ changes the 1-cocycle to gs [1].

All of this leads to the main theorem of this report:

Theorem 6.5. [1] Main theorem of mathematical crystallography
There exists a one-to-one correspondence between space groups in the arithmetic crystal class (H, M) and the orbits of $N(H, M)$ acting on the 1-dimensional cohomology group $H^1(H, V/M)$.

Remark. It can be shown that $H^1(H, V/M) \cong H^2(H, M)$, and actually, $H^2(H, M)$ seems to be more common to use.

The main theorem of mathematical crystallography turns out to be useful for classifying crystal structures and to find out how many different structures there are. In general, to count all n-dimensional crystal structures, it can be advantageous to represent the group elements as $n \times n$-matrices. Then the following algorithm can be used:[2]

1. Determine all possible point groups, H.
2. For each H, determine all unique representations of the generators and calculate $N(H, M)$.
3. For each representation, determine $H^1(H, V/M)$
4. Determine the orbits of $N(H, M)$ on $H^1(H, V/M)$

In the next section an example of how to use this algorithm will be shown.

7 2-dimensional space groups

In this section the 2-dimensional space groups, also called wallpaper groups, will be examined. The first thing that needs to be done, is to find all possible point groups. It turns out, as will be seen by the following results, that the number of possibilities is quite limited in the 2-dimensional case.

Proposition 7.1. [2] *Let $M \cong \mathbb{Z}^n$ and let g be an automorphism of finite order of M. Then g has order 1, 2, 3, 4 or 6.*

Proof. g must be an orthogonal transformation of M and therefore g is either a rotation or a reflection. If g is a reflection, it has order 2, therefore assume that g is a rotation through an angle θ. Since M is discrete, there exists a non-zero vector $m \in M$ of minimal length. The composition $t_m g^{-1} t_{-m}$ then describes a rotation through an angle $-\theta$ around the point m. Now let $v = t_m g^{-1} t_{-m}(0)$ and consider the difference $w = v - gu$. w must be a vector in the same direction as u. Since u is the shortest possible such vector and since $M \cong \mathbb{Z}^n$ w must be an integer multiple of u. Therefore, the only possible values of θ are $0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$. Thus the rotations all have order 1, 2, 3, 4 or 6. Since all reflections have order two, all g must be of order 1, 2, 3, 4 or 6. [2] ■

Proposition 7.2. [2] *Any finite group of real 2×2 matrices is either cyclic or dihedral.*

Propositions 7.1 and 7.2 show that the only possible 2-dimensional point groups are

$$e, \mathbb{Z}_2, \mathbb{Z}_3, \mathbb{Z}_4, \mathbb{Z}_6, D_1, D_2, D_3, D_4, D_6$$

The above-mentioned algorithm requires a lot of calculations for each point group, and therefore only a simple example concerning the trivial group will be shown here. (In [1] there is a thorough examination of $H = D_4$.)

Let $H = e$ and choose the basis $\mathbb{Z}e_1 \times \mathbb{Z}e_2$ for the lattice M, where e_1 and e_2 are the ordinary unit vectors. H has one generator, e, and it has order 1. Represented as 2×2-matrices, H is generated by

$$R = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Let $s : H \to V/M$ be a 1-cocycle. s transforms the elements of H and thus one needs to find out what $s(R)$ is. Since $s(R)$ is an element in V/M, it is a vector, so let

$$s(R) = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

However, R is the identity element, and by proposition 6.4 $s(1) = 0$, with 0 being the coset that contains 0. Thus $s(R)$ must always be the zero-vector, and the only 1-cocycle that exists is the trivial one that maps everything to 0. Thus $Z^1(H, V/M)$ only contains a single element and is isomorphic to the trivial group.

Since $Z^1(H, V/M)$ only contains one element, it must be equal to $H^1(H, V/M)$. The action of the normalizer will then generate only one orbit, and thus there is exactly one space group corresponding to the trivial point group.

Of course, the trivial group is generally considered uninteresting, but the reasoning is the same as in a non-trivial case. A non-trivial group can be presented on the form $H = \langle g_1, ..., g_m | r_1 = ... = r_n = 1 \rangle$, where the g:s are the generators and the r:s relations. Representing H with matrices and letting R_k be the matrix corresponding to the relation r_k one has that $s(R_k)$ must be an integer vector. This gives conditions on the elements of the vectors $s(G_k)$, where G_k is the matrix corresponding to the generator g_k. To further determine the possible values of $s(G_k)$ one can add appropriate 1-coboundaries and in that way see how many unique 1-cocycles there are. This is the number of possible choices of the vectors $s(G_k)$, and corresponds to the group $H^1(H, V/M)$. [1]

Doing this for all above mentioned two-dimensional point groups, gives the result shown in table 1. One sees that in total there are 17 different two-dimensional space groups.

Point group	Representation of generators	$H^1(H, V/M)$	Number of space groups	Notation
e	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	1	1	p1
$\mathbb{Z}_2$	$\begin{pmatrix}-1 & 0\\0 & -1\end{pmatrix}$	1	1	p2
$\mathbb{Z}_3$	$\begin{pmatrix}0 & -1\\1 & -1\end{pmatrix}$	1	1	p3
$\mathbb{Z}_4$	$\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	1	1	p4
$\mathbb{Z}_6$	$\begin{pmatrix}0 & 1\\1 & 1\end{pmatrix}$	1	1	p6
D_1	$\begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}$	$\mathbb{Z}_2$	2	pm, pg
D_1	$\begin{pmatrix}1 & 1\\0 & -1\end{pmatrix}$	1	1	cm
D_2	$\pm\begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}$	$\mathbb{Z}_2 \times \mathbb{Z}_2$	3	pmm, pmg, pgg
D_2	$\pm\begin{pmatrix}1 & 1\\0 & -1\end{pmatrix}$	1	1	c2mm
D_3	$\begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}, \begin{pmatrix}0 & -1\\1 & -1\end{pmatrix}$	1	1	p3m1
D_3	$\begin{pmatrix}-1 & 0\\1 & 1\end{pmatrix}, \begin{pmatrix}-1 & -1\\1 & 0\end{pmatrix}$	1	1	p31m
D_4	$\begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}, \begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$	$\mathbb{Z}_2$	2	p4m, p4g
D_6	$\begin{pmatrix}-1 & 0\\0 & 1\end{pmatrix}, \begin{pmatrix}0 & 1\\1 & 1\end{pmatrix}$	1	1	p6m

Table 1: Point groups with corresponding space groups in 2 dimensions. The fifth column shows the standard crystallographic notation used for space groups. [1, 10, 9]

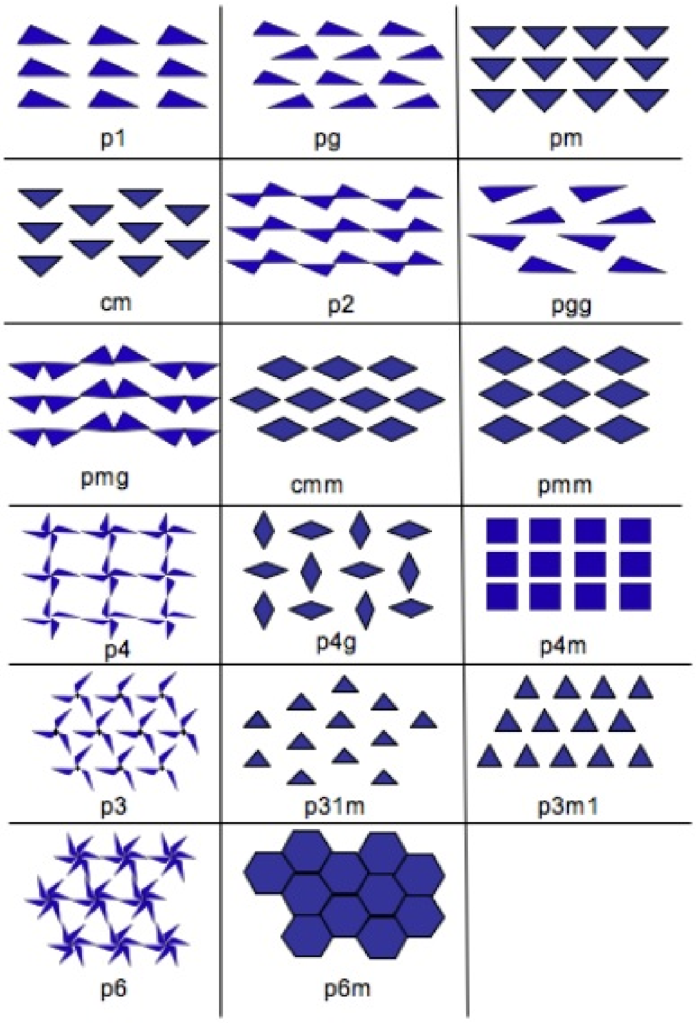

Figure 1: Pieces of the patterns that can be used to illustrate the 17 wallpaper groups. Image taken from [11]

Figure 1 shows patterns that correspond to these groups and is a nice way to illustrate the differences between them.

p1 is the space group that has the trivial group as point group. This means that the only maps that preserve the crystal structure are translations. Studying figure 1, one clearly sees that this is the case; the pattern cannot be rotated, reflected or glide reflected in any way without altering it. Similarly, in the case of p2, one sees in the picture that the pattern can be rotated 180° without altering it. This corresponds to the point group being $\mathbb{Z}_2$.

Figure 1 clearly shows the difference between space groups with different point groups. Take for example the space groups p6 and p6m. It is obvious that both patterns are invariant under rotation trough an angle $n60°$. However, one also sees that the p6m-pattern is invariant under certain reflections, which is not true for the p6-pattern. Therefore p6m must correspond to the point group D_6 and p6 to the point group $\mathbb{Z}_6$.

Instead of considering two different point groups, one can study the case where the same point group gives rise to different space groups. Take for example p4g and p4m. They both have D_4 as point group. Looking at the patterns in figure 1, one sees that both patterns have four lines of reflection meeting at one point. In the p4m-pattern, this point is also a center of rotation around which the pattern can be rotated trough an angle $n90°$. Also the p4g-pattern can be rotated through this angle, but the center of rotation is not located at the point where the lines of reflection meet. [1]

The 2-dimensional case is certainly nice when it comes to illustrating things, but in e.g. solid state physics it is the 3-dimensional case that is the most important. In three dimensions, according to mathematicians and the methods in this report, there are 219 space groups. According to crystallographers, however, there are 230. The difference arises because crystallographers consider crystals that are mirror-images of each other as being different. Mathematically, crystallographers use conjugation in the special affine group (i.e. affine mappings with positive determinant) as a definition of equivalence of space groups, in contrast to definition 4.7 and theorem 4.4 where conjugation in the affine group is used as criterion for equivalence [1].

In higher dimensions, the number of space groups grows fast, and according to [1] it has been shown that the number grows at least as fast as 2^{n^2}.

References

[1] Hiller, Howard. *Crystallography and cohomology of groups* The American Mathematical Monthly, Vol. 93, No. 10 (Dec., 1986), pp. 765-779.

[2] Webb, Peter J. *An Introduction to the Cohomology of Groups* Lecture notes, School of Mathematics, University of Minnesota, 2011

[3] Clapham, Christopher and Nicholson, James *The Concise Oxford Dictionary of Mathematics, 4th ed.* Oxford University Press, Oxford, 2009

[4] Conrad, Keith *Isometries of* $\mathbb{R}^n$ Lecture notes, Mathematics Department, University of Connecticut, 2012

[5] Conrad, Keith *Splitting of short exact sequences for groups* Lecture notes, Mathematics Department, University of Connecticut, 2008

[6] Fulton, William *Algebraic topology - A first course* Springer-Verlag New York, Inc. 1995

[7] Gamelin, Theodore W.; Greene, Robert Everist *Introduction to topology* Second edition, Dover publications, inc. Mineola, New York, 1999

[8] Moorhouse, Eric *Group Cohomology* Lecture notes, Topology II, Department of Mathematics, University of Wyoming, 2012

[9] Morandi, Patrick, J. *The Classification of Wallpaper Patterns: From Group Cohomology to Escher's Tessellations* Department of Mathematical Sciences, New Mexico State University

[10] Hrbek, Michal, *Group cohomology and wallpaper groups III*, Lecture notes, `http://www.karlin.mff.cuni.cz/jarniskola/files/prednasky/cohomology_3_hrbek.pdf`, visited 2014-12-10.

[11] Shakiban, Cheri, *Wallpaper Patterns* Lecture notes, Institute for Mathematics and its Applications, University of Minnesota