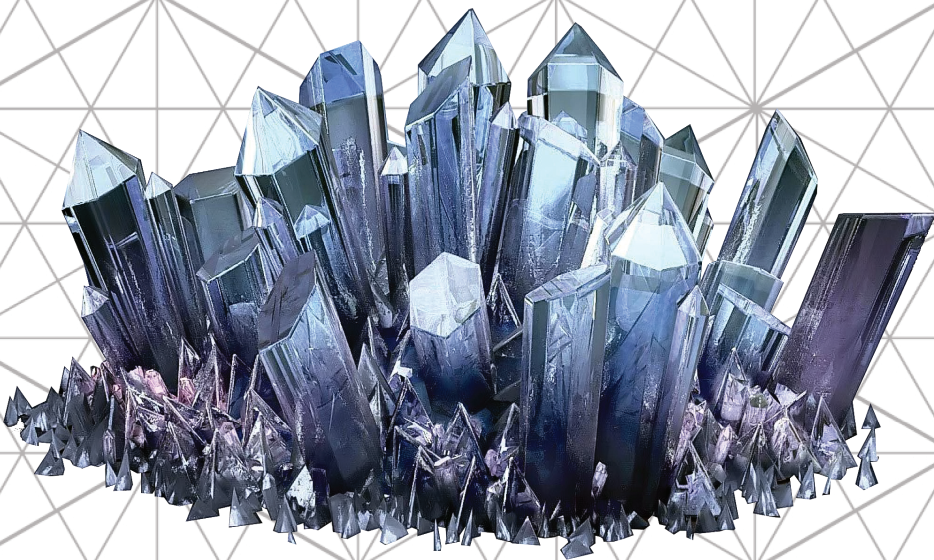
Ivan Červeň

CRYSTAL SYMMETRY

Historical development of ideas about symmetry from the beginning of the XVII. century to the middle of the XX. century
Authors, their publications and opinions



SPEKTRUM STU

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of the XVII. century to the middle
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Slovak University of Technology in Bratislava
2025

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PREFACE

We have a certain idea about the content of the concept of symmetry, but from the point of view of the theory of symmetry, its definition is needed. Arthur Schoenflies, one of the creators of the theory of crystal symmetry, wrote in 1889: "*There are objects whose peculiarity is that they can be identified with themselves in various ways - by rotation or mirroring." Such objects are said to be symmetric*".

In theoretical physics, other types of symmetries are also considered - time, space or charge symmetry of physical processes, but this text deals only with that type of symmetry, which we can call *shape symmetry*. The essence of shape symmetry is a certain regularity in the spatial arrangement of parts of the observed object, or in the sameness of its appearance when viewed from different sides. It is obvious that the shape symmetry of the sphere does not coincide with the shape symmetry of the cube, so we realize that there are objects with different types or degrees of shape symmetry. Various geometric shapes (cube, cone,...) are characterized by shape symmetry, but the symmetry of the external shapes of crystals has attracted special attention for a long time. According to current knowledge, external shapes are influenced by the arrangement of atoms, i.e. crystal structure, which can be characterized by one of 230 types of symmetry.

Considerations about symmetry can be supported by exact mathematics. From a mathematical point of view, symmetry of an object (not only shape) means the preservation of certain of its properties during certain changes (transformations) of the parameters that characterize its state. As for the symmetry of the shape, it is about rotations, mirroring, or displacements of the object, while these transformations are expressed with respect to the chosen frame of reference, in which each point of the object has its three spatial coordinates. If, during the transformation, the object reaches a position that we consider to be identical (equivalent) to the original position, then it is a so-called *symmetry operation*. For example, by rotating a square by 90° around an axis passing through its center and perpendicular to its plane, the vertices of the square get to new positions, but if we do not distinguish the vertices from each other - and this is how we will understand it in the next text - then the square gets to a position that is equal to original position. If it is a crystal, then its geometric and physical properties - with respect to the external reference frame - are preserved in all its points through the operation of symmetry. The symmetry of the crystal then means the set of all such operations.

Much effort has been devoted in the past to the description of the symmetry of crystals, i.e., to the description of the relevant set of symmetry operations and methods for their determination. This has led to the development of the theory of crystal symmetry. This text was written with the intention of conveying the development of this theory - from the first scientific experiments already in the XVII. century until its completion in the middle of the XX. century. But the symmetry of objects attracted attention already in ancient times - Egypt, Babylon, Greece. Not only ornaments are known from this period, on which we can observe certain elements of symmetry, but also texts related to symmetry. Plato already in the year 360 BC in the dialogues *Timaeus* described 5 ideal bodies with walls formed by equilateral polygons. The octahedral shape of diamond crystals was described by Plinius (16-79 AD) in the encyclopedia *Naturalis historia*, and Georgius Agricola described the geometric shapes of crystals in *De natura fossilium* published in 1564.

From the beginning of the XVII. century, Johann Kepler's work on the hexagonal shape of snowflakes (1611) *Strena Seu De Niue Sexangula* [1] is known, and his work from 1619 *De figurarum regularium* [2] also deals with the symmetry of bodies. Kepler did not yet have the knowledge to discover the reason for the hexagonal shape of snowflakes, but his reflections on possible causes are remarkable. In the first of the listed writings, considerations about the tightest placement of spheres in a plane and in space, but also about the possibilities of perfectly filling a plane or space with identical symmetrical objects, are also interesting. It is these considerations that make his work interesting even for contemporary crystallographers, who still use to quote it in their works. The tightest arrangement of spheres was also a mathematical problem for a long time, while its exact reasoning was mastered only at the end of the 20th century [30]. In 2014, Charles University honored Kepler's work [1], which is not large in scope, by publishing it with the original Latin text and a parallel Czech translation [3].

Some terms used in the theory of crystal symmetry are explained in the glossary at the end of this book, while the english terminology is in accordance with the publication *International tables for Crystallography* [34]. It was sometimes interestng to go back to the past and find out the genesis of crystallographic terms. In this context, it was primarily the thoughts of Fyodorov and Schoenflies, but they also followed on from important predecessors. That's why it was interesting to look deeper into the past, when and where considerations about the laws of crystal symmetry arose. We owe the possibility of looking into older original texts to their digitization and the Internet, through which one can literally flip through old books. Out of respect for older sources, many original names have been preserved in this text, including the names of books and magazines.

Special thanks go to the reviewers of original slovak text, who were willing to read it and point out its shortcomings. My wife Mileva also read the text before publication, and I am indebted to her for the succinct comments of the first reader.

Author

OUTLINE OF THE DEVELOPMENT OF THE THEORY OF CRYSTAL SYMMETRY

The timid beginning of the scientific perception of the symmetry of crystals can be placed in the XVII. century, when Nicolas Steno published his dissertation [4] in 1669, in which he described how rocks are formed and how crystals grow. In connection with crystals, he stated that during their growth, when new matter is deposited on their outer surfaces, the angles between the surfaces do not change; this fact was named the *law of constancy of angles*.

More than a century later, in 1784, René-Just Haüy published the results of measuring the angles between the walls of calcite, garnet and gypsum crystals [5]. He found that when the crystals were broken into smaller and smaller pieces, their shape in the main features was preserved. On this basis he concluded that the crystal was composed of a large number of repeating parts; it was essentially a hypothesis of the periodicity of the crystal structure. In 1801, in the *Traité de Mineralogie* [6], he formulated the *law of rationality of indices*, which expresses the fact that the ratio of the size of the sections on the crystal axes, which are cut on them by the outer surfaces of the crystal, can always be expressed as a ratio of whole numbers.

The study of the symmetry of crystals continued in the XIX. century and resulted in the determination of 32 types of external symmetry of crystals (so-called crystal clases), 14 types of space lattices and 230 types of symmetry of the arrangement of atoms in crystals. From a mathematical point of view, they are currently represented by 32 *point groups*, 14 *translation groups* and 230 *space groups*. The elements of **point groups** are rotations about the axes of symmetry and reflections in the planes of symmetry, in which the position of at least one point of the crystal does not change, hence their name. The types of point symmetry were already derived in 1830 by J.F. Ch. Hessel [7], but his work remained unnoticed. They were independently derived by the Finnish scientist A. Gadolin only in 1867 [9] and for a long time the primacy was attributed to him. Meanwhile, A. Bravais tried to derive them, but he failed to derive all of them. Types of space lattices represent possible ways of three-dimensional periodic arrangement of sets of points, which A. Bravais [8] derived in 1848. They are represented by **translation groups**, the elements of which are translations expressed as integral linear combinations of three basic vectors; with their help, the lattice gets into equivalent positions. The first works on **space groups**, where combinations of translations with rotations and reflections are considered, are associated with the names of C. Jordan [10] (1868) and L. Sohncke [11] (1879). Sohncke derived 65 space groups that contained only proper rotations, reflections were missing. A complete set of space groups, including reflections, was published in 1891 by E. S. Fyodorov [12] and A. Schoenflies [13], after a more extensive mutual correspondence; however, they have previously published articles containing an incomplete number of spacce groups. This completed the effort to derive all possible types of symmetry of the arrangement of atoms in crystals.

Although Schoenflies, unlike Fyodorov, already used the mathematical theory of groups, he did not use all its possibilities. Moreover, the representation of symmetry operations by matrices was absent in both authors.

Mathematicians also entered the construction of the theory of crystal symmetry, especially A. Speiser with his book on finite groups [14] and to some extent also G. Pólya, with his article in the Zeitschrift für Kristallographie [15]. Speiser did not derive symmetry groups, but pointed out the principles and possibilities of using mathematical group theory in this process, including the so-called factor group. Pólya showed how group theory can be used in the classification of symmetry groups of planar periodic structures (ornamentations, wallpapers, etc.).

Group theory was not consistently used until F. Seitz in a series of articles published in the Zeitschrift für Kristallographie in 1934–1936 and in his doctoral thesis [16] published in 1934. In 1945, W. H. Zachariasen published a book [17] in which, instead of the matrix algebra used by Seitz, he used the algebra of tensors, while also changing the procedure for constructing symmetry groups, which he demonstrated only with a few examples.

In the 1950s, Shubnikov [18] expanded the number of parameters characterizing an atom in a unit cell from three position coordinates to include a parameter that can take on two values. These were mainly two possible orientations of the magnetic moment, and the corresponding groups are known as **magnetic groups**, **black-white groups**, and **Shubnikov groups**. The number of possible types of symmetry thus increased to 1651. Shortly thereafter, Belov and Tarchova [19] considered the situation when the additional parameter can take on more values (different "colours"); the corresponding groups, the number of which has again increased significantly, are known as **colour groups**. Shubnikov and Belov summarized the results achieved in the book [20] published in 1964.

In the 1950s, the theory of so-called **OD structures** (Order-Disorder) came to the center of attention of crystallographers, dealing with structures that are not perfectly periodic in all three dimensions. The Slovak crystallographer Slavomil Ďurovič played a significant role in the development of this theory. His contribution to the theory of so-called **polytypes** is part of the International Crystallographic Tables [24].

In 1992, the International Union of Crystallographers defined the term **aperiodic crystal**, which means a crystal that appears crystalline from the point of view of X-ray diffraction, but in which the three-dimensional periodicity of the arrangement of atoms can be considered absent. Such types include **quasicrystals**, the discovery of which was published by D. Schechtman and his collaborators in 1984 [25], further so-called **incommensurate modulated structures** and also **incommensurate composite crystals**, which were pointed out in 1992 by the Slovak crystallographer Emil Makovicky [26].

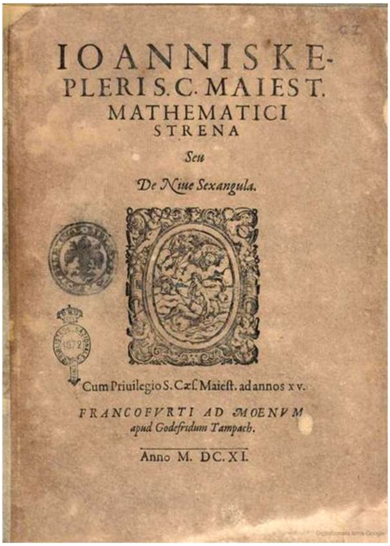
The following parts of the text describe in more detail the results achieved by the aforementioned authors, their references to other authors, as well as brief biographies illustrating their position and possibilities in the society of that time.

Johannes Kepler (1571 – 1630)

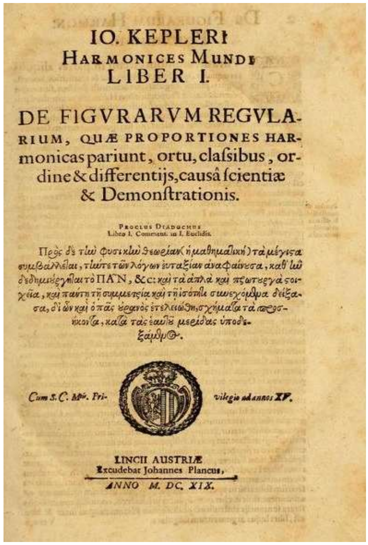
Kepler is considered by some authors to be the figure at the beginning of a series of important crystallographers, because already in the first half of the 17th century he considered the perfect filling of space with equal regular bodies and described the most compact arrangement of spheres in a plane and in space. Kepler is generally known as an astronomer, as the author of the three laws of planetary motion in the solar system, but his interests were much broader. Biographies state that he was a German mathematician, astronomer, physicist and astrologer. However, he was also interested in “earthly” matters and in 1611 he dedicated a thin treatise with reflections on the shape of snowflakes to his friend and patron Johann Matthäus Wacker [1]. The search for the causes of their hexagonal shape also led him to solve the problem of what bodies could perfectly fill space and how spheres could be arranged as compactly as possible in a plane and in space. The Russian crystallographer Shafranovsky wrote about this work of Kepler [29]:

Kepler's "Hexagonal Snowflake" of 1611 is the first work on the structure of crystals. Despite its small size, it is remarkably rich in ideas. One of his greatest discoveries is the geometry of the packing of spheres (as is well known, the principle of the closest packing is the basis of modern crystallography). He described the cubic closest packing and also described two less close-packed ones - hexagonal and simple cubic, but he did not realize that there was also a hexagonal closest packing. Based on considerations about the packing of spheres, Kepler came to conclusions about convex bodies that can fill space without gaps. In this regard, he anticipated the conclusions of R. J. Haüy (1784) and E. S. Fyodorov (1885). Kepler's work also indirectly points to the law of constancy of angles in a hexagonal snow crystal. Therefore, Kepler can be considered a predecessor of the discoverers of this law (N. Steno, 1669, M. V. Lomonosov, 1749, Romé de l'Isle, 1783). We are aware of Kepler's ideas about the dependence of all natural forms on the forming force of the Earth; in this respect, we consider him one of the first predecessors of Pierre Curie and his universal principle of symmetry (1894).

Johannes Kepler was born on December 27, 1571, in the town of Weil der Stadt near Stuttgart. He completed his studies at the University of Tübingen in 1593. From 1594 to 1600, he taught at the high school in Graz, where he published the book *Mysterium Cosmographicum* in 1596. In this book, he admirably connected Plato's five ideal solids with Copernican heliocentric system.



IOANNIS KE-
PLERI S.C. MAIEST.
MATHEMATICI
STRENA
Seu
De Niue Sexangula.
Cum Priuilegio S. Cæs. Maiest. ad annos XV.
FRANCOFVRTI AD MOENVM
apud Godefridum Tampach.
Anno M. DC. XI.



IO. KEPLERI
HARMONICES MUNDI
LIBER I.
DE FIGVRARVM REGVLA-
RIUM, QUÆ PROPORTIONES HAR-
monicas pariunt, ortu, classibus, or-
dine & differentijs, causâ scientiæ
& Demonstrationis.
Cum S. C. Mtis. Pri- vilegio ad annos XV.
LINCII AUSTRIÆ
Excudebat Johannes Plancus,
ANNO M. DC. XIX.

Title pages of Kepler's books - on the snowflake and on the regular solids

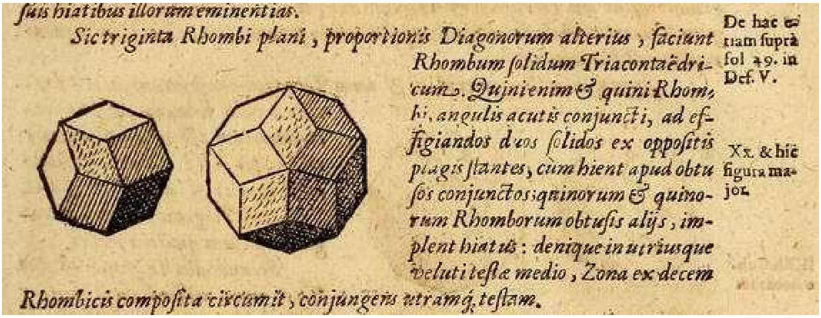
In 1600, he came to Prague at the invitation of Tycho Brahe, where he worked as his assistant. After Brahe's death in 1601, he became the imperial mathematician and astrologer to Rudolf II. During his stay in Prague, based on Brahe's precise measurements, he began to recalculate the orbit of Mars. After lengthy calculations, in which he also used logarithms, he discovered the first two of his laws. He published the results in 1609 in the work *Astronomia Nova*. In 1612 he went to Linz and then to Ulm in 1626. In his work *Harmonices Mundi* (1619) he also addressed the problem of convex and stellated polyhedra and published his third law. He died on 15 November 1630 in Regensburg.

In his treatise on the shape of snowflakes, Kepler asks himself at the very beginning of his reflections why there are only six-pointed ones, and not five- or seven-pointed ones. He realized that this was not a coincidence, that it must have some cause – either internal or external. He concluded that it was the result of some external influence, some kind of force. He further wondered what this force was, whether it was limited by the internal need of the substance, by the pattern of beauty hidden in the hexagon, or by the knowledge of the purpose to which it was directed? Kepler decided to solve this problem using geometry and first turned his attention to the hexagonal shape of the cells of honeycombs.

He stated that at first glance it is clear that the honeycombs are built on the basis of hexagons, but the bottoms of the cells are formed by three rhombic (diamond) faces. The cells are arranged in two layers with their bottoms touching each other. Each cell is thus surrounded on the sides by six others, with each of them sharing a common wall, but its bottom faces also touch three cells of the opposite layer. It was precisely the contact of the bottom walls that led him to consider whether it was possible to construct a body using only rhombic shapes. Kepler literally wrote:

"*I have discovered two such solids, one related to the cube and octahedron, the other to the dodecahedron and trisocahedron. The first of these solids can be constructed from twelve rhombuses, the second from thirty.*" [3]

The following image is Kepler's original drawing of these solids, included in the second of five books published under the title *Harmonices Mundi* [4], in which his wide interest in natural phenomena is documented. The image is taken from the original available on the Internet at archive.org.


ſuis hiatibus illorum eminentias.
Sic triginta Rhombi plani, proportionis Diagonorum alterius, faciunt Rhombum ſolidum Triacontaëdricum. Quini enim & quini Rhombi, angulis acutis conjuncti, ad effigiandos duos ſolidos ex oppoſitis plagis ſtantes, cum hient apud obtuſos conjunctos: quinorum & quinorum Rhomborum obtuſis aliis, implent hiatus: denique in utriusque veluti teſtæ medio, Zona ex decem Rhombicis compoſita circumit, conjungens utramq; teſtam.

De hac etiam ſuprà fol 49. in Def. V.

Xx. & hic figura major.

Other sentences in Kepler's text already concern the perfect filling of space with equal regular solids; they also require spatial imagination from the reader:

"*Just as eight cubes touching at one common corner completely fill the space so that no empty space remains between them, so the first of the rhombic solids with its four obtuse triangular corners and six square corners achieves the same. Space can therefore be completely filled with rhombic solids by always connecting either their four triangular corners or their six square corners at one point.*"

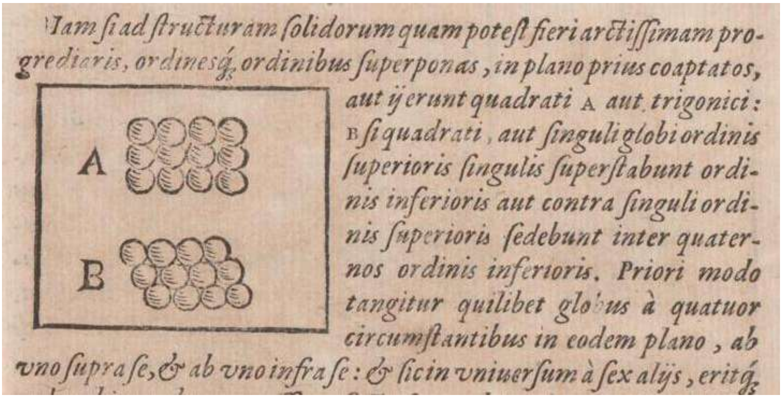
As an example of the number of solids touching each other when filling space perfectly, Kepler first gave cubes. Then he evaluated the number of touching rhombic solids:

"*However, if we fill the space with identical rhombic solids, each of them will touch six square corners and twelve other four corners - a total of eighteen solids. This is the geometric shape of a solid that can perfectly fill the space, just as a hexagon, a square, and a triangle can fill a plane. This is also the shape used by bees in building honeycombs, except that the honeycombs lack a roof resembling a bottom*."

In the next part of the text, he dealt with the arrangement of pomegranate seeds, whose originally spherical shape filled with juice changes to a rhombic shape when squeezed into a limited space. He tried to understand why they acquire such a shape and gave several speculative reasons. The original spherical shape of the seeds led him to consider ways of closely arranging the spheres in a plane and in space. And this is another moment that has something in common with crystallography, even with the theory of OD structures. He wrote about the possible shapes of the arrangement of spheres in a plane:

"*For if you place balls of the same size in the same plane as closely as possible side by side, so that they touch each other, they will form either a triangle or a square. In the former case one sphere touches six, in the latter case four, adjacent spheres. In both cases it is the same for all the bullets, apart from those on the edge. The pentagonal shape does not correspond to the tightest arrangement; the hexagonal shape can be put together from triangles: and so, as has been said, only two arrangements are possible*."

The following image is from Kepler's original text on the snowflake.



Iam ſi ad ſtructuram ſolidorum quam poteſt fieri arctiſſimam progrediaris, ordineſq; ordinibus ſuperponas, in plano prius coaptatos, aut ijerunt quadrati A aut trigonici: B ſi quadrati, aut ſinguli globi ordinis ſuperioris ſingulis ſuperſtabunt ordinis inferioris aut contra ſinguli ordinis ſuperioris ſedebunt inter quaternos ordinis inferioris. Priori modo tangitur quilibet globus à quatuor circumſtantibus in eodem plano, ab vno ſupra ſe, & ab vno infra ſe: & ſic in vniuerſum à ſex alijs, eritq;

He further considered the closest arrangement of balls in space:

"*If you want to achieve a structure with the closest possible arrangement of balls in space by layering one row of balls on top of another (as before in the plane), then the structure will be quadrangular (A) or triangular (B). In the quadrangular one, the individual balls of the upper layer will stand exactly above the balls of the lower layer, or they will be located between the four balls of the lower layer. In the first case, one ball touches four neighboring balls in its layer, and one each in the layer above and below, a total of six balls. This corresponds to a cubic structure; if they are pressed together, a cube is formed. But this is not the closest arrangement. In the next case, the ball touches, in addition to the four balls in its layer, four in the lower and* *four in the upper layer, a total of twelve balls. If we press them together, the balls will form rhombic bodies. This structure is more like an octahedron and a pyramid. This is the most compact arrangement: in no other arrangement can more balls be packed into the same container.*

However, if the balls are arranged in such a way that the layers are in the shape of a triangle, then in the spatial arrangement the individual balls of the upper layer will either stand on the balls of the lower layer as in the case of the looser arrangement mentioned above, or the ball of the upper layer will be located between three balls of the lower layer. In the first case, the ball touches six neighboring balls in its layer and one each from the layer above and below, i.e. a total of eight balls. This structure resembles a prism and when compressed, the balls will form columns with six sides in the shape of a square and two hexagonal bases. In the second way, we achieve the same result as in the second variant of the square structure".

He concludes these considerations with the sentence:

"*In the case of the closest possible arrangement in space, the triangular cannot exist without the quadrangular, nor vice versa.*"

Kepler's work on the shape of a snowflake is usually mentioned by some authors (e.g. A. Speiser in his book [14]), but it was not cited by the real creators of the theory of crystal symmetry, Fyodorov or Schoenflies, it is not included in the extensive list of literature contained in the book by the authors Bradley – Cracknell, and it is not mentioned in the first volume of the International Crystallographic Tables. Nevertheless, we believe that its originality deserves attention. It received recognition in 2014 with the publication of the original with a translation into Czech [3].

Some of Kepler's works:

1. Mysterium Cosmographicum, 1596
2. Astronomia nova (1609)
3. Strena Seu De niue sexangula (1611)
4. Harmonices Mundi, Lincii Austriae, Anno M. DC. XIX.

Sources:

1. https://archive.org/details/bub_gb_Nb8kgmlxUuUC
2. https://archive.org/stream/ioanniskepplerih00kepl#page/n9/mode/2up
3. Google books: The Harmony of the World by Johann Kepler
4. Quoted Kepler texts translated from Latin by Drahomíra Dobrovodská, 2017

Nicolas Steno (1638 – 1686)

The Danish scientist (Niels Stensen) is known in crystallography as the author of the law of constancy of angles. He was a pioneer in the field of anatomy and geology, and began to question the previous claims about geological development. For his research into fossils, rock formation, and the conclusions he drew from it, he is considered the founder of modern stratigraphy and modern geology. He made the first careful observations of crystal types and published them in his dissertation "*De solido intra solidum naturaliter contento*" in 1669. In his work, he stated that during the growth of crystals, when material is deposited on their outer surfaces, the angles between the surfaces do not change during this process. This finding is known as Steno's law, or Steno's law of constancy of angles, or the First Law of Crystallography. It was the first step on the path to modern crystallography, with the next step being taken more than 100 years later by R. J. Haüy with the formulation of the law of rationality of indices. Steno's dissertation – (Dissertationis Prodromus) – is often considered the beginning of crystal science.

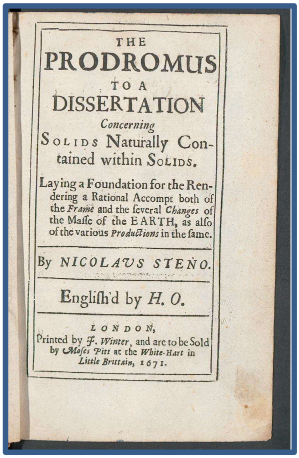
Steno was born in Copenhagen to a poor Protestant family. When he was three years old, he fell seriously ill, and so he lived in isolation for a long time during his childhood. At the age of 19, he began to study medicine at the University of Copenhagen. After completing his studies, he traveled extensively, visiting the Netherlands, Germany, France and Italy, where he settled permanently in 1666. He first worked as a professor of anatomy at the University of Padua, then in Florence as a house physician to the Medici family. He became a member of the Academie di Cimento. Meetings with leading physicians and scientists in various countries significantly influenced his further work, led to the use of his own judgment and ultimately to significant scientific discoveries that often contradicted previous views. After converting to the Catholic faith in 1667, his interest in natural sciences decreased significantly, and he became interested in theology. He was ordained a priest in 1675 and was soon appointed Vicar Apostolic and Titular Bishop by Pope Innocent XI. He was prominently involved in the Counter-Reformation in northern Germany and was venerated as a saint after his death. The canonization process began in 1938 and was completed in 1988 by Pope John Paul II.

A significant part of the dissertation is devoted to geological issues and fossils. Steno dealt with the explanation of the layered nature of rocks, the origin of mountain ranges and the origin of various stones. He came to the opinion that the layered structure of rocks is the result of sedimentation in the seas.

NICOLAI STENONIS
DE SOLIDO
INTRA SOLIDVM NATVRALITER CONTENTO
DISSERTATIONIS PRODROMVS.
AD
SERENISSIMVM
FERDINANDVM II.
MAGNVM ETRVRIÆ DVCEM.

GRATIA OBVIA VLTIO QVÆSITA

FLORENTIÆ
Ex Typographia ſub ſigno STELLÆ MDCLXIX.
SVPERIORVM PERMISSV.



THE
PRODROMUS
TO A
DISSERTATION
Concerning
SOLIDS Naturally Contained within SOLIDS.

Laying a Foundation for the Rendering a Rational Accompt both of the *Frame* and the ſeveral *Changes* of the Maſſe of the EARTH, as alſo of the various *Productions* in the ſame.

By *NICOLAUS STENO.*

Engliſh'd by *H. O.*

LONDON,
Printed by *J. Winter*, and are to be Sold by *Moſes Pitt* at the *White-Hart* in *Little Brittain*, 1671.

Title pages of the original dissertation from 1669 and the English translation from 1671

He also devoted part of his dissertation to crystals, specifically considering the method of their formation. He argued that crystals in rocks are formed in the same way as those that arise from aqueous solutions - by the gradual deposition of matter on the surface, and not like plants - by receiving "nutrition" from the soil. By crystal he meant mainly quartz, describing its hexagonal symmetry, the termination of a hexagonal prism with a hexagonal pyramid. He also notes its imperfections, for example, the disruption of the smoothness of the surfaces, or the inequality of the triangles of the top pyramid. He concluded that during the growth of a crystal, a new substance is not added to all surfaces at once, nor in the same amount. He discovered that the axis of the pyramidal part of a crystal is not always parallel to the axis of its prismatic part, that the pyramidal faces are not always triangular in shape, and the prismatic parts are not always tetragonal in shape. The most significant result of Steno's study of crystals, however, is the law of constancy of angles.

The beginning of the text about crystals is marked with a note in the margin of the text:

> Quod cryſtalli productionem attinet, quomo- *De Cry-*
> do prima ipſius delineatio peragatur, non auſim *ſtallo.*
> determinare; id ſaltem extra controuerſiam eſt,
> quæ apud alios ea de re legere mihi contigit, lo-
> cum ibi nullum habere : nec enim irradiationes,

Free translation: *As for the formation of crystals, I do not dare to express an opinion as to how their initial shape is formed; however, it is indisputable that much of what I have read from other authors on this problem was beside the point.*

To illustrate Sten's considerations, we will present his idea of the shape of a crystal (by which he means a quartz crystal) and the introductory definitions of the terms he used in the following text:

> Cryſtallus componitur ex duabus pyramidibus
> hexagonis, & columna intermedia itidem hexa-
> gona, vbi *angulos ſolidos extremos* illos appello, qui
> vertices pyramidum conſtituunt, *angulos* verò *ſoli-*
> *dos intermedios*, illos, qui in pyramidum cum co-
> lumna vnione conſtituuntur, eodem modo plana
> pyramidum

The crystal consists of two hexagonal pyramids and a prism between them, which is also hexagonal. The angles formed by the vertices of the pyramids I call terminal solid angles, *but those formed by the connection of the pyramids with the prism I* call intermediate solid angles.

Steno's essential contribution from the point of view of crystallography – on the constancy of angles during crystal growth – is in the following text and figure:

ret, duodecim lateribus continetur. 13. figura
indicat quomodo, dum planis pyramidum im-
ponitur noua materia cryſtallina, in plano baſis
laterum longitudo interdum, & numerus variè
mutantur non mutatis angulis.

13

The text about the constancy of angles is found at the end of the dissertation, on the last two pages, in the comments to the figures, specifically to figures number 5, 6 and especially to figure 13, where he formulated it particularly clearly:

Figure 13 shows that as new crystal mass is deposited on the surfaces forming the pyramid, in the plane of the base the length and number of sides change in various ways, but without changing the angles.

In Steno's native country, on the website

http://denmark.dk/en/meet-the-danes/great-danes/scientists/niels-stensen

his contribution to crystallography is evaluated in the following words:

"*Crystalography gained its scientific foundation with Steno's discovery that as crystals grow, material is* *deposited on their outer surfaces, the angles between the surfaces remaining unchanged during this process.*"

After its first edition in 1669, the dissertation was published as a copy of the original in 1679, 1763, 1904 and 1910, and in several translations – 1671 and 1916 in English, 1757 and 1832 in French and 1902 in Steno's native language – Danish. Other editions of the original work can also be found on the Internet.

The law of constancy of angles was generalized and established by Jean-Baptiste Romé de l'Isle (Cristallographie, Paris, 1783), who measured the angles between the walls of many types of crystals.

Steno's most important scientific publications point to his initial interest in anatomy:

Observationes anatomicae (1662)
De musculis et glandis (1664)
Discourse on the anatomy of the brain (1665)
Canis carchariae dissectum caput (1667)
Elementorum Myologiae Specimen, seu musculi descriptio geometrica (1667)
De solido intra solidum naturaliter contento dissertationis prodromus (1669)

Sources:

https://archive.org/details/ita-bnc-mag-00001426-001
https://archive.org/stream/prodromusnicola00wintgoog#page/n0/mode/2up
http://www.e-rara.ch/zuz/content/pageview/11339638
https://en.wikipedia.org/wiki/Nicolas_Steno

René – Just Haüy (1743 – 1822)

French scientist known for proposing that crystals are composed of a number of small, regularly arranged elementary particles (1784) [5] and for formulating the *law of rationality of indices* (1801) [6]. Often called Abbé Haüy, or the "Father of Modern Crystallography".

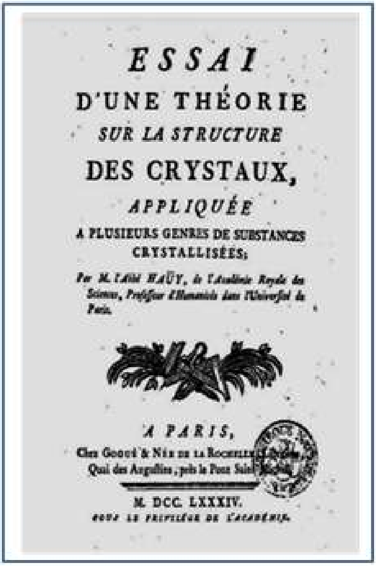
He was born in the town of Saint-Just-en-Chaussée, in the Oise region of northern France. He came from a poor family, and was able to study only thanks to the kindness of his parents' friends. After studying at the College de Navarre and the College de Lemoine, he was ordained a Catholic priest. He began as a teacher at the College de Lemoine, where he worked for 21 years. He was interested in botany, but an accident, when a calcite crystal fell out of his hand and broke, led him to study minerals. The pieces of the broken crystal had the same shape as the original one, which prompted him to experiment with crystals of other minerals (gypsum, topaz, garnet). He conducted a number of experiments, from which he concluded that crystals of the same composition always have a nucleus of the same shape, regardless of their external shape. He expressed the opinion that the basic building blocks of crystals are regularly arranged, which essentially meant their periodic arrangement. He published the first findings of his research in 1781 in the Journal de physique and then in 1784 in the book *Essai d'une théorie sur la structure des crystaux*. During his experiments, he also measured angles on crystals and confirmed the *law of constancy of angles* formulated by N. Steno over a century earlier, when he wrote (free translation):

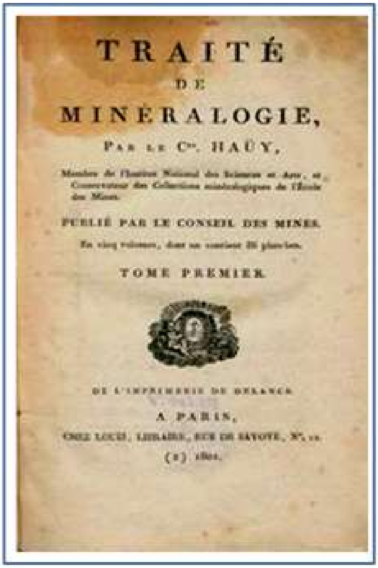
The angles and axes of crystals are constant, no matter the country the crystal comes from.

The second important finding, the *law of rationality of indices* – was published in the five-volume work *Traité de mineralogie* in 1801 (each volume had over 500 pages). The illustrations for the entire work are concentrated in the fifth volume and document the author's precision. He also wrote about crystals and minerals in the following years, the last such publication being published in the year of his death in 1822.

Haüy also had to create the necessary terminology. In his ideas about the structure of a crystal, he called the elementary building blocks "*molécules cristallines*" and "*molécules intégrantes*", while in special cases he specified them, e.g. "*molécules rhomboidales*". When splitting a crystal, he proceeded until he arrived at its "core". He recognized *primitive* and *secondary* shapes of the cores. He identified primitive shapes with integrating molecules and distinguished three of their types ("*types of the simplest regular bounded bodies*"), which have an impact on the external shape of the crystal:

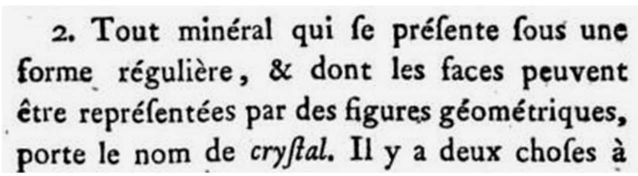
triangular pyramid, triangular prism and tetrahedral prism.


ESSAI
D'UNE THÉORIE
SUR LA STRUCTURE
DES CRYSTAUX,
APPLIQUÉE
A PLUSIEURS GENRES DE SUBSTANCES
CRYSTALLISÉES;
Par M. l'Abbé HAÜY, de l'Académie Royale des Sciences, Professeur d'Humanités dans l'Université de Paris.
A PARIS,
M. DCC. LXXXIV.


TRAITÉ
DE
MINÉRALOGIE,
PAR LE Cen. HAÜY,
PUBLIÉ PAR LE CONSEIL DES MINES.
TOME PREMIER.
A PARIS,

Title pages of two of Haüy's most important mineralogical publications

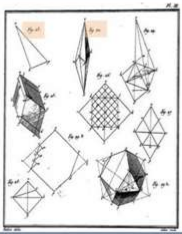
He also used the regularity of shape to define a crystal (1784):


2. Tout minéral qui ſe préſente ſous une forme régulière, & dont les faces peuvent être repréſentées par des figures géométriques, porte le nom de *cryſtal*. Il y a deux choſes à

"*A mineral characterized by a regular shape and walls that have the shape of geometric figures is called a crystal.*"

SPATH CALCAIRE A DOUZE FACES TRIANGULAIRES SCALENÈS, connu ſous le nom de *Dent de Cochon*. (*Pl. III*, *fig.* 22). *Id.* DAUB. *Tableau minér.*

Développement. Douze triangles ſcalènes (*fig.* 23) égaux & ſemblables entr'eux. L'angle *ehg* = 101° 32' 13". *egh* = 54° 27' 30". *geh* = 24° 0' 17".

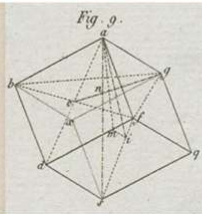


↑ Image and text from the book *Essai d´une theorie sur la structure des crystaux* (1784). In the image (fig. 22) the vertices of one of the crystal walls are marked, in the text the angles between the edges are given.

Dans le rhomboïde primitif de la chaux carbonatée, on a $g=\sqrt{3}.p=\sqrt{2}$ (1). Substituant ces valeurs à la place de g et de p, dans les rapports précédens, on trouve :

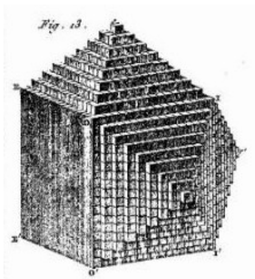
1°. $af : fm$ (*fig.* 9) :: 5 : 1, ce qui donne fam = 11d. 32' 13", donc baf = 101d. 32' 13".

2°. $am : im$ :: 4 : 1, ce qui donne pour l'angle ami, 75d. 31' 20".



↑ Text and image from the book Traité de mineralogie (1801). They concern the *law of rationality of indices*. The text indicates the ratios of the lengths of the sides, which are equal to the ratio of whole numbers.

It is remarkable how precisely Haüy expressed the angles between the edges of crystals, since he could not have had a goniometer of current quality at his disposal. A goniometer suitable for measuring the angles of crystals was constructed by Romé de l'Isle in 1780, and the reflective goniometer by Wollaston only in 1809.



The image on the side documents Haüy's idea of the structure of a crystal consisting of "molecules".

Haüy was also interested in physics, and wrote a textbook on electricity and magnetism, in which he also wrote about pyroelectricity. In 1795 he became a physics teacher at the Ecole Normale. He was a member of the commission appointed to determine the metric units of weights and measures (1793). In 1802 Napoleon appointed him professor of mineralogy at the Musée d'historie Naturelle in Paris, and from 1809 he held a similar position at the Faculté des sciences of the Sorbonne University. In 1814 he was dismissed from his position by the Bourbons and was left practically without funds. Despite this, he worked intensively and in 1821 he was accepted as a member of the Swedish Academy of Sciences. His name is listed among the names of the most important figures of France on the Eiffel Tower.

Haüy cited the works of both predecessors and contemporaries.

In the first book *Essai d'une théorie* (1784), the authors were:

M. Bergmann, M. Daubent (Tableau Mineralogique), I. Newton (Optics, birefringence), M. Sage (Eléments de Minéralogie).

In the introduction to *Traité de minéralogie* (1801), he mentioned the authors:

Wullerius: Systema mineralogica (1778), De l'Lisle: Cristallographie (1785),

Emmerling: Lehrbuch der Mineralogie (1793), Karsten: Mineralogische

Tabellen, 1800, Daubenton: Tableau méthodique des mineraux,

Borchant: Traité élementaires de mineralogie, Paris

He mentions M. Bergman in connection with the processes of crystallization, M. Daubent – his teacher – as the author of mineralogical tables and I. Newton in connection with optics, especially birefringence.

Haüy published a lot, wrote several books and articles.

Book publications related to crystals:

1. *Essai d'une théorie sur la structure des crystaux (1784)*
2. *Exposition abrégé de la théorie de la structure des cristaux (1793)*
3. *Traité de minéralogie (5 volumes, 1801)*
4. *Tableau comparatif des résultats de la cristallographie, et de l'analyse*
5. *chimique relativement à la classification des minéraux (1809)*
6. *Traité de cristallographie (2 volumes, 1822)*

He published articles mainly in the journals
Journal de physique and *Annales du Museum d'Histoire Naturelle*, of which 100 are registered in the Royal Society's catalogue.

Sources:

1. http://gallica.bnf.fr/ark:/12148/bpt6k97620795?rk=107296;4
2. http://gallica.bnf.fr/ark:/12148/bpt6k1060890?rk=128756;0
3. https://archive.org/details/TraiteDeMineralogieTomeQuatrieme
4. https://en.wikipedia.org/wiki/Ren%C3%A9_Just_Ha%C3%BCy

Johann Friedrich Christian Hessel
(1796 – 1872)

A German scientist who took the lead in the effort to develop a mathematically based systematics of the types of symmetry of crystals, as well as other bounded regular geometric objects. He derived the types of their symmetry, including 32 types of external symmetry of crystals (crystall classes). He published his more than 300-page work in 1830 in the fifth volume of the encyclopedia *Gehlers Physikalische Wörterbuch* as the entry *Krystall* [7], but the work did not reach the attention of crystallographers and remained unnoticed. L. Sohncke, who was the first (1876) to begin constructing crystallographic space groups, did not cite it either. But Sohncke atoned for his inattention when in 1891 published a 12-page article praising Hessel and his work in the journal Zeitschrift für Krystallographie und Mineralogie. The thirty-two types of symmetry were not derived again until 37 years later by Axel Gadolin. Hessel's work was published in book form under the title *Krystallometrie oder Krystallonomie und Krystallographie* only after his death in 1897, divided into two volumes. A year before his death, in 1871, he published another book on geometry: *Uebersicht der gleicheckigen Polyeder*, but he did not deal with the symmetry of crystals in it.

Hessel was born in Nuremberg to a merchant family. In 1813 he began studying medicine in Erlangen, continued in Würzburg, while simultaneously studying mathematics and natural sciences. He completed this study in 1817, went to Munich for further studies and soon became an assistant at the University of Heidelberg. There he continued his studies, devoting himself to crystallography, mathematics, physics and chemistry. In 1821 he received his doctorate in philosophy and at the same time the opportunity to work as a private lecturer at the university. In the same year he was invited as an extraordinary professor of mineralogy and applied sciences to Marburg, where after four years he became a full professor. He remained there for 50 years until his death. In 1830/31 he worked at the Philips-Universität Marburg as rector.

In the introduction to his work, Hessel stated the goal he pursued in writing it:

I have attempted to place on a purely mathematical basis the consideration of the equivalence of spatial forms and to distinguish the various types of these equivalences more strictly than has been done hitherto. To take into account not only the shapes of crystals, but the shapes of all conceivable forms, although – partly tacitly, sometimes explicitly – to give preference precisely to the shapes of crystals of all so-called crystall systems.

This is the only mention of crystall systems in the entire work. He built his theory by first determining the

possible types of symmetry axes and then their possible combinations. He divided the axes of symmetry primarily into non-polar (*gleichendig*) and polar (*ungleichendig*), and then in more detail into up to 7 types. He classified the types of symmetry mainly according to the presence of a main axis, its multiplicity and the number of secondary axes. He created the necessary terminology and symbols. When classifying the types of symmetry, he used the term "axis system" (*Axensystem*) in addition to the term "ray system" (*Strahlensystem*), by which he meant a set of line segments, originating from a single point, representing significant directions in the described type of symmetry (for example, a set of line segments that arise by successive rotations around an n-fold axis of symmetry). For bodies (objects) that can be identified by rotation, he used the term *ebenbildlich gleich* and for objects that can be identified by reflection, the term *gegenbildlich gleich*. For p-multiplicity of symmetry axes, he used the term *p-gliedrich*. He also introduced Latin equivalents of already common terms, e.g. *figura ternoradiata* and the like.
In the introduction to his work, Hessel defined a crystal, which he understood as a natural solid homogeneous body that is completely or partially bounded by plane surfaces.
His procedure for determining types of symmetry is documented in the chapter headings of the book *Krystallometrie*:
• On surfaces and ray systems in a plane
• On types of axes (symmetry)
• On the center (symmetry) and different types of axes of a body


KRYSTALLOMETRIE,
oder
Krystallonomie und Krystallographie,
auf eigenthümliche Weise und
mit Zugrundelegung neuer allgemeiner Lehren
der reinen Gestaltenkunde,
sowie mit vollständiger Berücksichtigung
der wichtigsten Arbeiten und Methoden
anderer Krystallographen,
bearbeitet von
JOH. FRIEDR. CHRISTIAN HESSEL,
Dr. d. Med. und Phil. und Prof. der Mineralogie zu Marburg.
(1830.)
Besonders abgedruckt aus Gehler's phys. Wörterbuche.
Erstes Bändchen.
Mit 8 Tafeln.
Herausgegeben
von
E. Hess.
LEIPZIG
VERLAG VON WILHELM ENGELMANN
1897.


Uebersicht
der
gleicheckigen Polyeder
und Hinweisung
auf die Beziehungen dieser Körper
zu den
gleichflächigen Polyedern
von
Johann Friedrich Christian
Professor Dr. Hessel.
MARBURG.
Oscar Ehrhardt's Universitäts-Buchhandlung.
1871.

Title pages of Hessel's books

• Ray systems and axis systems of objects with a principal axis
• Ray systems and axis systems of objects without a principal axis
• Description of simple objects with a principal axis and their surfaces
• Description of simple objects without a principal axis and their surfaces
• Calculation of important relations in figures with a principal axis
• Calculation of important relations in figures without a principal axis

• Über das Gerengesetz, und über gerengesetzliche Strahlenveraine...

loosely translated: On the law of the formation of parallelograms from rays

• The shape and structure of crystals

• Essential data from the history of crystallography

The main result of his work – the possible shapes of symmetrical objects, including crystals (Krystallgestalten), was clearly presented in four tables. Fig. 1 shows the first of the tables, which lists the shapes (types of symmetry) of crystals characterized by four threefold axes, i.e. crystals belonging to the cubic crystallographic system. Their number corresponds to the number of point groups of this system. (Following the Hessel's publications, the figures are included at the end of the text.)

36 types of symmetry are described in the four tables compiled by Hessel. The table with 32 types of point symmetry of crystals was compiled by the publisher of Hessel's book after his death and included in the appendix to the book (Fig. 2). Hessel also described the symmetries of objects in which "non-crystallographic" axes of symmetry occur (dodecahedron, icosahedron), as the text in Fig. 3 shows.

In addition to the derivation of 32 crystall classes, it is also necessary to mention Hessel's construction of a plane lattice and space lattice. This part of his publication has the difficult-to-translate title *Ueber das Gerengesetz*... The essence of the idea was to create a set of parallelograms based on two line segments (rays – *Strahlen*) emanating from one point, as can be seen from a copy of Hessel's text (Fig. 4) and the corresponding images (Fig. 5). The two rays (segments) *B* and *D*, which according to current terminology form the basis of the unit cell, allow the creation of a third ray, which is the diagonal *S'* of the cell (it is actually a sum of vectors). This ray and ray *B* again form a cell with diagonal *S''*, etc. Similarly, the ray *S'* can be combined with the ray *D*, thereby creating a plane network – a plane lattice. For the pair of fundamental rays (vectors) of a plane lattice he used the symbols [*B, 0D*], or [*0B, D*], for the rays formed by their combination the symbol [*mB, nD*], where *m* and *n* are integers, according to Hessel *Maasszähler*. In the three-dimensional case he used the notation [*lA, mB, nD*], while from today's point of view these are clearly *lattice vectors*. Although he did not yet use the term *lattice*, it is clear that his considerations were directed towards it. And this is a significant step, although probably not yet conscious, from the description of the external symmetry of crystals to the symmetry of their internal arrangement. Therefore, Hessel can be considered to some extent a predecessor of Bravais, although he did not yet distinguish between types of lattices.

In the chapter on the method of creating a space lattice, he also described a possibility of expressing the orientation of a plane in such a lattice. For this purpose, he used the coordinates of the normal of such a plane. He showed that if a plane cuts off segments *x, y, z*, (rational numbers) on the basic rays, then the coordinates of the normal are their inverse values. Figure 6 shows the conclusion of Hessel's original text (normal = *Träger*) concerning this problem. The results of his considerations are documented in a table (Fig. 7), the first column lists the symbols of specific planes and the last column lists the coordinates (*Maasszähler*) of the normal of the relevant surface, essentially their Miller indices. The comma above the number has the meaning of a negative sign before the number. Therefore, Hessel can also be mentioned as an unquoted predecessor of Miller.

In the text in Fig. 4, it can be seen that he writes about *rational numbers*, which the author of the assessment of Hessel's significance, published in the appendix to the book edition of his work, relates to the law of rationality of indices. Hessel cited Haüy's work from 1801, so it is likely that he was considering this connection.

Hessel thus entered the history of crystallography not only by determining 32 crystall classes, but also by his other considerations. He sensed the path of further development of the description of crystal symmetry, but his ideas only became known to crystallographers after his death, when they were already known as the results of the works of other authors.

Like Haüy, he cited authors whose works he referred to or wanted to draw attention to. The (incomplete) list of authors he cited in his work Krystallometrie is interesting, testifying to the development of crystallography in his time: *Haüy*: Traité de minéralogie, *Hoffmann*: Handbuch der Mineralogie, *Weiss*: Dynamische Ansicht der Krystallisation, *Neumann*: Beiträge zur Krystallonomie, *Naumann*: Grundriss der Krystallographie, *Mohs*: Grundriss der Mineralogie, *Grassmann*: Zur physischen Krystallonomie, *Marx*: Geschichte der Krystallkunde.

Figures

A. 3gliedrig 4axig

	Weiss'sche Benennung	*Mohs*'sche Benennung	Beispiel
1) 8strahlig	sphäroedrisch	tessularisch	Flussspath
2) 1fach 3gliedrig 8strahlig			
3) 4strahlig	hemisphäroedrisch tetraedrisch	semitessularisch von geneigten Flächen	Fahlerz
4) 1fach 3gliedrig 4strahlig			
5) 2 × 4strahlig	hemisphäroedrisch pyritoedrisch	semitessularisch von parallelen Flächen	Eisenkies

Krystallgestalten können sein: [258]

Krystallometrie. 95

Fig. 1

Hiernach lassen sich die 32 Krystallclassen, entsprechend den Anordnungen A., B., C., D. auf S. 95—98 kurz auf folgende Weise charakterisiren:

A. 3*gliedrig* 4*axig*.
(Reguläres Krystallsystem.)

1) $4^2 g^3$
2) $4^1 \varepsilon^3$
3) $4^2 u^3$
4) $4^1 g^3$
5) $4^1 u^3$.

B. 1- *und* 3*maassig*.
(Hexagonales Krystallsystem.)

1) $1^2 G^6$
2) $1^1 G^6$
3) $1^1 \varepsilon^6$
4) $1^2 u^6$
5) $1^1 u^6$
6) $1^2 g^3$
7) $1^1 g^3$
8) $1^1 \varepsilon^3$
9) $1^2 G^3$
10) $1^1 G^3$
11) $1^2 u^3$
12) $1^1 u^3$.

C. 1- *und* 2*maassig*.
(Tetragonales Krystallsystem.)

1) $1^2 G^4$
2) $1^1 G^4$
3) $1^1 \varepsilon^4$
4) $1^2 u^4$
5) $1^1 u^4$
6) $1^2 g^2$
7) $1^1 g^2$.

D. 1- *und* 1*maassig*.
(Rhombisches, monoklines und triklines Krystallsystem.)

1) $1^2 G^2$
2) $1^1 G^2$ = 6) $1^2 g^1$
3) $1^1 \varepsilon^2$
4) $1^2 u^2$ = 9) $1^2 G^1$
5) $1^1 u^2$ = 8) $1^1 \varepsilon^1$
7) $1^1 g^1$
10) $1^1 G^1$ = 11) $1^2 u^1$
12) $1^1 u^1$.

Fig.2

2) Die 3gliedrig 10axigen Gestalten.

A. ***Die 20strahligen Gestalten, Icosiarcta.***

1) Der *Zwölfflächner* (*Dodecaedrum*, regelmässiges Pentagondodekaeder). Ihn begrenzen 12 $|\cong|$ 2fach 5gliedrige 5seitige Flächen *d*, d. h. regelmässige Fünfecke; er hat 30 $|\cong|$ 2fach 2gliedrige Kanten *r*; 20 $|\cong|$ 3kantige 2fach 3gliedrige Ecken *i*. Grösse der Kanten 116°33′54″. Fig. 301.

2) Der *Zwanzigflächner* (*Icosaedrum*) hat 20 $|\cong|$ 2fach 3gliedrige 3seitige Flächen *i*; 30 $|\cong|$ 2fach 2gliedrige Kanten *r*; Fig. 302.

Fig.3

Es lässt sich in der Ebene zweier nach Länge und Lage gegebener Strahlen *B* und *D*, die nicht in einer und derselben geraden Linie liegen, stets ein neuer 3ter Strahl *S′* denken, welcher der Gerenstrahl von *B* und *D* und daher nach Länge und Lage bestimmt ist. Zwischen *S′* und *B* ist daher abermals ein neuer Strahl *S″* möglich, welcher Gerenstrahl von *S′* und *B* ist; ebenso entsteht auch ein Gerenstrahl *S‴* von

Dass man die beiden gegebenen Strahlen *B* und *D* auch darstellen könne durch [*B*, 0*D*] den ersten und [0*B*, *D*] den zweiten, ist gleichfalls einleuchtend. Es ist daher jeder bisher aus den beiden gegebenen Strahlen *B* und *D* gerengesetzlich abgeleitete Strahl in der Ebene *BD* unter dem allgemeinen Zeichen [*mB*, *nD*] begriffen, so dass jeder der Buchstaben *B* und *D* die ursprünglich gegebene Länge des seiner Richtung nach bekannten Strahles *B* oder *D* bedeutet, welche gleichsam als *Maass* dient für die in der Richtung von *B* oder *D* liegende Linie, während jeder der Buchstaben *m* oder *n* eine *rationale* Zahl ist, welche angiebt, wie vielmal dieses Maass zu nehmen sei, und die man daher den *Maasszähler* für *B* oder *D* nennen kann.

Fig. 4

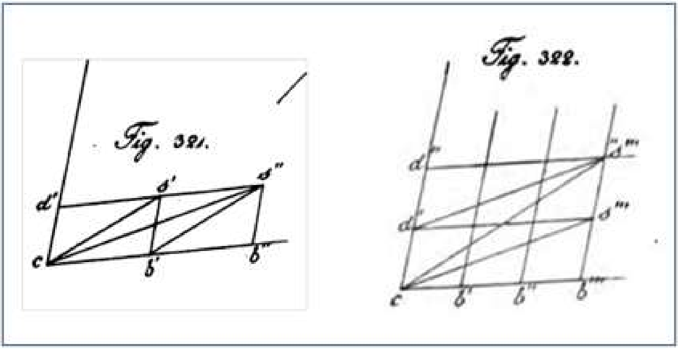


Fig. 5

Jede Fläche $(xa,\ yb,\ zd)$ fordert daher ihren Träger $\left[\frac{1}{x}\alpha,\ \frac{1}{y}\beta,\ \frac{1}{z}\delta\right]$ und umgekehrt. Dass nun ebenso wieder jeder kantenthümliche Strahl $[xa,\ yb,\ zd]$ eine Fläche $\left(\frac{1}{x}\alpha,\ \frac{1}{y}\beta,\ \frac{1}{z}\delta\right)$ eines von α, β, δ abhängigen neuen gerengesetzlichen Flächenvereins fordere, für die er Träger ist,

Fig. 6

Krystallometrie. 65

Man erhält so nach und nach folgende Entwickelung:

die Fläche	ist bestimmt dadurch, dass sie liegt in den bekannten zwei Zonen		daher das Ende ihres Trägers in der Zeigerfläche bestimmt durch	folglich die Maasszähler in Zeichen des Trägers $[x\alpha,\ y\beta,\ z\delta]$
A	. .	. .	. . . .	1 0 0
B	. .	. .	. . . .	0 1 0
D	. .	. .	. . . .	0 0 1
k	. .	. .	. . . .	1 1 1
l	AD	kB	$[0Am,\ 1Al] = [0\beta,\ 1\delta]$	1 0 1
m	AB	kD	$[1Am,\ 0Al] = [1\beta,\ 0\delta]$	1 1 0
f	BD	Ak	$\infty Ak = \infty [1\beta,\ 1\delta]$	0 1 1
a	ml	BD	$\infty [1\beta,\ 1\delta']$	0 1 1'*)
g	Aa	kl	$1\beta',\ 1\delta$	1 1' 1
b	gD	Ak	$1\beta',\ 1\delta'$	1 1' 1'
i	bB	kD	$1\beta,\ 1\delta'$	1 1 1'
o	bi	AD	$0\beta,\ 1\delta'$	1 0 1'
n	bg	AB	$1\beta',\ 0\delta$	1 1' 0
q	ka	AB	$2\beta,\ 0\delta$	1 2 0
r	ka	AD	$0\beta,\ 2\delta$	1 0 2
s	ba	AB	$2\beta',\ 0\delta$	1 2' 0
h	ba	AD	$0\beta,\ 2\delta'$	1 0 2'
t	mf	ka	$\frac{3}{2}\beta,\ \frac{1}{2}\delta$	2 3 1
y	na	gf	$\frac{3}{2}\beta',\ \frac{1}{2}\delta$	2 3' 1
x	nf	ba	$\frac{3}{2}\beta',\ \frac{1}{2}\delta'$	2 3' 1'

Fig. 7

Hessel's works on symmetries and polyhedra

1. *Krystall* – entry in the encyclopedia *Gehlers Physikalische Wörterbuch* 1830
2. *Uebersicht der gleicheckigen Polyeder*, Marburg 1871
3. *Krystallometrie oder Krystallonomie und Krystallographie*, Leipzig 1897

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3. https://de.wikipedia.org/wiki/Johann_Friedrich_Christian_Hessel

Auguste Bravais (1811 – 1863)

A French scientist who made his mark in the history of crystallography by deriving fourteen types of space lattices, which was the first step from describing the external symmetry of crystals to describing the symmetry of their internal arrangement. In December 1848, at a meeting of the French Academy of Sciences, he delivered a lecture, *Mémoire sur les systémes formés par des points distribués régulierement sur un plan au dans l'espace* [8], in which he described possible types of symmetry of periodically arranged points in a plane and in space. A year later, he published the work *Sur les polyèdres symétriques*, where he described polyhedra and their classification according to the elements of symmetry (axes, planes) they are characterized by, i.e. essentially the point symmetry of crystals. In the work *Études crystallographiques*, published in 1851, he also dealt with the symmetry of the internal arrangement of crystals. Bravais's collection of works on crystallography was published posthumously in 1866 as *Études crystallographiques*, together with a review by a commission of the French Academy of Sciences headed by the mathematician Cauchy. His works had a significant influence on both the morphological and structural study of crystals.

Bravais was born in Annonay and graduated from the Collège Stanislas in Paris. In 1829, he won first prize in a mathematics competition and was accepted at the École Polytechnique, where he was a classmate of the eminent mathematician Évariste Galois. Shortly before graduating, he became a naval officer, participated in hydrographic surveys along the Algerian coast, and also took part in research expeditions to Spitsbergen and Lapland. In 1840, he began lecturing a course in applied mathematics for astronomy students at the Faculty of Sciences in Lyon, where he headed the Department of Physics at the École Polytechnique from 1845 to 1856. He became a member of the *Académie Royale des Sciences*, the *Belles Lettres et Arts de Lyons*, and the *Académie de Sciences*.

He also studied magnetism, aurora borealis, meteorology, geobotany, astronomy, and hydrography. His work on the theory of measurement errors is known from 1846, and in 1847 he published his first reflections on crystallography.

In his most famous work – on systems of points regularly distributed in the plane and in space – he first defined the necessary concepts and created his own terminology. He distinguished between a rectilinear lattice (*rangée*), a planar lattice (*réseau*) and a space lattice (*assemblage*). The work has the following chapters:

On plane lattices in general, On symmetrical plane lattices, On space lattices in general, On symmetrical space lattices, On polar space lattices.

Bravais first described how a *space lattice* – a system of periodically spaced points – can be created by successively placing points on a line, in a plane and finally in space. He expressed the procedure as follows:

If we want to create a regular system of points in space, we take two arbitrary points, connect them with a line, which we extend to infinity on both sides. We place an infinite series of other points on this line, equidistant from each other. ... The basic distance between two adjacent points will be called the parameter of the line lattice (paramétre de la Rangée).

From such lines, parallel to each other with a constant distance between them, he created a planar lattice and from mutually parallel lattice planes a space lattice. In this construction, it was necessary to choose first the distance between the points, then the distance between the lines and finally the distance between the planes. In the following text, he set himself the opposite task – how to find these parameters of a three-dimensional lattice that already exists. He gradually sets out tasks in the text and solves them. For the first task (Problem I.), he set himself the task of finding lattice lines, lattice planes and a space lattice for a given system of points. In the original text:

Problème I. — *Un Assemblage étant donné, retrouver les Rangées, plans et Réseaux qui peuvent le produire.*

Problem number XIII was to find the so-called principal triangle in a plane lattice.

Problème XIII. — *Trouver le triangle principal d'un Réseau.*

Choisissez arbitrairement un Sommet O (*fig.* 4), et cherchez parmi tous les autres Sommets le plus rapproché de O.

He solved the problem as follows:

In a plane lattice, we choose an arbitrary lattice point O and among the other lattice points we search for the one that is closest to it. Let A be that point, then OA is the smallest lattice parameter. Through points O and A we draw lines Op *and* Am *perpendicular to line OA, and in the bounded space* pOAm *we search for the next closest lattice point* B.

The three points OAB form the *main (principal) triangle* of the lattice, by completing it with a parallelogram we obtain → *the main (principal) parallelogram*, i.e. according to current terminology a *unit cell*.

To determine the position of lattice points, he used integer coordinates, so that the basic length units in two basic directions in the plane were the parameters of the corresponding lattice lines. On their basis, he expressed the equations of the lattice lines and their (directional) indices.

Bravais first considered lattices regardless of their symmetry, in the following chapter he devoted himself to symmetric lattices (according to him, these are those *that contain a line dividing the lattice into two equal parts*, i.e. lattices with a plane of symmetry). In planar lattices, the "Bravais" axes of symmetry lie in the plane of the lattice, are lattice lines, and there is an axis perpendicular to each axis of symmetry. Already in the plane, he introduces a *centered lattice*, i.e. a lattice with a *main parallelogram* in the middle of which there is a lattice point.

According to the multiplicity of the axis of symmetry in the plane, he distinguished four "classes" of lattices (a class without an axis of symmetry, with a two-fold, four-fold and six-fold axis). In each of them there is a primitive *main parallelogram*, and in the case of a two-fold axis of symmetry also a centered parallelogram, which together represents five types of plane lattices. In the original French text, two "modes" - two types of lattices are distinguished for the third class:

Classification des Réseaux symétriques.

Au point de vue de leur symétrie, on peut distinguer quatre classes distinctes de Réseaux :

Première classe. — Réseaux à six axes de symétrie, trois d'une espèce et trois d'une autre espèce. Cette classe n'offre qu'un seul mode ; le Réseau à maille triéquiangle ayant pour parallélogramme générateur un rhombe à angles de 60 et 120 degrés (*voyez* théorème XIX).

Deuxième classe. — Réseaux à quatre axes de symétrie, deux d'une espèce et deux d'une autre espèce. Cette classe n'offre qu'un seul mode ; le Réseau à maille carrée (*voyez* théorème XVIII).

Troisième classe. — Réseaux à deux axes de symétrie. Cette classe offre deux modes distincts : le Réseau à maille rhombe, ou rectangle centrée : le Réseau à maille rectangulaire, ou rhombe centrée (théorèmes XV et XVI). Les deux axes sont rectangulaires entre eux et d'espèces différentes.

Quatrième classe. — Réseaux asymétriques ; la maille est un parallélogramme à côtés inégaux, et dont les angles diffèrent de 90 degrés.

He also used integer coordinates of lattice points in describing spacelattices, gave equations of lattice planes, used Miller indices, and defined the elementary tetrahedron. (W. H. Miller introduced indices in 1839 in his work *Traetice on Crystallography*.) For symmetric space lattices, he proved that only two-fold, three-fold, four-fold, and six-fold axes of symmetry are possible, and that the planes of symmetry are the lattice planes or planes parallel to them. He classified fourteen types of space lattices into seven crystallographic systems (*Classe*), and in each he stated the number of lattices:

cubic (terquaternaires) 3, hexagonal (senaires) 1, tetragonal (quaternaires) 2, trigonal (ternaires) 1, rhombic (terbinaires) 4, monoclinic (binaires) 2, triclinic (asymetrique) 1, a total of **14** types.

In the French original, the part of the text describing the three types of lattices of the cubic system has the following form:

> Trois modes d'arrangement distincts :
>
> 1°. Le cube;
>
> 2°. Le cube centré, que l'on peut remplacer par le rhomboèdre de 120 degrés;
>
> 3°. Le cube à faces centrées, que l'on peut remplacer par le rhomboèdre de 70°31'44", ou par le prisme centré, à base carrée, dont la hauteur égale le côté de la base multiplié par $\sqrt{2}$. Le tétraèdre régulier et l'octaèdre régulier peuvent aussi servir à la dérivation de ce troisième mode.

In english translation:
Three different types of arrangement:

1. Cube;
2. A centered cube, which can be replaced by a rhombohedron with an angle of 120 degrees;
3. A cube with centered faces, which can be replaced by a rhombohedron with an angle of $70^\circ\ 31'\ 44''$, or a centered prism with a square base, whose height is $\sqrt{2}$ times the length of the base. The regular tetrahedron and the regular octahedron can also serve for this third type.

Bravais also attempted to describe the types of symmetry of polyhedra, i.e. bounded figures, in today's terminology *point groups*. In his article on polyhedra – *Sur les polyèdres symétriques*, published in 1849, he distinguished 23 types of symmetry based on his criteria. He distinguished

- asymmetric polyhedra,
- polyhedra without axes of symmetry (with only a center of symmetry, or a plane of symmetry),
- polyhedra with a principal axis of symmetry and
- spherohedral polyhedra (they have more than one equivalent axis of symmetry).

In doing so, he defined the elements of symmetry (center, axis, plane) and also considered 5-fold axes. He proved that in every bounded polyhedron there can be at most one center of symmetry, that the axes and planes of symmetry must intersect at one point. However, he did not derive all types of symmetry of polyhedra, he overlooked those in which a four-fold rotoinverse axis occurs, which Hessel had already included under the name "Gerenstelligkeit" before him and Gadolin after him under the name "sphenoidische Symmetrie".

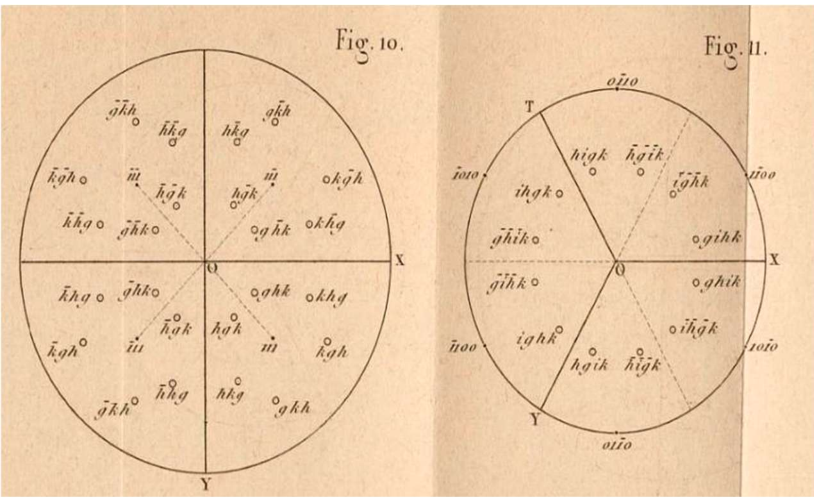
Eintheilung der Polyeder nach der Art ihrer Symmetrie
[61] mit Angabe der Minimalzahl ihrer Ecken.

Polyeder	Symbol der Symmetrie des Polyeders	Classe des Polyeders	Minimalzahl der Ecken der 1. Art	2. Art	3. Art	4. Art
asymmetrisch	$0L, 0C, 0P$	1.	1	1	1	1
symmetrisch, ohne Axen	$0L, C, 0P$	2.	2	2	2	
	$0L, 0C, P$	3.	1	1	1	
symmetrisch, mit einer Hauptaxe, von gerader Ordnung	$\Lambda^{2q}, 0L^2, 0C, 0P$	4.	$2q$	$2q$		
	$\Lambda^{2q}, 0L^2, C, \Pi$	5.	$2q$	$2q$		
	$\Lambda^{2q}, qL^2, qL'^2, 0C, 0P$	6.	$4q$			
	$\Lambda^{2q}, 0L^2, 0C, qP, qP'$	7.	$2q$	1		
	$\Lambda^{2q}, qL^2, qL'^2, C, \Pi, qP^2, qP'^2$	8.	$2q$	0 od. $2q$*]		
	$\Lambda^{2q}, 2qL^2, 0C, 2qP$	9.	$4q$			
symmetrisch, mit einer Hauptaxe, von ungerader Ordnung	$\Lambda^{2q+1}, 0L^2, 0C, 0P$	10.	$2q+1$	$2q+1$		
	$\Lambda^{2q+1}, 0L^2, C, 0P$	11.	$4q+2$	$4q+2$		
	$\Lambda^{2q+1}, 0L^2, 0C, \Pi$	12.	$2q+1$	$2q+1$		
	$\Lambda^{2q+1}, (2q+1)L^2, 0C, 0P$	13.	$4q+2$			
	$\Lambda^{2q+1}, 0L^2, 0C, (2q+1)P$	14.	$2q+1$	1		
	$\Lambda^{2q+1}, (2q+1)L^2, C, (2q+1)P^2$	15.	$4q+2$			
	$\Lambda^{2q+1}, (2q+1)L^2, 0C, \Pi, (2q+1)P$	16.	$2q+1$			
symmetrisch, sphäroedrisch, quaterternär	$4L^3, 3L^2, 0C, 0P$	17.	12			
	$4L^3, 3L^2, C, 3P^2$	18.	12			
	$4L^3, 3L^2, 0C, 6P$	19.	4			
	$3L^4, 4L^3, 6L^2, 0C, 0P$	20.	24			
	$3L^4, 4L^3, 6L^2, C, 3P^4, 6P^2$	21.	6			
symmetrisch, sphäroedrisch, decem-ternär	$6L^5, 10L^3, 15L^2, 0C, 0P$	22.	60			
	$6L^5, 10L^3, 15L^2, C, 15P^2$	23.	12			

Bravais' table of types of symmetry of polyhedra in German translation

In his work *Études cristalllographiques*, published in 1851, Bravais also dealt with the symmetry of the internal arrangement of crystals. He considered points distributed regularly in space to be the geometric centers of the molecules of which the crystals are composed. Based on the reticular density of these points, he was able to explain the cleavability and also the external symmetry of crystals. He devoted a separate chapter to considerations of crystals consisting of molecules:

This work includes a picture (on next side), showing that he used stereographic projection to indicate the positions of symmetry elements. It was later consistently used by Axel Gadolin (1867).



ÉTUDES

CRISTALLOGRAPHIQUES,

PAR

M. AUGUSTE BRAVAIS,

MEMBRE DE L'INSTITUT (ACADÉMIE DES SCIENCES).

PARIS,

GAUTHIER-VILLARS, IMPRIMEUR-LIBRAIRE

DU BUREAU DES LONGITUDES, DE L'ÉCOLE IMPÉRIALE POLYTECHNIQUE,

SUCCESSEUR DE MALLET-BACHELIER,

Quai des Augustins, 55.

1866

ABHANDLUNG

über

die Systeme von regelmässig auf einer Ebene oder im Raum vertheilten Punkten

von

A. BRAVAIS,

Lieutenant zur See und Professor an der École Polytechnique.

(1848.)

Uebersetzt und herausgegeben

von

C. und E. Blasius.

Mit 2 Tafeln.

LEIPZIG

VERLAG VON WILHELM ENGELMANN

1897.

Title pages of Bravais' crystallographic publications
in French (1866) and German (1897)

Bravais's important works related to crystallography:

1. Mémoire sur les systémes formés par des points distribués régulierement sur un plan au dans l'espace, Paris 1848, 1850, Leipzig 1897, New York 1969, 2005
2. Sur les polyèdres symétriques, Paris 1849, Leipzig 1890
3. Études cristalllographiques, Paris 1851
4. Collected edition of these works under the title Études cristalllographiques Paris 1866

Bravais cited authors:
Poisson, Cauchy, Frankenheim, Gauss, Weiss, Haüy, Miller
He did not cite Hessel

Sources used

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3. https://en.wikipedia.org/wiki/Auguste_Bravais

Axel Gadolin (1828 – 1892)

A Finn by origin, who made a significant contribution to the modern view of the systematics of crystals in terms of their external symmetry types. He published the results of his considerations in an article entitled *Derivation of all crystallographic systems and their separations on the basis of a single principle*, which he published in 1869 in the journal *Zapiski imperatorskogo russkogo mineralogičeskogo obšestva* [9]. It was published in French two years later in the journal *Acta Societatis Scientiarum Fennicae*. However, the title page of the German edition (1896) states that the work was "read" as early as March 1867. Since Hessel's work on the derivation of the 32 point groups was not yet in the consciousness of crystallographers at that time, practically until the end of the 19th century Gadolin's primacy was acknowledged. For this work, he was awarded the M. V. Lomonosov Prize, received a doctorate in mineralogy, and became a member of several domestic and foreign scientific societies.

Gadolin was born in the city of Somero, in what is now Finland, which at that time was part of Tsarist Russia. He served his entire life as an officer in the Tsarist army, where he achieved the rank of general towards the end of his life (1890). He prepared for a military career at the cadet school and after graduating in 1847 became captain of the Guards Artillery. As early as 1849, he began working as a teacher at the Artillery School and in 1856 became its director. He dealt with artillery technology, mechanical metalworking, mineralogy and crystallography. He became a member of the St. Petersburg Academy of Sciences and the Imperial Academy of Sciences. He died in St. Petersburg.

It should be noted that several crystallographers had tried to derive the point groups of crystals before him, for example Bravais, but – with the exception of the forgotten Hessel – they had not derived all of them. In the introduction to his work, Gadolin cites this fact as the reason why he undertook this task.

He was already aware that the external shapes of crystals are conditioned by the action of molecular forces, as evidenced by a part of the text from the introduction to the work:

im gewöhnlichen Sinne dieses Wortes, zu gründen. Berücksichtigt man aber, dass die äussere Form der Krystalle selbst [2] nur eine Folge der Wirkungsweise der Molekularkräfte ist, so ist man berechtigt, die Gesetze, welche diese Formen beherrschen, als physikalische Qualitäten zu betrachten. Diese

"*However, it should be remembered that the external shape of crystals is only a consequence of the* *action of molecular forces, which entitles us to consider the laws that determine these shapes as physical qualities.*"

Abhandlung

über

die Herleitung aller

KRYSTALLOGRAPHISCHER SYSTEME

mit ihren Unterabtheilungen

aus einem einzigen Prinzipe

von

AXEL GADOLIN.

(Gelesen den 19. März 1867.)

Deutsch herausgegeben

von

P. Groth.

Mit 26 Textfiguren und 3 Tafeln.

LEIPZIG

VERLAG VON WILHELM ENGELMANN

1896.

Gadolin, unlike Hessel, was concerned only with crystallographic symmetries, and he divided the types of symmetry into six crystall systems. In the introduction to this work he wrote:

In addition to the general laws governing crystals (the planar shape of the surfaces, the constancy of the angles, and the rationality of the ratios of the surface parameters on certain axes), several special laws can be discovered that apply only to certain groups of crystals. These are the groups known as crystall systems, with their further division into holohedral, hemihedral, tetartohedral, and hemimorphic.

An important part of his work was the use of stereographic projection to depict the positions of symmetry elements. This is probably related to his artillery profession, which required him to deal with cartography. Some authors give him precedence in this respect, but indications of the use of stereographic projection in crystallography can be found already in Bravais.

The sequence of Gadolin's considerations can be seen through the headings of the individual chapters: *On the equivalence of directions* (Gleichheit der Richtungen), *On the axes of symmetry* (Deckaxen), *On the laws of symmetry, General overview of crystall groups, Arrangement and multiplicity (Dimension) of characteristic crystall axes* and the last chapter *List of simple shapes of some crystall groups.*

It should be noted that by the term group he did not mean its mathematical content, but a set, or rather a group, whose members (elements) meet certain criteria:

in der Weise, dass wir in die gleiche Gruppe diejenigen Krystalle stellen, in denen die Zahl und die Anordnung der gleichen Richtungen dieselbe ist, und dass wir als verschiedenartig nur

"... we group together those crystals in which the number and arrangement of equivalent directions are the same..."

He proceeded consistently in his reasoning, after stating a statement, he always followed it with proof. Some of his statements:

§ 4. *It can be easily proved that the smallest cover angles cannot have other values than* 60°, 90°, 120° *and* 180°.

§ 10. *It is now not difficult to find all possible combinations of sixfold, fourfold, or twofold axes.*

§ 12. *Apart from the six cases of combinations of axes of symmetry given in § 10. and § 11., the four cases where there is a single axis of* 60° *(Fig. 50),* 90° *(Fig. 35),* 120° *(Fig. 53), or* 180° *(Fig. 41), and the last case without an axis of symmetry, there is no other case.*

§ 15. *A twofold, fourfold, or sixfold axis of rotation, in combination with the laws of parallelism, conditions the existence of a plane of symmetry perpendicular to it.*

§ 19. *In Chapters II and III, 32 crystallographic groups were introduced, which can be divided into six classes. These classes are nothing other than the generally accepted crystall systems.*

He did not present the summary of the derived point groups in a table, but in condensed text, as shown by the detail of the page on which he listed the 5 point groups of the cubic system; next to the text is a stereographic projection of one of them:

A. Die Gruppen des regulären Systems.

1) und 2) Fig. 28 und 27. In diesen beiden Gruppen, welche der Holoëdrie und der Hemiëdrie mit abwechselnden Flächen entsprechen, giebt es drei auf einander senkrechte Axen von 90°. Dieselben sind nothwendig mögliche krystallographische Axen von gleichem Werthe (§ 27, Nr. 1 und 4).

3) Fig. 31. In dieser, der tetraëdrischen Hemiëdrie entsprechenden Gruppe halbiren die Normalen der Symmetrieebenen die Winkel zwischen den Axen von 180°. Aus der Anmerkung des § 13 ist bekannt, dass in Bezug auf die absoluten Werthe der Parameter diese Normalen dieselbe Rolle spielen, wie Deckaxen von 180°, woraus sich die Gleichwerthigkeit der in dieser Gruppe vorhandenen Axen von 180°, welche ebenfalls mögliche krystallographische Axen sind, ergiebt, weil dieselben durch Drehungen von 180° um die Normalen der Symmetrieebenen vertauscht werden (§ 27, Nr. 2).

4) und 5) Fig. 30 und 29. In diesen Gruppen, welche der dodekaëdrischen Hemiëdrie und der Tetartoëdrie entsprechen, sind die drei Axen von 180° zugleich orthogonale krystallographische Axen, gleichwerthig aber nur dann, wenn die Axen von 120° ebenfalls mögliche krystallographische Axen

He included not only the geometric shape of the crystal but also its physical properties in the properties of symmetry. He wrote:
Two directions that are equivalent with respect to the external shape of the crystal also exhibit identical physical behavior.

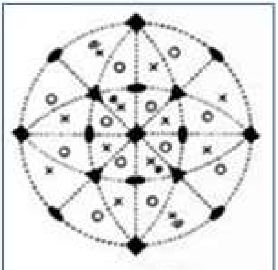

Fig. 27

And a little further on:

We consider those groups to be different which differ in the number and arrangement of equivalent directions, and when it is true that directions which are in the same relation to the shape of the crystal also show the same physical properties. This principle is so generally accepted that it is not uncommon for the definitive belonging of a group of crystals to one or another crystallographic group to be determined on the basis of physical properties.

In one of the appendices he also dealt with the law of rationality of indices, as follows from the following heading:

[63] Anhang A.

Das Gesetz der Rationalität der Parameterverhältnisse der Krystallflächen.

Gadolin's work *Derivation of all crystall systems and their separations on the basis of a single principle*, which he developed as early as 1867, was successively published in Russian, French and German:

- Вывод всех кристаллографических систем и их подразделений из общего начала, Записки Имп. русского минерал. общ., IV, 1869.
- *Mémoire sur la déduction d'un seul principe de tous les systémes cristallographiques avec leurs subdivisions*, Acta Societatis Scientiarum Fennicae, IX, 1871.
- Abhandlung über die Herleitung aller Kristallographischer Systeme mit ihren Unterabtheilungen aus einem einzigen Prinzipe, Leipzig 1896.

Gadolin cited the authors: von Naumann, Haidinger, Kokscharov, Pasteur, Sacchi, Miller, Weiss, but did not cite Bravais or Hessel.

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3. https://de.wikipedia.org/wiki/Axel_Wilhelmowitsch_Gadolin

Leonhard Sohncke (1842 – 1897)

German mathematician, physicist and crystallographer, whose name is associated with the beginning of the work on the derivation of space groups, i.e. groups in which combinations of point and translational symmetry are already considered. He published the work on the derivation of 65 types of symmetry groups in 1879 [11]. He did not derive all space groups, he only used point operations of the first kind related to rotational and screw axes; he did not consider reflections. He used the name *systems of regularly spaced points* for the derived groups, but they are also known under the names *chiral space groups* or *Sohncke groups*. He did not know Hessel's or Gadolin's work on point groups, and for translational symmetries (space lattices) he relied on Bravais's work. He also followed up on the work of C. Jordan from 1868 [10], who derived 174 space groups, but more than 100 of them were not applicable to crystallography, especially those that contained rotations by an arbitrarily small angle. When deriving individual groups, he proceeded according to the type of the principal axis of symmetry (similar to Hessel). He created his own terminology, already in considerable agreement with the current one – *screw axis, fourfold axis*, etc. He accepted 7 crystallographic systems.

He was born into a family of mathematicians in Halle, where he studied mathematics and natural sciences at the university from 1859. From 1865 he worked as a teacher at the gymnasium in Königsberg, while continuing his studies at the university there, which he completed in 1866 with a graduation in Halle. The title of Dr. phil. he received for his work on differential equations "*De aequatione differentiali seriei hypergeometricae*". In 1869 he received a docentship for his work "*Kohäsion des Steinsalzes*". Two years later, on the recommendation of G. R. Kirchhoff, he was appointed professor of experimental physics at the Polytechnic in Karlsruhe and at the same time head of the meteorological observatory. In 1883 he became a full professor of physics at the University of Jena and at the same time the first head of the Physical Institute there. Three years later, he moved to Munich to the Department of Experimental Physics, where he headed the Physics Institute of the Technical University until his death (1897).

In connection with the goal of deriving space groups, he expressed his opinion as follows:

> **Beitrag zu liefern bestimmt ist. Man findet hier die ganze Mannichfaltigkeit der überhaupt möglichen Krystallstrukturformen aus einem einzigen Princip, nämlich aus dem selbstverständlichen Grundsatze von der regelmässigen Anordnung, auf streng mathematischem Wege abgeleitet. Die geome-**

The entire variety of all possible crystal shapes can be derived from a single principle in a strictly mathematical way, using the obvious assumption of regular arrangement.

He based his work on Jordan's work [10], which he also critically evaluated:

Despite the principled agreement with Jordan's work, which must have occurred during my research, there are also significant differences, which lie primarily in the fact that I always placed the main emphasis on the geometric meaning of the results, because finding the shapes of the structures was my main goal.


ENTWICKELUNG

EINER

THEORIE DER KRYSTALLSTRUKTUR

VON

DR. LEONHARD SOHNCKE,

LEIPZIG,

DRUCK UND VERLAG VON B. G. TEUBNER.

1879.

He formulated his idea of crystals as follows:

A crystal is a homogeneous solid body whose geometric and physical properties are generally different in different directions and which, in undisturbed development, is bounded by plane surfaces. ... Since a crystal grows by depositing particles of matter on its outer surfaces, it is inconceivable that it would not be built up from these particles. Therefore, the structure of a crystal should be *understood as the arrangement of the particles of which it is composed.*

He further writes:

For the following geometric considerations, the crystal will be replaced by a system of discrete material points, between which there is a certain minimum distance.

He considers such a point to be the center of a group of particles – atoms, or the center of a molecule.

In the following text he writes:

Crystals, if we understand them as unbounded, represent regular infinite systems of points, such that around each of the points the arrangement of the other points is the same.

In doing so, he sets himself the goal:

To find all possible regular systems of points that are infinite in all directions.

Sohncke stated that he was not the first to attempt to extend Bravais's lattice theory. That before him, the situation of how the symmetry changes when an atom is placed inside the unit cell of a Bravais lattice had already been considered. In this connection, he wrote:

"*Every regular system of points, infinite in all directions, is either a space lattice or consists of several congruent space lattices nested within each other.*"

Sohncke increased the number of Bravais types of regularly arranged points (i.e. lattices) by types in which screw axes occur. He thus combined rotation with translation into one symmetry operation, which is an operation that does not belong to the point or translation group, but to the space group. The following figure from his work represents a text about a structure with such possible operations. He marked the symmetry operation representing a rotation by 90°, i.e. by $2\pi/4$ combined with a translation by a quarter of the lattice parameter λ with the symbol

$$A_{\frac{2\pi}{4},\frac{\lambda}{4}}\,,$$

other operations have analogous designations.

Für die der Axe parallele kleinste Deckschiebung λ gilt nach Satz 47 die Gleichung

$$p\,.\,\lambda = 4\,.\,l,$$

worin p nacheinander die Werthe 1, 2, 3, 4 annehmen kann.

1) *Bei* $p = 1$ wird $l = \frac{\lambda}{4}$. Die Deckbewegungen $A_{\frac{2\pi}{4},\frac{\lambda}{4}}$ und λ charakterisiren eine Vierpunktschraube (Taf. II. Fig. 26).

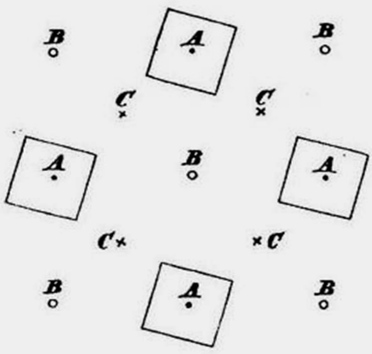

Fig. 23.

2) *Bei* $p = 2$ wird $l = \frac{2\lambda}{4}$. Die Deckbewegungen $A_{\frac{2\pi}{4},\frac{\lambda}{2}}$ und λ bestimmen 2 ineinandergewundene kongruente 4-punktschrauben mit der Schraubenhöhe 2λ, ausgehend von 2 diametral gegenüber liegenden Punkten des Schraubencylinders. Die Verbindungslinie des um $\frac{\lambda}{2}$ höher gelegenen Punktpaars kreuzt die Verbindungslinie des Ausgangspaars rechtwinklig im Raum (Taf. III. Fig. 29).

The next figure presents a summary of such operations in the tetragonal system.

Zusammenstellung der Punktsysteme dieser Abtheilung.

1) und 2) Rechtes und linkes 4-punktschraubensystem.

$$A_{\frac{2\pi}{4}, \pm\frac{\lambda}{4}}, \lambda, e, \left(B_{\frac{2\pi}{4}, \pm\frac{\lambda}{4}}\right).$$

3) Vierzähliges Gegenschraubensystem.

$$A_{\frac{2\pi}{4}, \pm\frac{\lambda}{4}}, \lambda, \sigma, \left(B_{\frac{2\pi}{4}, \mp\frac{\lambda}{4}}\right).$$

4) Zweigängiges 4-punktschraubensystem.

$$A_{\frac{2\pi}{4}, \frac{\lambda}{2}}, \lambda, e, \left(B_{\frac{2\pi}{4}, \frac{\lambda}{2}}\right).$$

5) Quadratsäulensystem. $A_{\frac{2\pi}{4}, 0}, \lambda, e, \left(B_{\frac{2\pi}{4}, 0}\right).$

6) Quadratoktaëdersystem. $A_{\frac{2\pi}{4}, 0}, \lambda, \sigma, \left(B_{\frac{2\pi}{4}, \frac{\lambda}{2}}\right).$

In 1876 he published a paper in which he presented 54 types of space groups, but three years later he published another in which he distinguished between right-handed and left-handed screw axes, bringing the total number of groups to 66. In 1891 Schoenflies repeated Sohncke's derivation and found that the two groups were identical, so the final number of Sohncke groups is 65. The following figure shows the end of the table published in the 1879 book

VII) Systeme mit 4-zähligen Hauptaxen von mehr als 2 Richtungen.

59. Kubisches
60. Oktaëdrisches
61. Rhombendodekaëdrisches

} 24-punktnersystem.

62. Reguläres Gegenschraubensystem erster Art.
63. „ „ zweiter „
64. Reguläres zweigängiges 4-punktschraubensystem.
65. Rechtes
66. Linkes

} reguläres 4-punktschraubensystem.

He classified the derived types of space groups according to the type of symmetry axes (by multiplicity and their number), which ultimately agreed with the classification into crystall systems. His naming of these seven systems, which, given in the original, can be seen in the following figure, is noteworthy.

Krystalle mit sich selbst wieder zur Deckung gelangen. So erhält man folgende Uebersicht:

1. Klinorhomboidisches Krystallsystem. Keine Drehungsaxe.
2. Klinorhombisches Krystallsystem. 1 zweizählige Drehungsaxe.
3. Rhombisches Krystallsystem. Zweizählige Drehungsaxen nach 3 senkrechten Richtungen.
4. Quadratisches Krystallsystem. 1 vierzählige Drehungsaxe.
5. Rhomboëdrisches Krystallsystem. 1 dreizählige Drehungsaxe.
6. Hexagonales Krystallsystem. 1 sechszählige Drehungsaxe.
7. Reguläres Krystallsystem. 3 zweizählige oder 3 vierzählige, und 4 dreizählige Drehungsaxen, bezüglich parallel den Kanten und Diagonalen eines Würfels.

From a terminological point of view, it is interesting that he used the term *Krystallsystem*, as opposed to Gadolin's term *Krystallografische system*.

Sohncke's work on the derivation of 65 space groups was often cited by both Fyodorov and Schoenflies, who essentially independently and practically simultaneously derived all 230 space groups.

Sohncke's work on crystallography:

1. *Die unbegrenzten regelmässigen Punktsysteme als Grundlage einer Theorie der Krystallstruktur*. 83 Seiten. 2 Tafeln, Karlsruhe 1876. Separatabdruck aus dem 7. Heft der Verhandlungen des naturwissensohaftl. Verein zu Karlsruhe.
2. *Universalmodell der Raumgitter*. Repertorium für Experimentalphysik. Bd. XII. 1876. 6 Seiten.
3. *Entwickelung einer Theorie der Krystallstruktur*. B.G. Teubner, Leipzig 1879
4. *Erweiterte Theorie von der Krystallstruktur*, Zeitschrift für Kristallographie 14, 426-446 (1888).

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2. https://de.wikipedia.org/wiki/Leonhard_Sohncke

Arthur Moritz Schoenflies (1853 – 1928)

German mathematician, famous in crystallography for the derivation of 230 space groups describing types of symmetry of crystal structure. Originally, in 1889, he published in the journal Mathematische Annalen the derivation of 227 groups, but after correspondence with E. S. Fyodorov (29 letters surviving) he published in 1891 a book *Krystallsysteme und Krystallstruktur* [13] with the derivation of all 230 groups. In his search for types of symmetry of crystals, he was the first to use the mathematical theory of groups. He introduced the symbols of the groups, which are still used in the International Crystallographic Tables (in addition to the International Symbols) and are actively used in solid state theory.

Schoenflies was born in Prussia in Landsberg an der Warthe (now the Polish town of Gorzów). From 1870 to 1875 he studied mathematics at the Friedrich Wilhelm University in Berlin (later renamed Humboldt University), where the eminent mathematician Karl Weierstrass was then a professor. He was interested in set theory and topology. He received his doctorate in 1877, and the following year began teaching in Berlin, where he habilitated after six years. In 1891 he was appointed to the chair of applied mathematics in Göttingen, and in 1899 he began to work as a professor at the University of Königsberg and in 1911 at the Academy of Social and Commercial Sciences in Frankfurt. In 1922 he ended his career as rector of the university there. During his active career, he became a member of the Leopoldina in Halle, the Bavarian Academy of Sciences in Munich, an honorary member of the German Scientific Society, and was one of the founders of the German Mathematical Society, which he led as president in 1922.

Of his crystallographic works, the most frequently cited is the book *Krystallsysteme und Krystallstruktur* (Fig. 1; the figures are at the end of the article on Schoenflies), in which he summarized the results of his earlier work. In the introduction of the book he wrote:

... to move more and more from the empirical to the deductive method. We owe this step to the discovery that the systematics of crystals can be deduced from a single fundamental law and the theory of structure from a single fundamental hypothesis in a mathematical way.

By mathematical method he probably understood the theory of groups. In the introduction of the book he wrote what he meant by a group in the case of symmetry of crystals:

By a finite group of operations we mean a finite series of non-equivalent operations with the property that the product of any two of this series is always equal-valued with some operation of this series.

And further: *all the operations of symmetry that transform a symmetric body into itself form a finite group of operations*.

By the product of operations Schoenflies understood their successive execution, and he attributed the same meaning to the powers of operations. He described the properties of such products and introduced the appropriate symbolism:

If A and B are two rotations whose axes pass through a point O, and C is their equivalent resultant rotation, we shall henceforth express this relation by the equation $AB = C$, and call C the product of the rotations A and B .

The first part of Schoenflies' book is the derivation of 32 crystall classes (32 Krystallclassen) of finite formations – symmetric polyhedra. In doing so, he quoted J. F. Ch. Hessel, who derived them already in 1830, admittedly without using the theory of groups. He also mentioned Bravais's incomplete attempt and Gadolin's derivation. He began by describing the symmetry of formations characterized by a single axis of symmetry. He gave the name rotation groups (*Drehungsgruppen*) to the groups in question. He proved that in the case of crystals, in accordance with the law of the rationality of indices, only four such groups are possible, with axes of symmetry twofold, threefold, fourfold, or sixfold. He then considered formations with multiple axes of symmetry, proving that there are 11 types (classes) of such symmetry (Fig. 2).

In the following he dealt with figures whose symmetry is described by combinations of rotation with reflection or inversion, as well as by reflection or inversion alone; the corresponding symmetry operations he called *rotations of the second kind*. In the case of reflection he wrote:

Ist $\mathfrak{S}$ irgend eine Spiegelung, so bilden die Operationen 1 und $\mathfrak{S}$ eine Gruppe; wir bezeichnen sie einfacher durch

$$S = \{\mathfrak{S}\}.$$

Lehrsatz II. ***Es giebt eine Krystallclasse, deren Symmetrie in der Existenz einer einzigen Symmetrieebene besteht.***

Translated:
If S is some reflection, then the operations I (identity) and S form a group; we denote it simply as S = {S } .
Theorem II. *There is a class of crystals whose symmetry is based on the existence of a single plane of symmetry.*

He made analogous claims about inversion. In the conclusion of the chapter on operations of the second kind, he included a table of such point groups (there are 21 of them), which, together with the eleven point groups of the first kind, represent 32 types of symmetry.

After obtaining the 32 point groups, he classified them into 6 main classes (Fig. 3). He used multiplicity and the number of axes of symmetry as sorting criteria, thus essentially mimicking Hessel's procedure. He placed types with multiple equivalent axes of symmetry in the first class, and formed the other groups according to the multiplicity of the major axis of symmetry. In doing so, he considered purely rotational axes and axes combined with inversion or reflection to be equivalent. In the group called *Digonaler* *typus* he included groups in which only twofold axes occur, which includes the groups we now classify in two crystall systems, the monoclinic and the rhombic.

He also supported his classification in terms of the theory of groups. In this context he stated:

In every crystall system, the respective groups of operations are related in such a way that one of them - the main group - contains the others as subgroups.

On the basis of this criterion he repeated the classification of the groups. For example, the monoclinic system includes three point groups, which Schoenflies designated by the symbols C_2, C_s and C_{2h}, the first two being subgroups of the third.

Groups were also used in the chapter on **space lattices**. He wrote:

By a group of translations we mean an infinite series of translations of such a kind that any two translations made in succession constitute a translation which is equivalent to some translation belonging to that group.

Theorem IV. *The set of all translations which a regular series of points, or a planar network of points, or a space lattice, identify with each other, forms a group of translations.*

The space lattice and the space translation group are formations which are inseparably connected.

For plane lattices, in addition to the non-symmetric lattice, he distinguished four types of symmetric lattices, noting that a plane symmetric lattice can only be orthogonal or rhombic. He did not explicitly mention the centred lattice, which is, however, the rhombic lattice (*rhombische*

Netz). For space lattices he distinguished 14 types, which he classified into seven crystall systems and where he had already used the term *centred lattice*.

In describing space translation groups, he used a triple of translations $2\tau_1, 2\tau_2, \ 2\tau_3$, which he called *primitive*: If *OA* = $2\tau_1$, OB = $2\tau_2$, *OC* = $2\tau_3$ are *primitive translations of a space lattice, then each of them transforms the space lattice into itself.*

Denoting the primitive translations in this way - as doubles - allows one not to use fractional expressions for centered lattices, but only τ_1, τ_2 and τ_3 respectively. The translations $2\tau_1, 2\tau_2, \ 2\tau_3$, are thus simultaneously the edges of a primitive unit cell (Schoenflies' name: *primitive Palallelepipedon*). He wrote:

When characterizing symmetric space lattices, we preferably use the set of primitive translations, or the corresponding tetrahedra and parallelograms. For each symmetric lattice, these can be chosen more or less arbitrarily.

The space lattices were obtained (constructed) on the basis of their compatibility with the point groups describing their symmetry. He proved that in every space lattice there is a set of symmetry centers; that a space lattice can be characterized only by twofold, threefold, fourfold and sixfold axes of symmetry; that there is a perpendicular lattice plane to every symmetry axis; and that every symmetry plane must be parallel to some lattice plane.

In deriving the space lattices, he relied on evidence from the preceding sections of the text. He justified the two types of lattices in the monoclinic system by the following reasoning (loosely modified):

If a point O is the center of symmetry of a space lattice, and if a twofold axis of symmetry $\boldsymbol{a}$, passes through this point, then there is a plane of symmetry perpendicular to this axis. The corresponding point group has the label C_{2h}. It is the holohedral group of the monoclinic system. The lattice of the plane of symmetry perpendicular to the axis may be orthogonal or rhombic. Thus, there are two types of monoclinic lattice – primitive (corresponding to an orthogonal lattice) and centred; Schoenflies denoted them by the symbols Γ, and Γ', respectively. He expressed the result in the theorem:

Theorem XII. *There are two different space lattices of monoclinic type.*

At the end of the text on lattices, he included a table of them - in this text it is shown in Fig. 4 in a modified abbreviated form with the original German text.

Before the chapter on space groups, he described in a separate chapter Bravais's procedure for deriving space lattices, but he also mentioned Bravais's work on filling the lattice with "molecules". He used the term *Molekelgitter* for such a lattice and wrote in terms of its symmetry:

Lehrsatz IV. *Die Symmetrie eines Molekelgitters ist niemals höher als die Symmetrie des zugehörigen Raumgitters.*

The symmetry of the molecular lattice is never higher than the symmetry of the corresponding space lattice.

This statement is consistent with his reasoning about the subgroups of the holohedral group of the corresponding crystall system. By filling the lattice with "molecules", his thoughts on possible types of symmetry of the crystal structure begin.

He introduced the chapter on space groups with a definition:

By a space group of operations we mean an infinite set of space operations such that the product of any two of them is equivalent to an operation which also belongs to this set.

Then he stated how one can construct (create) a space group:

Lehrsatz XXI. ***Enthält die zur Punktgruppe G isomorphe Raumgruppe Γ die Gruppe G als Untergruppe, so kann sie durch Multiplication der Gruppe G mit der Translationsgruppe Γ_t erzeugt werden.***

If a space group Γ isomorphic to a point group G contains this group as its subgroup, then it can be created by multiplying the point group G by the translation group Γ_τ .

However, only so-called symmorphic space groups arise in this simple way; for the others, Schoenflies had to consider the cases of screw axes and glide planes conditioned on the shape or symmetry of the "molecules".

He started the construction (derivation) of space groups with the triclinic system. When considering the monoclinic system, he wrote:

There are four different kinds of space groups characterized by the symmetry of monoclinic hemihedra.

Two of them contain Γ_m, the remaining two Γ_m', as translation groups.

And further:

These four groups, in which operations of the second kind stand out, can be denoted by the following symbols. The group G_s^1 contains only the ordinary symmetry plane. The group G_s^3 contains a plane of symmetry and, in addition, planes with translational symmetry, and for all these planes the translational component is equally large. The groups G_s^2 and G_s^4 do not have pure reflection planes. For the former, the translational component is the same everywhere, but for the latter, there are two different kinds of translational operations with unequal magnitudes.

The text on the derivation (construction) of space groups is supplemented by a summary table (Fig. 5), followed by a sentence:

***Main theorem**. There are a total of 230 crystallographically usable space groups.*

Schoenflies did not yet use the reciprocal lattice, the decomposition of the group into cosets and hence the factor group, which could have streamlined the procedure for constructing symmetry groups. But he did take a decisive step towards the mathematization of crystal symmetry theory. He correctly cited his predecessors, referring in the introduction to the book mainly to the work of Hessel, Bravais, and Sohncke, but mentioning a number of other crystallographers: Naumann, Groth (definition of a crystal), Gadolin, Minnigerode, Liouville, Curie, Moebius, Poisson, and Wulf. However, he paid special attention to the works of E. S. Fyodorov, with whom he corresponded intensively before completing his work on the types of symmetry of crystal structure.

KRYSTALLSYSTEME

UND

KRYSTALLSTRUCTUR

VON

Dr. ARTHUR SCHOENFLIES,

LEIPZIG,

DRUCK UND VERLAG VON B. G. TEUBNER.

Fig. 1

Tabelle I.

Die Krystallclassen, die nur Symmetrieaxen enthalten.

No.	Drehungsgruppen	Zahl der Drehungen	Die einseitigen Symmetrieaxen	Die zweiseitigen Symmetrieaxen
1	Identität C_1	1	—	—
2	Cyclische Gruppe C_2	2	h_2	—
3	Cyclische Gruppe C_3	3	h_3	—
4	Cyclische Gruppe C_4	4	h_4	—
5	Cyclische Gruppe C_6	6	h_6	—
6	Vierergruppe V	4	—	l_2, l_2', l_2''
7	Diedergruppe D_3	6	$3l_2$	h_3
8	Diedergruppe D_4	8	—	$h_4, 2l_2, 2l_2'$
9	Diedergruppe D_6	12	—	$h_6, 3l_2, 3l_2'$
10	Tetraedergruppe T	12	$4l_3$	$3l_2$
11	Octaedergruppe O	24	—	$3l_4, 4l_3, 6l_2$

Fig. 2

I. Regulärer Typus.
Symmetriecharacter: Vier dreizählige Axen.

II. Hexagonaler Typus.
Symmetriecharacter: Eine sechszählige Axe.

III. Tetragonaler Typus.
Symmetriecharacter: Eine vierzählige Axe.

IV. Trigonaler Typus.
Symmetriecharacter: Eine dreizählige Axe.

V. Digonaler Typus.
Symmetriecharacter: Nur zweizählige Axen.

VI. Monogonaler Typus.
Symmetriecharacter: Keinerlei Symmetrieaxe. (Eine einzählige Axe.)

Fig. 3

Gitter von Typus	Symmetriegruppe	Translationsgruppen
triklinen	S_2	Γ_τ
monoklinen	C_{2h}	Γ_m , Γ'_m
rhombischen	V_h	Γ_v , Γ'_v , Γ''_v , Γ'''_v
rhomboedrischen	D_{3d}	Γ_{rh}
tetragonalen	D_{4h}	Γ_q , Γ'_q
hexagonalen	D_{6h}	Γ_h
regulären	O_h	Γ_c , Γ'_c , Γ''_c

Fig. 4

	Reguläres System.	Γ_c,	Γ'_c,	Γ''_c.
O^h.	Holoedrie.	4	4	2
O.	Enantiomorphe Hemiedrie.	4	2	2
T^d.	Hemimorphe Hemiedrie.	2	2	2
T^h.	Paramorphe Hemiedrie.	3	2	2
T.	Tetartoedrie.	2	1	2

Wir schliessen mit folgendem

Hauptsatz. *Es giebt im Ganzen 230 krystallographisch verwendbare Raumgruppen.*

Fig. 5

Schoenflies' papers on crystallography:

1. Ueber Gruppen von Bewegungen Mathem. Ann., **28**, 1887, 319-42; **29** 1887, 50-80
2. Ueber regulare Gebietstheilungen des Raumes Götting. Nachr., 1888, Nr 9;
3. Beitrag zur Theorie d. Kristallstructur Götting. Nachr., 1888, Nr 9.
4. Ueber Gruppen von Transformationen des Raumes in sich, Math. Ann., Bd. **34**, 1889, 172-203. ← derivattion of 227 groups
5. Ueber das gegenseitige Verhältniss der Theorien über die Struktur d. Kristalle, Götting. Nachr., 1890, Nr 6).
6. Krystallsysteme und Krystallstruktur, Teubner, Leipzig 1891
7. Theorie der Kristallstruktur. Ein Lehrbuch. Gebr. Borntraeger, 1923.

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Evgraf Stepanovič Fyodorov (1853 – 1919)

Russian crystallographer, mineralogist and mathematician, who is known in crystallography for deriving 230 types of symmetry of crystal structure, in today's understanding 230 space groups. The work was published in 1891 in the journal of the Russian mineralogical society *Zapisky mineralogicheskogo obshestva*. Fyodorov is also known as the inventor of the universal turntable used in light microscopes in the analysis of geometric and optical properties of minerals (Fyodorov table).

E. S. Fyodorov was born in Orenburg in the family of an engineer serving in the tsarist army with the rank of major general. In 1866 he was admitted to a military grammar school and already there he showed a greater interest in mathematics. He did not finish his studies at the grammar school, because after a very successful audition he was admitted to the Military Engineering School in St. Petersburg, although only at the age of 16. After graduating in 1872, he joined a military unit in the city of Bielaya Tserkv, Ukraine. Two years later, he left military service and began studying at the Military Medical Academy in St. Petersburg. In 1879 he became more seriously interested in crystallography and in the same year he completed the first major work on the shapes and symmetry of polyhedra, *Начала учения о фигурах* (Beginnings of the doctrine of figures). However, the reviewers did not recommend publishing the work, it was commissioned for printing later – in 1883, but it was not published until 1885; this caused problems in recognizing Fyodorov's priority, since a similar work by P. Curie was published in 1884. For Fyodorov, it became the basis for further reflections and publications on the symmetry of bodies. In an effort to improve his skills in crystallography, in 1880 he enrolled in the third year of the Mining Institute (Gorny Institute in St. Petersburg). He completed his studies in 1883 so successfully that his name was engraved on the marble slab of the school's excellent students. From 1885 to 1890 he was the leader of the group that compiled the geological map of the northern Urals, but in the winter months he devoted himself to science at home in St. Petersburg.

In 1889, his work *Симметрия конечных фигур* (Symmetry of finite figures) was published in the journal of the Mineralogical Society, where he expanded his reflections on the symmetry of polyhedra. Already in December of the same year, he completed a substantial part of his most important and most cited work, *Симметрия правильных систем фигур* (Symmetry of regular systems of figures) [12] with the derivation of space groups, but it was not published until 1891 (at the end of the introduction in the manuscript is the date "*December 1889*"). In 1890, in the journal of the Mineralogical Society, Fyodorov published three papers on the achievements of theoretical crystallography, in which he also presented part of the results of his work on space groups. The German mathematician A. Schoenflies was also working on their derivation at that time, who in 1889 published a work with the derivation of 227 groups. Fyodorov also managed to derive only 229 groups at first, they agreed on the final number of 230 only after mutual correspondence. 29 letters to Fyodorov have been preserved, the first dated December 14, 1889, in which Schoenflies accepted Fyodorov's priority. But even Fyodorov stated in the introduction to the article *Симметрия правильных систем фигур* that Schoenflies had overtaken him in his efforts to complete the derivation of space groups initiated by Jordan. The correct number of groups was stated by Fyodorov only in the appendix to the article, as follows from the minutes of the meeting of the Mineralogical Society of October 1890. There it is written that Fyodorov omitted one of the groups because it coincided with another, but added two more. Fyodorov and Schoenflies agreed on the total number of groups, despite the fact that they used a completely different methodology for their construction. Schoenflies already used the mathematical theory of groups, Fyodorov was able to derive them without it, without using the term group. Their works were published in 1891, that is, almost at the same time. It can be said – in a sense, given the extensive correspondence with each other – that the derivation of space groups is their joint work. As late as 1891, Fyodorov wrote an article for the German journal *Zeitschrift für Krystallographie und Mineralogie*, in which he described the similarities and differences between his views and those of Schoenfies. Between 1894 and 1902, three more articles on the structure of crystals were published in this magazine, where he repeated the derivation of 32 point and 230 space groups, basically in his original procedure and symbolism, but in German. In 1891, Fyodorov also published a work on 17 types of symmetry of planar periodic structures, even in the same issue of the journal of the Mineralogical Society in which the work on space groups was published.

The invention of the *Fyodorov table* is associated with 1892, and a year later he published another original work – a monograph on the use of theodolite in mineralogy and petrography to measure the angles between the outer faces of crystals. In 1894, he went with his family to the Urals (Bogoslovskij gornyj okrug), where he worked as a head of exploration geological work and compiled a geological map of the area. In 1895 he became a professor of geology at the Moscow Agricultural Institute (later the Timiriazev Academy), while also going to St. Petersburg to lecture. A year later, he was accepted as a member of the Bavarian Academy. In 1905, he was elected director of the Mining Institute (Gorny Institute) for a three-year term, where he served as the head of the department until his death. In February 1919, four months before his death, he was elected a full member of the Russian Academy of Sciences.

Before deriving space groups, Fyodorov dealt with the types of symmetry of finite formations – polyhedra, not just crystals. He published the results in the article *Симметрия конечных фигур* (Symmetry of finite figures), in which, along with the symmetries of polyhedra, he also derived 32 types of point symmetry of crystals. He followed the work of his predecessors Hessel, Bravais, Gadolin, but used his own method of derivation and original symbolism.

First, he proved what the multiplications of axes of symmetry can be, he also included fivefold axes in his considerations. He described the types of symmetry of objects with a single axis of symmetry, as well as objects with multiple axes of symmetry, where he distinguished the main axis, minor axes, axes with even and odd multiplicity, generating axes and other axes. He continued with objects with planes of symmetry, parallel to and perpendicular to the axes of symmetry. This was followed by a section on composite symmetry (rotoreflection). For the symmetry characterized by the presence of the axis of symmetry, he used the quite obvious name *simmetria sovmeščenija* (symmetry of identification), but in the case of reflection, he used the special term *direct simmetry*. He called the number of elements of the symmetry group the *veličina simmetrii* (magnitude of symmetry). It is noteworthy that he did not consider the center of symmetry as a separate element, but as the intersection of axes and planes of symmetry.

When reading Fyodorov's works, it is first necessary to understand the peculiar symbolism used to express the positions of points that arise from one point by transformations corresponding to the respective type of symmetry. In the case of the axis of symmetry, he proceeded from the following reasoning: a *p*-fold axis from one line will form *p* equivalent lines, each of which can be chosen as a coordinate axis; He marked them with the symbols $y_0, y_1, y_2, \dots y_{p-1}$ and the coordinates of a specific point on these axes with the symbols $b_0, b_1, b_2, \dots b_{p-1}$. Three coordinate axes are sufficient to determine the position of a point in space, of the possible *p* lines, he marked the selected three with the symbols y_0, y_1, y_2. The coordinates of the point on these axes, taking into account the presence of a *p*-fold axis of symmetry, were expressed by

$$y_0 = b_i^p, \qquad y_1 = b_{i+1}^p, \qquad y_2 = b_{i+2}^p$$

where the subscript *i* = 0, 1, 2, ..., *p* – 1, represents the *i*-th position of the point and the superscript *p* the multiplicity of the axis of symmetry. When the corresponding axis of symmetry is chosen as one coordinate axis, both the subscript and the superscript are omitted for such an axis, for the other coordinate axes *p* is retained and the subscripts are reduced by one:

$$y = b; \quad y_0 = \overset{p}{b}_i; \quad y_1 = \overset{p}{b}_{i+1}$$

He expressed the relationship between the coordinate y_i on another of the possible axes and the three chosen coordinates by the relationship:

$$y_i\, Sn\,(y y_o y_1) = y\, Sn\,(y_i\, y_o y_1) + y_o\, Sn\,(y\, y_i\, y_1) + y_1\, Sn\,(y y_o\, y_i),$$

where the symbol Sn represents the sine of the "spatial" angle between three non-co-linear lines 1, 2, 3 passing through one point, expressed using the determinant:

$$
\mathrm{Sn}\ (123) = \begin{vmatrix} \mathrm{cs}\,(1x_0)\ \mathrm{cs}\,(1x_1)\ \mathrm{cs}\,(1x_2) \\ \mathrm{cs}\,(2x_0)\ \mathrm{cs}\,(2x_1)\ \mathrm{cs}\,(2x_2) \\ \mathrm{cs}\,(3x_0)\ \mathrm{cs}\,(3x_1)\ \mathrm{cs}\,(3x_2) \end{vmatrix}
$$

where, for example, the symbol $\mathrm{cs}(1x_0)$ represents the cosine of the angle between the first line and the x_0 coordinate axis of the orthogonal coordinate system. In essence, this is not far from the matrix representation of symmetry operations.

Example of symbols of two groups with fivefold axes of symmetry:

Додекаэдроикосаэдрическая система

1) **Гомоэдрия** (6) $y = n^k b;\ y_0 = n^k \overset{5}{b}_i;\ y_1 = n^k \overset{5}{b}_{i+n}.$ (35)

2) **Гемиэдрия** (6) $y = n^k b;\ y_0 = n^k \overset{5}{b}_i;\ y_1 = n^k \overset{5}{b}_{i+n^k}$ (20)

Using the symbol n^k, where $n \equiv (-1)$ and $k = 0$ or 1, Fyodorov expressed mirroring; If $k = 1$, then $(-1)^k = -1$, so the corresponding coordinate changes the sign. Thus, the values of 0 and 1 represent two mirror-symmetrical positions of a point on a specific axis of symmetry to which the plane of symmetry is perpendicular. The n^k symbol also serves in the case of twofold axes of symmetry; Its placement in front of the coordinates of the points on the co-coordinate axes perpendicular to the axis of symmetry expresses two positions related to the rotation of 180°. The symbol is also suitable for describing the inversion that occurs when the sign of all three coordinates changes at the same time. In the cubic system, there are more indices (Fyodorov called them *parameters*) and also other symbols of the coordinate axes – instead of the symbols *y*, the symbols *x* and instead of *b* the symbol *a*.

Fyodorov wrote:

As an example, let us mention the relation representing the thetardohedra of the cubic system

$$x_0 = n^j \overset{3}{a}_{\,i};\; x_1 = n^k \overset{3}{a}_{\,i+1};\; x_2 = n^{j+k} \overset{3}{a}_{\,i+2}$$

The parameter i refers to one of the threefold octahedral axes of symmetry, and the parameters j and k to the two twofold cubic axes of symmetry. The first parameter has 3 values and both other 2 values; Therefore, their product has a value of 12, which represents the magnitude of the given type of symmetry.

In this case, the option of 0, 1 applies to the both exponents *j* and *k*.

The example above (groups numbered 20 and 35) is taken from the final table of point groups, which, as can be seen, also contains non-crystallographic groups (fivefold axis of symmetry). The notations of the groups testify to their relative complexity, but on the other hand, knowing the meaning of the symbols, it is possible to read from them what symmetry operations the respective point group contains.

The next stage of Fyodorov's work was the derivation of 230 space groups, which he published in the article *Симметрия правильных систем фигур* (Symmetry of Regular Systems of Figures). In it, he mainly quoted A. Bravais, A. Gadolin, P. Curie, but the name of L. Sohncke occurs most often. At the beginning of the article, he accepted Schoenflies' partial primacy in the effort to complete the derivation of space groups, begun by Jordan:

В первом отношении я отчасти предупрежден Шенфлисом (Schönflies), который явился прямым продолжателем Жордана.

... I was partially overtaken by Schoenflies, who was the direct successor of Jordan.

Let us state what Fyodorov means by the name *Regular System of Figures* (free translation):

By a regular system of objects, I mean such an infinite set of objects of finite dimensions in all respects, that if, in accordance with the laws of symmetry, we identify two of the objects belonging to the system by transformation, then the whole system will also be identified.

He had a clear idea of how such a system (space group) is determined:

Ясно, что система вполне определена, если дана одна из ее фигур и движения совмещения.

It is clear that a system is fully determined if one of its objects and the operations of symmetry (identification) are known.

The object, according to current terminology, is apparently a structural motif.

Fyodorov distinguished systems with structural motifs without reflection, which he called *simple*, as opposed to systems with motifs also containing reflection, which he called *double*.

When working on space groups, he used the results published in the previous article *Симметрия конечных фигур* (Symmetry of Finite Figures), because symmetry operations belonging to a space group are combinations of point and translational operations. At the same time, it is interesting that he did not pay special attention to space lattices, i.e. translation groups, before deriving space groups. About operations belonging to the space group, he wrote (free translation):

All regular system symmetry operations can be composed of existing S rotations, which convert any given direction to all other equivalent directions (which correspond to rotations of a given type of symmetry), and of translations.

At the beginning of the article on space groups, Fyodorov introduced the necessary terms and divided space groups into three main groups:

symmorphic systems – their structural motifs have the same symmetry as the whole system, they have a center of symmetry, they can be identified with each other by translations,

hemisymorphic systems – can be understood as two connected symorphic systems, whose structural motifs are mirror-symmetrical to each other; the motif itself has a center of symmetry, but it does not have planes of symmetry,

asymorphic systems – all other groups.

He proceeded according to this scheme when deriving space groups in individual crystall systems. In each system, he derived first symorphic groups, then hemisymorphic and finally asymmorphic, progressing in these groups from point groups with the fewest operations to holohedral groups.

When deriving space groups, he used seven theorems, which he proved in the first part of the article. The theorems concerned the multiplicity of the axes of symmetry, the positions and directions of the axes of symmetry in the lattice, the orientation and positions of the planes of symmetry in the lattice, the relationship of the planes and their normals to the lattice lines. This was followed by the derivation of space groups.

For space groups, he used symbolism based on the symbolism of point groups, extended by elements of translational symmetry. For example, in the hemihedra of the triclinic system, he symbolized a group without an axis and a plane of symmetry by writing:

$$y = b + B\lambda; \quad z = c + C\lambda_0; \quad v = d + D\lambda_1$$

where y, z, v represent the coordinates of a point on the three selected coordinate axes, the symbols b, c, d represent their initial values, λ, λ_o, and λ_1 the identity periods along these axes, and B, C, D represent integers from the range from minus to plus infinity. This expresses the coordinates of all points representing equivalent positions in a given structure (*regular system of points*). Fyodorov stated that he would deliberately omit integers in the symbolism of space groups, so he ended up writing the previous expression in the form:

$$y = b + \lambda;\ z = c + \lambda_0;\ v = d + \lambda_1$$

For a space group in a triclinic system with a holohedral point group (containing an inversion), he used the symbol:

$$y = n^k b + \lambda;\ z = n^k c + \lambda_0;\ v = n^k d + \lambda_1$$

where n^k – has the same meaning as for point groups.

As an example of Fyodorov's considerations, we will present a part of the derivation of two space groups in the monoclinic system (free translation):

In the case of hemimorphia, there is a twofold axis that, according to theorem 3, has the direction of a lattice line; we determine it for the y - axis. In a plane that is perpendicular to the axis, and based on theorem 4 is a lattice plane, we choose the coordinate axes z and v perpendicular to the lattice lines of this plane. We place the beginning of the coordinate system on the y - axis. The identity periods in the direction of these axes are marked with the symbols λ_0 and λ_1 .

When an axis passes through a lattice point, Fyodorov characterized the space group by notation

$$y = b + \lambda; \; z = n^k c + \lambda_0; \; v = n^k d + \lambda_1 \qquad (3\text{ s})$$

With k = 1, the coordinates c and d of the starting point change the sign, so it is obviously a 180° rotation around the y - axis. It is a space group that has the designation $P2$ in international tables and the Schoenflies designation C_2^1. The case when it comes to a structure with a base-centered cell, where screw axes are also applied, Fyodorov commented as follows:

In this case, based on theorem 2, there is an equally acting twofold axis of symmetry in the middle between every two equivalent axes of the system. Based on theorem 7, we get the system that is easiest to write in the form

$$y = b + f\lambda/2; \quad z = n^k c + f\lambda_0/2; \quad v = n^k d + \lambda_1 \qquad (4\text{ s})$$

It is a space group $C2$, according to Schoenflies C_2^3. In the symbolism of this space group, the parameter f can take the values of 0 or 1, respectively, while in the latter case it is an operation related to the screw axis.

The table of derived space groups in the article *Symmetry of Regular System of Figures* no longer contains their analytical expressions, only numbers in six crystall systems. In the columns, the numbers belonging to the groups symorphic, hemisymorphic, asymorphic are listed in turn, and in the last column there is their total number. In crystall systems, the numbers are divided according to their affiliation into 32 point groups with their names (holohedral, hemihedral, tetartohedral...). The following images show the beginning and end of the space group table:

Таблица правильных систем фигур

Системы кристаллографические	Правильные системы фигур			
	симморф-ные	гемисим-морфные	асимморф-ные	Сумма
А. Триклиноэдрическая система				
1. Гемиэдрия	1	—	—	1
2. Голоэдрия	1	—	—	1
Итого . . .	2	–	—	2
F. Кубооктаэдрическая система				
28. Тетартоэдрия	3	—	2	5
29. Додекаэдрическая гемиэдрия	3	2	2	7
30. Тетраэдрическая гемиэдрия	3	2	1	6
31. Гироэдрическая гемиэдрия	3	—	5	8
32. Голоэдрия	3	2	5	10
Итого . . .	15	6	15	36
Всего систем	73	54	103	230

The table ends with a row expressing the sum of the groups: *Total Systems . . . . 230.*

In this table, Fyodorov's names of six crystall systems are noteworthy:

triklinoedričeskaja,	*(triclinohedral)*
monoklinoedričeskaja,	*(monoclinohedral)*
rombičeskaja,	*(rhobic)*
tetragonal'naja,	*(tetragonal)*
gexagonal'naja,	*(hexagonal)*
kubooktaedričeskaja.	*(cubooktahedral)*

Both Fyodorov and Schoenflies used the term *rhombic system*, for which the term *orthorhombic* is used in International tables for crystallography. Fyodorov used the term *Kristalograficheskaya systema*, Schoenflies *Krystall system*.

In an article on the theory of crystal symmetry from 1894, Fyodorov wrote a sentence from which it follows that he realized the importance of generating operations, that is, generating elements of a group of symmetry. In connection with the point groups, he wrote:

We can see that ultimately the whole group can be constructed using two independent symmetry elements. All other symmetry elements arise as a combination of rotations about the initial ones, and we will call them generating symmetry elements.

In an article published in *Zeitschrift für Krystallographie und Mineralogie* (1891), Fyodorov commented on the correspondences and differences between his and Schoenflies' views. He noted that they agreed on the definition of the term *symmetry*, but disagreed on terminology and the classification of groups into crystall systems. Schoenflies referred to seven crystall systems for space groups, Fiodorov to six. Fyodorov did not accept the centre of symmetry as a separate element of symmetry, but as the intersection of all the elements of symmetry of a finite figure. Schoenflies limited the derivation of point groups to groups corresponding to crystal shapes, Fyodorov also considered other symmetric polyhedra. For point groups, Fyodorov used the term digonal system, in which he included those in which at most twofold axes occur (monoclinic, rhombic). Rejecting Schoenflies' content of the term *regular system* restricted to the cubic system, Fyodorov also included some non-crystallographic systems.

Schoenflies used the theory of groups, adapted the relevant terms, introduced the product of operations, and their powers. There is also a significant difference in the symbolism; while Schoenflies used a brief notation for groups, Fyodorov used (by his own account) *analytic relations* to denote groups.

There are over 400 entries in the list of Fyodorov's publications; only a minor part is on symmetry, most of it is on geology.

Fyodorov's most important works on symmetries:

1. Начала учения о фигурах. Зап. Мин. общ., 2-я серия, 1885, т. XXI, 1-289.
2. Симметрия конечных фигур. Зап. Мин. общ., 2-я серия, 1889, т. XXV, 1-52.
3. Симметрия правильных систем фигур. Зап. Мин. общ., 2-я серия, 1891, т. XXVIII, 1-146
4. Симметрия на плоскости. Зап. Мин. общ., 2-я серия, 1891, т. XXVIII, 345 Zusammenstellung der kristallographischen Resultaten des Herrn Schoenflies und der meinigen. Zeitschr. f. Krist. u. Min., 1891, Bd. XX, 25-75.
5. Theorie der Kristallstructur. Einleitung. Regelmässige Punktsysteme. Zeitschr. f. Krist. u. Min., 1894, Bd. XXIV, 210-252.
6. Theorie der Kristallstructur. I. Mögliche Structurarten. (Mit graphischer Darstellung der Symmorphen

Structurarten). Zeitschr. f. Krist. u. Min., 1895, Bd. XXV, 113-224.
7. Theorie der Kristallstructur. II. Reticulare Dichtigkeit und erfahrungsgemasse Bestimmung der Kristallstructur. Zeitschr. f. Krist. u. Min., 1902, Bd. XXXVI, SS. 209-233.

Sources:

1. https://en.wikipedia.org/wiki/Evgraf_Fedorov
2. http://books.e-heritage.ru/book/10080293 – in this book is a collection of Fyodorov's papers on crystal symmetry + an article Bokij, Šafranovskij: History of derivation of 230 space groups

Frederick Seitz (1911 – 2008)

American physicist, pioneer in the field of solid state physics, known in crystallography for using matrix algebra and group theory to derive 230 space groups of crystal structure symetries. Matrices and groups, together with the lattice postulate, i.e. the postulate of the three-dimensional periodicity of the crystal structure, were sufficient for him to cope with this vast task. He published the results between 1934 and 1936 in four articles in the journal *Zeitschrift für Kristallographie*. He introduced concise and succinct symbols for operators representing rotations, reflections and translations. In the introduced symbol $\{\Phi, \boldsymbol{t}\}$ – mark Φ represented the matrix of rotation or reflection, and $\boldsymbol{t}$ – the vector of translation. In 1934, his dissertation entitled "A matrix-algebraic development of the crystallographic groups" was published in book form [16].


A Matrix-algebraic Development of the Crystallographic Groups[1]). I.

By

F. Seitz in Princeton, New Jersey (U.S.A.).

The title of the first of a series of four articles

Together with E. Wigner, he developed one of the first quantum theories of crystals, e.g. the Wigner-Seitz cell is known. He also addressed the problem of global warming, he was a co-author of a book on this issue, in which he expressed his skepticism about the question of humanity's guilt.

Born in San Francisco, he began his undergraduate studies at Stanford University, where he graduated with a bachelor's degree in mathematics in 1932. His next path led to Princeton University, where he studied physics and received his PhD in 1934. He began writing articles on the use of matrices to derive space groups as a doctoral student under the guidance of E. Wigner. From 1935 to 1937 he worked at the Faculty of Physics of the University of Rochester. From there he went to General Electric, where he worked as a researcher (1937 – 1939), then worked at the University of Pennsylvania (1939 – 1942) and in the period 1942 – 1949 at the Carnegie Institute of Technology. From 1946 to 1947, he also worked at Oak Ridge National Laboratory as part of the atomic energy research program. In 1949, he was appointed professor of physics at the University of Illinois, where he became head of the department in 1957 and dean in 1964. In 1940, his most important book, *The Modern Theory of Solids*, was published.

He achieved a prominent position in the scientific community, was president of Rockefeller University (1968–1978) and president of the National Academy of Sciences of the United States from 1962 to 1969. He has been awarded the National Medal of Science, NASA's Distinguished Public Service Award, Franklin Medal, and honorable mentions from 31 universities in the U.S. and abroad. He founded the Frederick Seitz Materials Research Laboratory at the University of Illinois, as well as several other laboratories for materials research in the United States. Seitz was also the director of the well-known Texas Instruments company (1971–1982). He retired from Rockefeller University in 1979 as Professor Emeritus.

Seitz's contribution to the derivation of space groups lay in a more consistent use of mathematics. His predecessors, including Schoenflies and Fyodorov, relied to some extent on spatial imagination – for example, to assess the resulting position in which a crystal would reach after rotations around two different axes in succession. Euler's theorem about the possibility of converting a crystal to its final position by a single rotation around the next axis, which several of Seitz's predecessors cited, but did not use the relevant mathematical relationships, applies here. Fyodorov, in his article *Symmetry of Finite Figures* (1889), approached the matrix representation when he gave relations for calculating the coordinates of a point in positions after rotation around the axis of symmetry. In them, he used a specially introduced sine of the "spatial" angle between three non-complanar directions expressed by a determinant, but he had not yet arrived at the matrix notation of the rotation operator. The advantage of writing rotations and reflections using matrices lies in the fact that the product of two matrices (according to the specified rules), representing two different rotations, provides a matrix of the resulting rotation, from which the direction of the third axis and the angle of rotation of the object (crystal) can be read. This simplifies and also clarifies the construction of point groups, which are part of space groups of symmetry. It should be added, however, that when applying the theory of groups, Seitz did not use the possibilities of the so-called factor group, which were pointed out as early as 1923 by the Swiss mathematician Andreas Speiser in his book *Die Theorie der Gruppen von Endlicher Ordnung, mit Anwendungen auf Algebraische Zahlen und Gleichungen sowie auf die Kristallographie*, but also by his supervisor E. Wigner in his book *Gruppentheorie* published in 1931.

In the introduction to the first of four articles, Seitz wrote that he would use exclusively algebraic methods, so that the derivation of space groups would be based on a purely analytical-group basis.

Each of the four articles represented a coherent part and characterized the individual articles as follows:

I. ***Macroscopic groups*** (32 point groups represented by matrices).

II. ***Microscopic symmetry, part one*** (elements of microscopic theory, derivation of 14 Bravais lattices and their representation in a shape suitable for the construction of space groups).

III. ***Microscopic symmetry, part two*** (elements of the theory of operators representing spatial transformations from the point of view of matrix algebra, a set of theorems and conditions that must be met by groups of these operators from a crystallographic viewpoint; the beginning of the construction of space groups).

IV. ***Microscopic symmetry, conclusion*** (completion of the derivation of space groups).

In the first of a series of four papers, he derived matrices representing 32-point group symmetry operations describing the macroscopic symmetry of crystals – rotations "1, 2, 3, 4, 6" and mirroring. In doing so, he used a matric form in which (in the Cartesian system) the axis of rotation is identical to the X axis, which simplified the writing of matrices. The following figure shows a part of Seitz's text in which the left matrix represents its proper rotation, the right rotation with mirroring, i.e. improper rotation.

In all of our work it is essential that we restrict ourselves to such transformations and a may be reduced only to either of the forms

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{pmatrix} \qquad (11a, b)$$

For example, the symmetry operation of a point group, which has the symbol D_3in Schoenflies' designation (symbol 32 in the international tables), is represented by 6 matrices (a copy from Seitz's article):

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & -\sqrt{3}/2 \\ 0 & \sqrt{3}/2 & -1/2 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & \sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1/2 & -\sqrt{3}/2 \\ 0 & -\sqrt{3}/2 & 1/2 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1/2 & \sqrt{3}/2 \\ 0 & \sqrt{3}/2 & 1/2 \end{pmatrix} \quad D_3.$$

The fact that only the so-called "allowed" rotations "1, 2, 3, 4, 6" can be applied in crystals was proved only in the second article and on their basis he created the corresponding cyclic point groups.

In determining the permissible rotations, like his predecessors (e.g. Schoenflies), he relied on the fact that the existence of a three-dimensional periodic lattice with lattice vectors $n_1\boldsymbol{t}_1 + n_2\boldsymbol{t}_2 + n_3\boldsymbol{t}_3$, where n_1, n_2, n_3 are integers, places constraints on the matrices representing the rotations (on the angles φ appearing in them). His procedure on the case of the plane lattice was original, but cumbersome. He wrote the shortest lattice vector $\boldsymbol{t} \equiv (t_1, 0)$ in the form of a column matrix, and the rotation with a square matrix, which applied to this vector:

$$\begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \cdot \begin{pmatrix} t_1 \\ 0 \end{pmatrix} = \begin{pmatrix} t_1\cos\varphi \\ -t_1\sin\varphi \end{pmatrix} = \boldsymbol{u}\,.$$

Difference of vectors $\boldsymbol{u} - \boldsymbol{t}$

$$\boldsymbol{u} - \boldsymbol{t} = \begin{pmatrix} t_1\cos\varphi - t_1 \\ -t_1\sin\varphi \end{pmatrix} = \boldsymbol{w}$$

is the vector $\boldsymbol{w}$, which cannot be shorter than the original vector $\boldsymbol{t}$, because according to the assumption this is the shortest. Therefore, inequality must be met

$$t_1^2 \cos^2 \varphi + t_1^2 - 2t_1^2 \cos \varphi + t_1^2 \sin^2 \varphi \ \geq \ t_1^2 \ \Rightarrow \ 2t_1^2(1 - \cos \varphi) \geq \ t_1^2 \ \Rightarrow$$

$$\Rightarrow 4 \sin^2 \left(\frac{\varphi}{2}\right) \geq 1$$

This condition is met by angles from the interval:

$$\frac{\pi}{3} \leq \varphi \leq 5\frac{\pi}{3}$$

He made a similar consideration for the sum of $\boldsymbol{u} + \boldsymbol{t}$ and for the inversion of the vector $\boldsymbol{t}$. Thus, he obtained the permissible angles of rotation. From these, he created several combinations that, from a mathematical point of view, form groups; these are five cyclic groups, as can be seen in the copy from Seitz's second article (groups marked with the letters a, b, c, d, e):

only the values

$$0,\ \pi/3,\ \pi/2,\ 2\pi/3,\ \pi,\ 4\pi/3,\ 3\pi/2,\ 5\pi/3\ .$$

These may not all be taken simultaneously, and it is readily seen that if $\boldsymbol{\alpha}$ forms the basis of a cyclic subgroup of rotations the permissible combinations are

a) 0 $(n = 1)$
b) $0,\ \pi$ $(n = 2)$
c) $0,\ 2\pi/3,\ 4\pi/3$ $(n = 3)$
d) $0,\ \pi/2,\ \pi,\ 3\pi/2$ $(n = 4)$
e) $0,\ \pi/3,\ 2\pi/3,\ \pi,\ 4\pi/3,\ 5\pi/3$ $(n = 6)$.

Cyclic groups

In the second paper, Seitz also included the derivation (construction) of **Bravais lattices**, i.e. **translation groups**. The derivation relies on the compatibility of a particular point group with the corresponding lattice represented by a triple of basic vectors. Essentially, the process is as follows:

The set of symmetry operations of a point group from one vector produces the set of other vectors. Their endpoints form the basis of the space lattice. The entire space lattice is expressed as an integral linear combination of a triplet of basis vectors $\boldsymbol{t}_1, \boldsymbol{t}_2, \boldsymbol{t}_3$, which must be chosen appropriately in the lattice. The point group is therefore tightly coupled to the triplet of basic vectors.

As an example, the fourfold axis of symmetry requires a lattice characterized by a pair of perpendicular, equal-length basis vectors. Or another example - if the lattice is brought into congruent position by rotating it by 60°, then two of the basis vectors must take the same angle.

In constructing the Bravais lattices, Seitz used only 11 of the 32 point groups, the so-called Laue groups, which contain an inversion as a symmetry operation. He justified this by claiming that inversion as a symmetry operation is typical of all types of three-dimensionally periodic lattices. Moreover, it suffices to consider the effect of the generating elements of these groups. A copy of two lines from Seitz's second paper introduces these groups, containing inversion:

There are eleven groups which contain this element, namely S_2, C_2^h, V^h, C_4^h, D_4^h, S_6, C_6^h, D_3^d, D_6^h, T^h, O^h. In each of these there exists a number

The first of these, the group S_2, belongs to the triclinic system and contains only two elements - *identity* and *inversion*. Since the inversion is typical of all possible three-dimensional periodic lattices, this group imposes no restrictions on the triplet of basis vectors - neither on their sizes nor on their relative angles. For the other Laue groups, the constraints must already be taken into account.

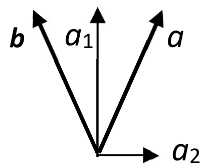
The second in order - the point group C_2^h (the holohedral group of the monoclinic system, by the designation in the International Tables C_{2h}) contains four elements - *identity, inversion, rotation* by 180° and *reflection* in a plane perpendicular to the rotation axis. Rotation and inversion can be chosen as the generating elements of the group. Their matrix representation looks like the following:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The symmetry operations of this point group allow the existence of two types of lattice - a lattice denoted by the symbol Γ_m with a primitive unit cell and a lattice Γ_m' with a base-centred cell (he used the notation after Schoenflies). The type of lattice depends on whether the shortest lattice vector is parallel to the rotation axis. Seitz identifies the rotation axis with the X axis of the Cartesian system; the other two principal directions in the lattice are perpendicular to it and, by convention, make an angle with each other greater than 90°. If the shortest lattice vector is parallel to the rotation axis, then it and the second shortest vector, perpendicular to the first, form a primitive orthogonal plane cell in its plane. In the second case, when the shortest lattice vector is not parallel to the rotation axis, Seitz chose this vector so that one component of it (with coordinate a_1) is identical to the X -axis (the rotation axis) and that the other component is perpendicular to it (with coordinate a_2, in the direction of the Y-axis). The shortest vector as a column matrix then has the form

$$\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ 0 \end{pmatrix}$$

noting that neither a_1 nor a_2 are then the shortest distances between lattice points, which is the square root of the sum of their squares. Rotating the vector $\boldsymbol{a}$ about the X -axis by 180° produces the vector $\boldsymbol{b}$, whose second coordinate is changed to $-a_2$:

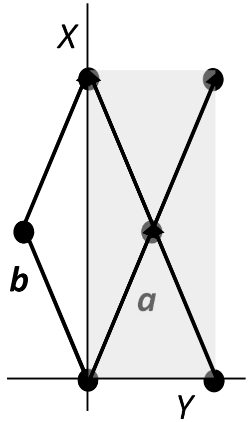


$$\boldsymbol{b} = \begin{pmatrix} a_1 \\ -a_2 \\ 0 \end{pmatrix}$$

In matrix notation, the transformation takes the form:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} a_1 \\ a_2 \\ 0 \end{pmatrix} = \begin{pmatrix} a_1 \\ -a_2 \\ 0 \end{pmatrix}$$

The endpoints of the vectors resulting from an integral linear combination of the vectors $n_1\boldsymbol{a} + n_2\boldsymbol{b}$, form a Γ'_m, lattice, whose base cell is centered (shaded part in the figure).



Vector $\boldsymbol{c} = \boldsymbol{a} + \boldsymbol{b}$:

$$\boldsymbol{a} + \boldsymbol{b} = \begin{pmatrix} a_1 \\ a_2 \\ 0 \end{pmatrix} + \begin{pmatrix} a_1 \\ -a_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 2a_1 \\ 0 \\ 0 \end{pmatrix}$$

has the first coordinate $2a_1$, the other two are zero. The distance $2a_1$ is the smallest distance between lattice points on the X -axis , which is related to the nature of the lattice. The notation of the triplet of basis vectors for Γ_m and Γ'_m lattices then looks like this:

$$\boldsymbol{t}_1 = \begin{pmatrix} t_{11} \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{t}_2 = \begin{pmatrix} 0 \\ t_{22} \\ 0 \end{pmatrix}, \quad \boldsymbol{t}_3 = \begin{pmatrix} 0 \\ t_{32} \\ t_{33} \end{pmatrix}, \quad \Gamma_m$$

$$\boldsymbol{t}_1 = \begin{pmatrix} t_{11} \\ t_{12} \\ 0 \end{pmatrix}, \quad \boldsymbol{t}_2 = \begin{pmatrix} 0 \\ 2t_{12} \\ 0 \end{pmatrix}, \quad \boldsymbol{t}_3 = \begin{pmatrix} 0 \\ t_{32} \\ t_{33} \end{pmatrix}, \quad \Gamma'_m$$

Seitz used a similar procedure for the other Laue point groups, and in other cases centred cells were also produced. The symbols of the derived 14 Bravais lattices are given in the first row of the following table, the second row being the corresponding Laue point groups in Schoenflies' notation:

Table IV.

Γ_t	Γ_m	Γ'_m	Γ_v	Γ'_v	Γ''_v	Γ'''_v	Γ_q	Γ'_q	Γ_{rh}	Γ_h	Γ_c	Γ'_c	Γ''_c
S_2	C^h_2	C^h_2	V^h	V^h	V^h	V^h	D^h_4	D^h_4	D^d_3	D^h_3	O^h	O^h	O^h.

The symbol Γ in the table represents the Bravais lattice (translation group), the apostrophe above the symbol represent the centred lattices (basal, face, body) and the subscripts the crystall system: t – triclinic, m – monoclinic, v – Vierergruppe (= rhombic system), q – quadratic, rh – rhomboedric, h – hexagonal, c – cubic.
As can be seen from the table, only 7 of the 11 Laue groups were sufficient to derive the 14 translation groups. These are holohedral point groups characterizing the symmetry of the lattices of the corresponding crystall system.

In the third and fourth articles, Seitz included the derivation of space groups. He also rationalized the procedure formally by introducing the notation $\{\Phi|\boldsymbol{a}\}$ for the symmetry operators in which he represented rotation and reflection by the matrix Φ and translation by the vector $\boldsymbol{a}$. With this notation he expressed a general symmetry operation consisting of rotation and translation. He expressed the action of such a symmetry operator on the position vector $\boldsymbol{x}$ of a point in space by the relation:

$$\{\Phi|\boldsymbol{a}\}\cdot\boldsymbol{x} = \Phi\cdot\boldsymbol{x} + \boldsymbol{a}\,.$$

That is, first a rotation is applied to the vector $\boldsymbol{x}$ (expressed by the scalar product of the square matrix Φ and the column matrix of the vector $\boldsymbol{x}$), which moves the point marked in space by the position vector $\boldsymbol{x}$ to a new position, and then this point is further shifted by the vector $\boldsymbol{a}$. Seitz expressed the successive application of two symmetry operations as a product of the corresponding operators, and gave a rule for obtaining the operator of the resulting symmetry operation:

$$\{\Phi|\boldsymbol{a}\} \cdot \{\Psi|\boldsymbol{b}\} = \{\Phi \cdot \Psi \mid \Phi \cdot \boldsymbol{b} + \boldsymbol{a}\}.$$

That is, the resulting rotation is represented by the product of the matrices $\Phi \cdot \Psi$ and the resulting translation by the sum of the two translations $\Phi \cdot \boldsymbol{b} + \boldsymbol{a}$, where $\Phi \cdot \boldsymbol{b}$ represents the vector $\boldsymbol{b}$ rotated by the rotation represented by the matrix Φ .

Each of the space groups was represented by Seitz using several (at most four) generating elements, expressed by operators, e.g.:

$$\{\Phi \mid \boldsymbol{v}(\Phi)\}, \quad \{\Psi \mid \boldsymbol{v}(\Psi)\}, \quad \{\varepsilon \mid \Gamma\},$$

which he also used for mutual differentiation (marking) of groupes. In such a notation of generating elements (i.e. symmetry operations), the symbol ε represents an identical operation (rotation by 0°) and Γ a translation belonging to one of Bravais's 14 translation groups. Thus the symbol $\{\varepsilon \mid \Gamma\}$ as a whole represents only translations without rotation or reflection. The symbols $\boldsymbol{v}(\Phi)$ and $\boldsymbol{v}(\Psi)$ represent the so-called non-lattice translations inseparably associated with the corresponding rotations and reflections, respectively. They are translations whose magnitudes are fractions of the lengths of the basis vectors, so they do not belong to the translation group, which includes only integral linear combinations of the basis vectors. Non-lattice translations occur for so-called screw axes (the combination of a rotation with a non-lattice translation in the direction of the rotation axis) and for glide planes (the combination of a reflection with a non-lattice translation parallel to the reflection plane).

In the construction of space groups, Seitz followed the multiplicity of the principal axis of symmetry, starting with the groups C_1, C_{1h}, continuing with the cyclic groups C_2 and S_2. The point group C_1 contains a single element - the identity - and the only space group associated with it is represented by a single generating element $\{\varepsilon|\Gamma_t\}$, where ε is the identity represented by the unit matrix and Γ_t is the translation group of the triclinic lattice (no restriction conditions are imposed on the triple of its basis vectors).

The point group C_{1h} contains only the identity represented by the unit matrix and the reflection represented by the matrix $\boldsymbol{\rho}_h$:

$$\boldsymbol{\rho}_h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Combining the C_{1h} group with the monoclinic translation groups Γ_m and Γ_m' results in four space groups, each represented by two generating elements:

$$\{\boldsymbol{\rho}_h|\mathbf{0}\},\{\varepsilon|\Gamma_m\} \quad \{\boldsymbol{\rho}_h|\boldsymbol{t}_p/2\},\{\varepsilon|\Gamma_m\} \quad \{\boldsymbol{\rho}_h|\mathbf{0}\},\{\varepsilon|\Gamma'_m\}$$
$$\{\boldsymbol{\rho}_h|\boldsymbol{t}_p/2\},\{\varepsilon|\Gamma'_m\}$$

The symbol $\{\boldsymbol{\rho}_h|\mathbf{0}\}$ represents reflection, $\{\boldsymbol{\rho}_h|\boldsymbol{t}_p/2\}$ represents glide reflection, which in this case is due to the configuration of the atoms in the unit cell of the crystal. Both cases are combined with both translation groups, the primitive Γ_m and the centred Γ'_m.

Seitz successively generated all possible combinations of cyclic groups with the corresponding Bravais translation groups, for which only two generating operators were ever sufficient, as in the case of the C_{1h} group - one from the point group, the other from the translation group. Having exhausted the cyclic groups, he combined the cyclic groups expressing rotations about different axes with each other to form non-cyclic groups, and combined these with the translation groups; here additional generating operators were needed.

The three space groups of the rhombic system belonging to the point group C_{2v} are already represented by three generating elements (ρ_v represents reflection in the plane parallel to the rotation axis, $\boldsymbol{\delta}_2$ rotation about the twofold axis, and $\boldsymbol{t}_1/2$ non-lattice translation):

$$\{\boldsymbol{\varrho}_v\,|\,\mathbf{0}\},\ \{\boldsymbol{\delta}_2\,|\,\mathbf{0}\},\ \{\boldsymbol{\varepsilon}\,|\,\Gamma'_v\} \qquad \mathfrak{C}_{2v}^{11}$$
$$\{\boldsymbol{\varrho}_v\,|\,\boldsymbol{t}_1/2\},\ \{\boldsymbol{\delta}_2\,|\,\mathbf{0}\},\ \{\boldsymbol{\varepsilon}\,|\,\Gamma'_v\} \qquad \mathfrak{C}_{2v}^{13}$$
$$\{\boldsymbol{\varrho}_v\,|\,\mathbf{0}\},\ \{\boldsymbol{\delta}_2\,|\,\boldsymbol{t}_1/2\},\ \{\boldsymbol{\varepsilon}\,|\,\Gamma'_v\} \qquad \mathfrak{C}_{2v}^{12}.$$

The four space groups of the hexagonal system belonging to the point group D_{6h} are represented by four generating elements:

$$
\begin{array}{ll}
\{\boldsymbol{\sigma}_2' \mid \mathbf{0}\},\ \{\boldsymbol{\iota} \mid \mathbf{0}\},\ \{\boldsymbol{\sigma}_6 \mid \mathbf{0}\},\ \{\boldsymbol{\varepsilon} \mid \Gamma_h\} & \mathfrak{D}_{6h}^1 \\
\{\boldsymbol{\sigma}_2' \mid \boldsymbol{t}_1/2\},\ \{\boldsymbol{\iota} \mid \mathbf{0}\},\ \{\boldsymbol{\sigma}_6 \mid \mathbf{0}\},\ \{\boldsymbol{\varepsilon} \mid \Gamma_h\} & \mathfrak{D}_{6h}^2 \\
\{\boldsymbol{\sigma}_2' \mid \mathbf{0}\},\ \{\boldsymbol{\iota} \mid \mathbf{0}\},\ \{\boldsymbol{\sigma}_6 \mid \boldsymbol{t}_1/2\},\ \{\boldsymbol{\varepsilon} \mid \Gamma_h\} & \mathfrak{D}_{6h}^4 \\
\{\boldsymbol{\sigma}_2' \mid \boldsymbol{t}_1/2\},\ \{\boldsymbol{\iota} \mid \mathbf{0}\},\ \{\boldsymbol{\sigma}_6 \mid \boldsymbol{t}_1/2\},\ \{\boldsymbol{\varepsilon} \mid \Gamma_h\}. & \mathfrak{D}_{6h}^3
\end{array}
$$

Although Seitz did not provide a summary table of space groups in the four articles, he pointed to his own article in which he described representations of all 230 space groups. His derivation (construction) of space groups did not introduce a new type of crystal symmetry, but was a demonstration of the connection of crystal symmetry with mathematics.

Seitz's major works on crystallography and crystalline substances:

1. Zeitschrift für Kristallographie: 88 (1934) p. 433, 90 (1935) p. 289, 91 (1935) p. 336, 94 (1936) p. 100.
2. A matrix-algebraic development of the crystallographic groups, Princeton University, 1934.
3. The modern theory of solids, McGraw-Hill, 1940.

Sources:

1. Original articles by Seitz in Zeitschrift für Kristallographie
2. https://en.wikipedia.org/wiki/Frederick_Seitz

William Houlder Zachariasen (1906 – 1979)

Originally a Norwegian, he focused his entire scientific activity on the study of the structure of mainly inorganic substances by X-ray diffraction methods. In his 1945 book *Theory of X-ray Diffraction in Crystals* [17] he devoted one chapter to the theory of symmetry of crystals, in which he presented his original method of derivation of 230 space groups based on the theory of groups and tensor algebra. He used these two mathematical tools more rigorously than his predecessors, not excluding F. Seitz. He became well known in the crystallographic community after the publication of his work on the structure of glass (1932).

He has worked in the USA most of his life, but was born in the south of Norway in the town of Langesund, about 100 km southwest of the capital Oslo. He also began his university studies at the Mineralogical Institute in the capital in 1923. He published his first paper at the age of 19 and over the course of 55 years of active work he published over 200 papers, most of them as a single author. He received his PhD from the *Universitetet i Oslo* at the age of 22, and was mentored by the well-known geochemist V. M. Goldschmidt. Immediately after completion of doctoral studies, from 1928 to 1929, he worked at *Manchester University* in the laboratory of L. Bragg, where he began to study the structure of silicates. He returned briefly to his home university, but after only a year of work accepted the offer of A. Compton and went to the USA. Thus, in 1930, he became a member of the Physics Faculty at the *University of Chicago* and in 1941 an American citizen.

Although he was primarily an experimentalist, he contributed to the theory of diffraction whenever he found it inconsistent with experiment. He published results on the determination of the structure of minerals, inorganic crystals, radii of atoms and ions, wrote on the amorphous (glassy) state, the structure of liquids, the chemical and crystallographic properties of actinides, phases at high pressures, the structure of superconductors, and the dependence of the binding strength on the binding distance. His contributions to the theory concern thermal diffuse scattering of X-rays, the phase problem of structure factors, as well as extinction, including the so-called Borrmann phenomenon. The correctness of each of these theoretical contributions has been carefully verified experimentally by Zachariasen.

In 1932, he published a paper *The Atomic Arrangement in Glass*, which significantly influenced material structure scientists at the time. The paper was a breakthrough on the structure of glass and its relationship to chemical composition. Between 1943 and 1945, as part of the Manhattan Project, he determined the structures of the crystalline phases of the transuranic elements. In 1945 he published a major monograph, *Theory of X-ray Diffraction in Crystals*, and continued to publish extensively (e.g., up to 19 papers between 1948 and 1949). From 1945-1950 and again from 1955-1959 he was head of the Department of Physics at the *University of Chicago*. Zachariasen's major scientific contribution was the experimental and theoretical assessment of relations expressing the intensity of diffracted radiation concerning corrections for secondary extinction. In 1967 and 1968 he published papers on the theory of X-ray diffraction on mosaic crystals.

The aim of this text is to describe Zachariasen's contribution to the theory of crystal symmetry, namely to the method of deriving 230 space groups. The means he used for this purpose can be summarised as follows:

- He used *tensors* to represent symmetry operations and in this context he also used the *reciprocal lattice* of crystals.
- In the construction of space groups he took advantage of the *factor group*, which other authors before him had not used (Schoenflies, Fyodorov or Seitz - with the exception of A. Speiser, who, however, only pointed out this possibility).
- He used the *lattice postulate* to obtain allowed symmetry operations.
- He used *Seitz's notation* for symmetry operators: $[\Phi, \boldsymbol{t}]$, where the symbol Φ represented tensors (rotations, reflections) and the symbol $\boldsymbol{t}$ represented vectors (translations).

Zachariasen's approach to the derivation (construction) of space groups is captured by the headings of the individual chapters:

- *Concept of symmetry* - equivalent points, trivial symmetry operations, group of symmetry operations
- *Possible symmetry operations of crystal lattices* – lattice postulate
- *Classification of possible symmetry operations and elements of symmetry* - centre of symmetry, axis of symmetry (proper, improper), screw axis, plane of symmetry, glide plane
- *Point groups* - general properties of space groups, factor group, cyclic group, number of cyclic groups (formula), possible angles between symmetry axes (formula)
- *Translation groups* - procedure for their construction according to crystall systems
- *Space groups* - symmorphic groups and other groups, table of space groups

The first mathematically formulated problem Zachariasen set himself was to obtain possible (allowed) symmetry operations in three-dimensional periodic crystal structures. Since he represented the operations by operators in the symbolic notation $[\Phi, \boldsymbol{t}]$ it was actually a matter of exploiting the conditions imposed by the lattice postulate on both the tensor part Φ of the operators (i.e., on rotations and reflections) and on their translational part $\boldsymbol{t}$.

He wrote the tensors in the form

$$\mathbf{\Phi} \equiv \Phi_{jk}\, \boldsymbol{a}^j \boldsymbol{a}_k$$

where Φ_{jk} are the scalar coordinates of the tensor, the symbol $\boldsymbol{a}_k$ represents the triplet of basis vectors of the direct lattice of the crystal, and $\boldsymbol{a}^j$ represents the triplet of basis vectors of the reciprocal lattice. The tensor coordinates can be written in rows and columns, i.e., in matrix form, making Zachariasen tensors essentially identical to Seitz matrices:

$$\begin{pmatrix} \Phi_{11} & \Phi_{12} & \Phi_{13} \\ \Phi_{21} & \Phi_{22} & \Phi_{23} \\ \Phi_{31} & \Phi_{32} & \Phi_{33} \end{pmatrix}$$

The difference in the notation of symmetry operations using tensors or matrices thus appears to be only formal. However, the notation using tensors is particularly advantageous in that it allows the illustrative use of the so-called *natural coordinate system*. The basis of this system is a triplet of non-complanar vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$, which is characteristic of each crystal because the directions of the vectors and their lengths are related to the arrangement of the atoms and the distances between them. The directions of the triplet of basis vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ determine the directions of the coordinate axes, while the "unit" lengths on these axes are determined by the magnitudes of the corresponding vectors. That is, the units of length in different directions in crystal space need not be the same, and are chosen to coincide with the repetition interval of the structural motif in the corresponding direction.

When the matrix and tensor of rotation about the Z axis (the "third" axis), are written in the Cartesian system $X,\ Y,\ Z$ with unit vectors $\boldsymbol{i},\ \boldsymbol{j},\ \boldsymbol{k}$ in the corresponding directions, they have the form:

$$\begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{matrix} \cos\varphi\ \boldsymbol{ii}\ + & \sin\varphi\ \boldsymbol{ij}\ + & 0 \\ -\sin\varphi\ \boldsymbol{ji}\ + & \cos\varphi\ \boldsymbol{jj} + & 0 \\ 0 & 0 & +\boldsymbol{kk} \end{matrix}$$

(A)

The rotation by 60° about the Z axis is then represented by a matrix resp. tensor

$$\begin{pmatrix} (1/2) & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & (1/2) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{matrix} (1/2)\ \boldsymbol{ii}\ + & \sqrt{3}/2\ \boldsymbol{ij}\ + & 0 \\ -\sqrt{3}/2\boldsymbol{ji} & (1/2)\ \boldsymbol{jj} + & 0 \\ 0 & 0 & +\boldsymbol{kk} \end{matrix}$$

In a natural system of basis vectors $\boldsymbol{a}_1,\ \boldsymbol{a}_2,\ \boldsymbol{a}_3$ in which the first two vectors make an angle 120° and the third is perpendicular to their plane, this matrix and tensor have the form

$$\begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{matrix} \boldsymbol{a}^1\boldsymbol{a}_1 & +\boldsymbol{a}^1\boldsymbol{a}_2 & +0 \\ -\ \boldsymbol{a}^2\boldsymbol{a}_1 & +0 & +0 \\ +0 & +0 & +\boldsymbol{a}^3\boldsymbol{a}_3 \end{matrix}$$

or tensor written in one-line form:

$$\boldsymbol{a}^1\boldsymbol{a}_1 + \boldsymbol{a}^1\boldsymbol{a}_2 - \boldsymbol{a}^2\boldsymbol{a}_1 + \boldsymbol{a}^3\boldsymbol{a}_3 \ .$$

As you can see, there are only integers in the matrix, and the same is true for the tensor coordinates. Their integer values are important for further considerations.

The unit matrix representing the identity (i.e., the rotation by 0°), whose diagonal terms are all 1 and the others 0, corresponds to the identity tensor, which has the following form in the Cartesian resp. in natural system:

$$\boldsymbol{ii} + \boldsymbol{jj} + \boldsymbol{kk}\,, \quad \boldsymbol{a}^1\boldsymbol{a}_1 + \boldsymbol{a}^2\boldsymbol{a}_2 + \boldsymbol{a}^3\boldsymbol{a}_3\,.$$

An important role in Zachariasen's procedure is played by the first scalar of the tensor, which coincides with the trace of the matrix, i.e. with the sum of its diagonal terms ($\rightarrow$ relation A). As long as we do not consider a particular rotation angle, both the trace of the matrix and the scalar of the tensor are expressed by the relation:

$$1 + \ 2\cos\varphi.$$

The value of this relation depends only on the rotation angle and, as can be shown, does not depend on the choice of the reference frame.

Zachariasen's reasoning concerning the rotation part of the operator $[\Phi,\ \boldsymbol{t}]$, i.e., the determination of the possible values of the rotation angle, is based on the fact that the lattice vectors $\boldsymbol{t}_j$ of the direct lattice of a crystal are integral linear combinations of a triple of basis vectors:

$\boldsymbol{t}_j \equiv n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$, where n_j are integers. The symmetry operation transforms an arbitrary lattice vector $\boldsymbol{t}_j$ into another lattice vector $\boldsymbol{t}_k$, whose coordinates n_k are also integers, which are a linear combination of the three coordinates of the original vector. The transformation is expressed in the symbolic notation $\boldsymbol{t}_k = \Phi \cdot \boldsymbol{t}_j$, where the transformation for the first coordinate of the vector $\boldsymbol{t}_k$ provides an expression:

$$n_1^k = \Phi_{11}n_1^j + \Phi_{12}n_2^j + \Phi_{13}n_3^j \, .$$

Similar expressions hold for the remaining two coordinates of the $\boldsymbol{t}_k$ vector. If all coordinates of any pairs of vectors $\boldsymbol{t}_j$ and $\boldsymbol{t}_k$ are to be integers, then the coordinates Φ_{ij} of the tensor (in the natural coordinate system) must also be integers. Then the scalar of the tensor must also be an integer N, which leads to the condition:

$$1 + 2\cos\varphi = N \;\; \Rightarrow \;\; \cos\varphi = (N - 1)/2 \, .$$

This condition is satisfied only by the rotation angles φ : 60°, 90°, 120° a 180°.

As stated by Zachariasen, the tensor representing a rotation of φ about an axis whose direction is determined by the unit vector $\boldsymbol{u}$, can be written in the form

$$\Phi = \pm\, \boldsymbol{uu} \pm (\mathbf{I} - \boldsymbol{uu})\cos\varphi \pm (\mathbf{I} \times \boldsymbol{u})\sin\varphi,$$

where $\mathbf{I}$ is the identity tensor (corresponding to the unit matrix). The expression $(\mathbf{I} \times \boldsymbol{u})$ represents the vector product of the identity tensor with the unit vector $\boldsymbol{u}$, which results in a tensor with the property that it projects any vector into a plane perpendicular to the vector $\boldsymbol{u}$. When the sign "+" is applied, these are tensors representing proper rotations, the sign "-" representing non-proper rotations. Substituting the allowed values of the angles φ yields the corresponding tensors, which Zachariasen has listed in a summary table:

The complete list of possible dyadics $\mathbf{n}$ is

$$\begin{aligned} \mathbf{1} &\equiv \mathrm{I} \\ \mathbf{2} &\equiv 2\bar{u}\bar{u} - \mathrm{I} \\ \mathbf{3} &\equiv \tfrac{3}{2}\bar{u}\bar{u} - \tfrac{1}{2}\mathrm{I} + \tfrac{1}{2}\sqrt{3}\,\mathrm{I} \times \bar{u} \qquad [2{\cdot}24] \\ \mathbf{4} &\equiv \bar{u}\bar{u} + \mathrm{I} \times \bar{u} \\ \mathbf{6} &\equiv \tfrac{1}{2}\bar{u}\bar{u} + \tfrac{1}{2}\mathrm{I} + \tfrac{1}{2}\sqrt{3}\,\mathrm{I} \times \bar{u} \end{aligned}$$

He further showed that the vector $\boldsymbol{u}$ cannot have an arbitrary direction, that it must be parallel to the lattice vector of a direct and at the same time reciprocal lattice - which is only possible in lattices of a certain type.

For the translational part $\boldsymbol{t}$ of the operator $[\Phi,\ \boldsymbol{t}]$ in the case of combination with rotations Zachariasen derived the condition

$$(\boldsymbol{t} \cdot \boldsymbol{u})\boldsymbol{u} = (j/n)\boldsymbol{A}_L\ ,$$

where $\boldsymbol{u}$ is a unit vector parallel to the rotation axis, $\boldsymbol{A}_L$ – the shortest lattice vector parallel to the rotation axis, n – nultiplicity of the rotation axis, where the number j can take values 0, 1, ... , n - 1. He derived a similar condition for the cases of combination of translation with reflection. The result of these considerations was a table of the allowed symmetry operations that are parts of the point groups and space groups.

Before he started constructing point and translation groups (all his predecessors started with this), Zachariasen outlined a method for how he wanted to construct space groups. Space groups contain various combinations of rotations, reflections and translations, i.e., they represent certain combinations of point and translation groups. He stated that a translation group (Γ) as a part of a space group (G), is always an invariant subgroup of it. This means, in other words, that a space group containing an infinite number of elements (due to the translation group) can be decomposed into a finite number of parts, the so-called *cosets* with respect to the translation group (Γ):

$$(G) = (\Gamma) + \Psi_1 \cdot (\Gamma) + \Psi_2 \cdot (\Gamma) + \ldots$$

In this relation, $\Psi_i \cdot (\Gamma)$ are the *cosets* of the group (G), with $\Psi_i \equiv [\Phi_i,\, \boldsymbol{t}_i]$ themselves being the *representatives of the cosets*. In doing so, Φ_i represents rotation or reflection (= elements of the point group) and $\boldsymbol{t}_i$ represents translation, which is a fraction of lattice translation, so it does not belong to the translation group. These, the so-called *non-lattice translations*, occur for screw axes and glide planes.

The set of cosets of the space group, together with the translation group, again forms a group, the so-called *factor group*. The elements (members) of the factor group are individual cosets (i.e., sets of elements, not individual elements), and the meaning of the unit (neutral) element in this group is the entire translation group. The space group can then be expressed as the so-called direct product of the translation group (Γ) with the factor group (G/Γ):

$$\text{space group} \quad (G) = (\Gamma) + \Psi_1 \cdot (\Gamma) + \Psi_2 \cdot (\Gamma) + \ldots$$
$$\text{factor group} \quad (G/\Gamma) = \{(\Gamma),\ \Psi_1 \cdot (\Gamma), \Psi_2 \cdot (\Gamma) + \ldots\}$$
$$\Rightarrow \ \text{space group} \quad (G) = (\Gamma) \cdot (G/\Gamma)$$

Zachariasen also considered a factor group to be a group (IG) of coset representatives, which is isomorphic to the factor group and in which the translation group is represented by an identical operation I (unit tensor or matrix):

$$\begin{aligned}
(G/\Gamma) &= \{(\Gamma),\ \Psi_1 \cdot (\Gamma), \Psi_2 \cdot (\Gamma) + \ldots\} \\
(IG) &= \{\mathrm{I},\quad \Psi_1,\quad \Psi_2, \ldots\ \} \\
(BG) &= \{\mathrm{I},\quad \Phi_1,\quad \Phi_2, \ldots\ \}
\end{aligned}$$

In the third row is the point group (BG), which is formed from the factor group when the translation parts $\boldsymbol{t}_i$ are omitted in all elements $\Psi_i \equiv [\Phi_i,\ \boldsymbol{t}_i]$. This point group is isomorphic to the factor group, what was used by Zachariasen in the construction of the space groups.

When screw axes or glide planes are present in the crystal structure, the representative of some coset is the $[\Phi, \boldsymbol{t}]$ operator, i.e., a combination of rotation or reflection with a non-lattice translation. If the representatives of all cosets are only elements of the point group (i.e., elements of type $[\Phi, \mathbf{0}]$, then these are so-called *symmorphic space groups*, of which there are 73, and for which Zachariasen used the name *point space groups*. He has included a table of them in the text, giving three symbols for each group: his own, the international (Hermann-Mauguin) and symbol by Schoenflies.

What is significant about the consideration of the factor group is that it is isomorphic to the point group, which is important to realize when the representatives of the cosets are not purely elements of the point group. This means that in the construction of space groups one needs to know all point groups, all translation groups, but also the allowed non-lattice translations that are part of some of the coset representatives. Therefore, the natural next step was to derive the possible point groups and translation groups, but also to determine what combinations of elements with non-lattice translations can form a group.

Zachariasen began the construction of point groups by creating so-called cyclic groups, which describe the symmetry of crystals with a single rotational axis. Such groups can be created (generated) by successive application of a single symmetry operation (the smallest allowed rotation), which after *n* steps brings the object to the initial position (e.g., four rotations of 90° about the fourfold axis). In terms of group terminology, this is the case of a group with a single generating element. Zachariasen divided these cyclic groups into two parts, proper and improper groups. Both proper and improper symmetry operations (*e.g.*, combinations of rotation with inversion) occur in the improper groups, and he pointed out that proper operations make up half of the entire group and constitute its cyclic subgroup. Therefore, the improper cyclic group can be decomposed into the sum of the proper cyclic group and its only coset whose representative is an improper operation. This reasoning implies that it is sufficient to find all proper cyclic groups and to know the improper operations, which Zachariasen has already listed in the table of allowed symmetry operations.

If the crystal contains more than one rotational axis of symmetry, the point group is no longer cyclic, but contains cyclic groups as its subgroups. Zachariasen derived a relation expressing the connection between the number of cyclic subgroups

$$s_2 = 3 + s_4 + 3s_6,$$

where s_n is the number of cyclic subgroups related to the *n*-fold axis of symmetry.

He further gave a relation expressing the total number k of elements (symmetry operations) in a non-cyclic point group (already given by Bravais):

$$k = 1 + s_2 + 2s_3 + 3s_4 + 5s_6 .$$

Zachariasen also derived a relation expressing the possible angles between the axes of symmetry, which allowed him to consistently construct all possible point symmetry groups of crystals. The result was a clear table of point groups, broken down into proper and improper point groups, with, moreover, an indication of the shape of the tensors representing the generating elements of the groups.

The next step was the construction of 14 types of Bravais lattices - translation groups, rigorously mathematically grounded. As far as the formulation of the problem using operators was concerned, Zachariasen's procedure was not different from Seitz's, except that he used tensors instead of matrices. The basis of the procedure was the condition that the translation group must be invariant with respect to the operations of the corresponding point group. In other words – each of the point group symmetry operations transforms all lattice vectors into other, also lattice vectors. This eventually leads to the requirement that the triple of vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ determining an acceptable translation group, for a given point group represented by tensors Φ, satisfies the relation

$$\Phi_{jk} = \boldsymbol{a}_j \cdot \Phi \cdot \boldsymbol{a}^k = \text{ integer number} \tag{B}$$

In this relation, Φ_{jk} are the coordinates of the tensor Φ and the expression $\boldsymbol{a}_j \cdot \Phi \cdot \boldsymbol{a}^k$ represents the so-called scalar products of the tensor with vectors from both the left and right sides, while from the left the basis vector of the direct lattice, from the right the basis vector of the reciprocal lattice. In the computations, it is sufficient to consider the constraints imposed only by the generating elements of the groups. In contrast to Seitz, who used Laue groups in the construction of translation groups (all of which are improper, because they contain an inversion), Zachariasen stated that it is sufficient to consider the influence of proper point groups, because if relation (B) holds for the $+\Phi$ tensor of an proper rotation, it also holds for the $-\Phi$ tensor of the corresponding improper protation.

Prior to the construction of translation groups, Zachariasen pointed out that in a primitive lattice, the lattice vectors $\boldsymbol{A}_L$ are integral linear combinations of a triple of basis vectors: $\boldsymbol{A}_L = L_1\boldsymbol{a}_1 + L_2\boldsymbol{a}_2 + L_3\boldsymbol{a}_3$. That is, the lattice translations then correspond to the operators $\Gamma_L \equiv [\mathbf{I}, \boldsymbol{A}_L]$ and the translation group can be expressed by the group symbol (Γ_L). However, in centered lattices, the position vectors of some lattice points also contain halves of the basis vectors, so that a translation group, in a body centered lattice, can be assigned the symbol: $(\Gamma) \equiv (\Gamma_L) \cdot (E, \Gamma_{1/2\,1/2\,1/2})$. The term $(E, \Gamma_{1/2\,1/2\,1/2})$ in this expression represents the identity E and the displacement by $(1/2)(\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3)$, so that the corresponding translation group consists of the so-called *integer translations* $\boldsymbol{A}_L = L_1\boldsymbol{a}_1 + L_2\boldsymbol{a}_2 + L_3\boldsymbol{a}_3$ and the translations that are the sum of the *integer and half-integer* ones: $\boldsymbol{A}_L + (1/2)(\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3)$.

The point groups he used in the construction of the translation groups were classified by Zachariasen into the traditional 7 crystall systems, where he then placed the corresponding translation groups obtained. In doing so, he also used the relations valid in the crystall systems for the directions of the basis vectors and for the angles between them, which simplified his further considerations.

As specific examples, we will mention the triclinic and monoclinic crystall systems.

In the *triclinic system*, there are point groups 1 and $\bar{1}$, where the generating elements are identity or inversion, represented by tensors $\Phi = \pm \mathbf{I}$; the relation (B) is then fulfilled for any triple of fundamental vectors, regardless of the sign before the identity tensor. After all, any three-dimensional periodic lattice, regardless of the type of symmetry, is characterized by inversion.

In a *monoclinic system*, the proper point group is the group denoted by the symbol $\mathbf{2}$, where the generating element is represented by the tensor

$$\mathbf{2} \equiv -\boldsymbol{a}^1\boldsymbol{a}_1 + \boldsymbol{a}^2\boldsymbol{a}_2 - \boldsymbol{a}^3\boldsymbol{a}_3 \ .$$

This allows the existence of both a primitive and a base-centered cell (the calculation is quite long). If lattice vectors are expressed in the form

$$\boldsymbol{A}_L + \Sigma f_k \boldsymbol{a}_k \ ,$$

thus, from the corresponding analysis, he emerged two options for f_k : 0 or 1/2, which represents a primitive or centered cell.

After obtaining all of the permitted operations, point groups and translation groups, Zachariasen proceeded to construct space groups. As mentioned above, the space group is expressed as the direct product of the translation group and the factor group, where the factor group is isomorphic to the point group. If the point group is cyclic, it has a single generating element $[\mathbf{\Phi},\ 0]$ and the whole group as a set of elements is denoted by the symbol $(\mathbf{\Phi},\ 0)$, or only by the symbol $(\mathbf{\Phi})$. In doing so, the representatives of some cosets of space group may also have non zero translation terms $\boldsymbol{t}$: $[\mathbf{\Phi},\ \boldsymbol{t}]$, but these must be such that the set of elements $(\mathbf{\Phi},\ \boldsymbol{t})$ forms a group. If the point group is not cyclic, then it has a maximum of three generating elements: $[\mathbf{\Phi}_1,\ 0], [\mathbf{\Phi}_2,\ 0], [\mathbf{\Phi}_3,\ 0]$, and the group is then the direct product of three cyclic groups: $(\mathbf{\Phi}_1)\cdot(\mathbf{\Phi}_2)\cdot(\mathbf{\Phi}_3)$. The generating elements of point group are, generally expressed in the form $[\mathbf{\Phi}_1,\ \boldsymbol{t}_1]$, $[\mathbf{\Phi}_2,\ \boldsymbol{t}_2]$, $[\mathbf{\Phi}_3,\ \boldsymbol{t}_3]$. The corresponding space group (G) is then the product of the factor group $(\mathbf{\Phi}_1,\ \boldsymbol{t}_1)\cdot(\mathbf{\Phi}_2,\ \boldsymbol{t}_2)\cdot(\mathbf{\Phi}_3,\ \boldsymbol{t}_3)$ with translation group (Γ):

$$(G) = (\Gamma)\cdot(G/\Gamma) = (\Gamma)\cdot(\mathbf{\Phi}_1\,,\boldsymbol{t}_1)\cdot(\mathbf{\Phi}_2\,,\boldsymbol{t}_2)\cdot(\mathbf{\Phi}_3\,,\boldsymbol{t}_3)\,.$$

In order for the product of $(\mathbf{\Phi}_1,\ \boldsymbol{t}_1)\cdot(\mathbf{\Phi}_2,\ \boldsymbol{t}_2)\cdot(\mathbf{\Phi}_3,\ \boldsymbol{t}_3)$ to be a group, it is not enough for the groups to be independent terms $(\mathbf{\Phi}_j,\ \boldsymbol{t}_j)$, but the non-lattice translations $\boldsymbol{t}_1,\ \boldsymbol{t}_2,\ \boldsymbol{t}_3$ must meet the additional conditions specified by Zachariasen in a separate paragraph of the text.

As mentioned above, space groups that are formed by the direct product of the translation group and the point group are the so-called *symorphic groups*. He divided the other space groups (non-symmorphic) into three sets, according to the shape of the translational member of the first of the two or three generating elements of the factor group.

In the first set of non-symmorphic groups, which he denoted with the letter $\mathbf{A}$, he included space groups in which the first of the three generating elements of the factor group has the form $[\overline{\boldsymbol{n}},\ \boldsymbol{t}]$, where the tensor $\overline{\boldsymbol{n}} = \overline{\mathbf{1}},\ \overline{\mathbf{3}}, \overline{\mathbf{4}}$, or $\overline{\mathbf{6}}$, e.g. inversion $(\overline{\mathbf{1}})$ and rotoinversions $(\overline{\mathbf{3}},\ \overline{\mathbf{4}},\ \overline{\mathbf{6}})$. This set includes space groups constructed on the basis of the following point groups:

C_i, C_{2h}, D_{2h}, S_4, C_{4h}, D_{2d}, D_{4h}, C_{3i}, D_{3d}, C_{3h}, C_{6h}, D_{3h}, D_{6h}, T_h, O_h.

In the second set, marked with the letter $\mathbf{B}$, he included non-symmorphic space groups, in which the first of the three generating elements of the factor group has the form $[\boldsymbol{n},\ \boldsymbol{t}]$, where the tensor $\boldsymbol{n} = \mathbf{2},\ \mathbf{3},\ \mathbf{4},$ or $\mathbf{6}$. So these are proper rotations. This set includes space groups constructed on the basis of the following point groups:

$$C_2, D_2, C_{2v}, C_4, D_4, C_{4v}, C_3, D_3,\ C_{3v}, C_6, D_6, D_{6v}, T, O, T_d.$$

The third set, marked with the letter $\mathbf{C}$, includes space groups related to the point group C_s . The generating element of the factor group is $[\overline{2},\ \boldsymbol{t}]$ so it is a reflection, which can also be understood as a combination of rotation by

180° with inversion, i.e. as an operation according to the twofold rotoinverse axis.

A different view of the three types of space groups, or the generating elements of the factor group, is also possible. In the case of type $\mathbf{A}$, the translational part of the operator can be zeroed by suitable choosing the position of the origin of the coordinate system. In type $\mathbf{B}$, the translational part of the operator must be parallel to the rotational axis of symmetry, so it has the form $\boldsymbol{t}\cdot\boldsymbol{uu}$, where $\boldsymbol{u}$ is the unit vector parallel to the axis of rotation. So these are screw axes. In type $\mathbf{C}$, the translational part of the operator must be parallel to the mirror plane, so it has the form $\boldsymbol{t}-\boldsymbol{t}\cdot\boldsymbol{uu}$, where $\boldsymbol{u}$ is the unit vector perpendicular to this plane. Given these circumstances, the three types of non-symmorphic space groups can be expressed by relationships:

$$\mathbf{A}\ \ (G)=(\Gamma)\cdot(\Phi_{\mathbf{1}},\ 0)\cdot(\Phi_2,\ \boldsymbol{t}_2)\cdot(\Phi_3,\ \boldsymbol{t}_3),$$

screw axes $\mathbf{B}\ \ (G)=(\Gamma)\cdot(\Phi_{\mathbf{1}},\ \boldsymbol{t}\cdot\boldsymbol{uu})\cdot(\Phi_2,\ \boldsymbol{t}_2)\cdot(\Phi_3,\ \boldsymbol{t}_3),$

glide planes $\mathbf{C}\ \ (G)=(\Gamma)\cdot(\Phi_{\mathbf{1}},\ \boldsymbol{t}-\boldsymbol{t}\cdot\boldsymbol{uu})\cdot(\Phi_2,\ \boldsymbol{t}_2)\cdot(\Phi_3,\ \boldsymbol{t}_3).$

In a similar way, two other members of the factor group can be analyzed, but Zachariasen did not do this in detail. He did not use this method to derive all 230 space groups, arguing that they were derived more than half a century ago. He gave only a few typical examples of the construction of non-symmorphic space groups.

In type $\mathbf{A}$, he used his method to show that 4 non-symmorphic groups are related to the point group C_{4h} in addition to the two symorphic ones.

For type $\mathbf{B}$, he gave the example of groups related to the point group D_3 and derived 4 non-symmorphic groups.

In type $\mathbf{C}$, starting from the point group C_S derived two non-symmorphic groups, one with a primitive lattice, the other with a base-centered lattice.

At the end of the chapter on crystal symmetries, he listed all 230 space groups, with three symbols:

his own, international (Hermann-Mauguin) and Schoenflies.

Zachariasen, like Seitz, could no longer discover new types of space groups, all of which had already been derived by Fyodorov and Schoenfkies, but he took their derivation – construction – to a higher mathematical level.

Authors quoted by Zachariasen:
Bravais, Sohncke, Fyodorov, Schoenflies, Seitz, he did not quote the authors of the point groups – Hessel and Gadolin. He also cited the International Tables for Cystallography.

Some of Zachariasen's works:

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BLACK-WHITE AND COLOUR GROUPS

The systematics of space groups representing types of symmetry of crystal structure was developed at the end of the XIX century and is associated with the names of Fyodorov and Schoenflies. The work of Seitz and Zachariasen in the first half of the twentieth century was a contribution only in terms of the methodology of derivation of space groups, a more complete and elegant use of the possibilities of mathematics. However, the development did not stop there, and the extension of symmetry types began to be considered. In addition to the three spatial coordinates of the atom expressing its position in the unit cell of the crystal, another parameter began to be considered which could characterize the atom and take on two or even more values. A parameter with two values was already in 1929 the subject of consideration of the German mathematician Heinrich Heesch [21], who in his doctoral thesis gave the name **black-white** to the respective symmetry groups. Allegedly already in that period Russian crystallographer A. V. Shubnikov corresponded with Heesh. Later, in 1951 Shubnikov published a rigorous derivation of 58 black-white point groups. In his work, Shubnikov began to use the term *antisymmetry*, which seems to have originated in the oppositeness of the states corresponding to the two possible values of this *antisymmetry parameter*. For example, in antiferromagnetics there are possible two opposite orientations of the magnetic moments of the atoms, which contributed to the use of the threefold naming of these groups - the *black-white*, *magnetic*, and *Shubnikov groups*. Shubnikov at that time collaborated with N. V. Belov, who in 1956, together with R. F. Tarchova, considered the case of several possible values of this additional parameter. Under the influence of the name black-white groups, the name **coloured groups** [19] was coined. The number of possible types of symmetry thus grew considerably, and this involved an increase in the number of point, translation and space groups. On groups of this type, Shubnikov and Belov published a book in 1964, *Colored symmetry* [20].

It is convenient to illustrate the construction of black-white groups by the example of a crystal in which the magnetic moment of a particular atom can have only one of two orientations opposite to each other. Consider the case in which an atom is moved from a particular location in the unit cell of the crystal by an operation of symmetry to another position (equivalent from the point of view of space symmetry), but in which it should have an oppositely oriented magnetic moment. Thus, complete identification is achieved only when the magnetic moment of the displaced atom is flipped over. From a mathematical point of view, the flipping can be expressed symbolically by the number –1, which is understood as the magnetic moment flipping operator (spin inversion, colour inversion, antisymmetry operator), which is added to the operator representing the corresponding space operation (rotation, reflection or translation). However, by another symmetry operation, the atom can be brought to a position where the same orientation of the magnetic moment is required; the conservation of its direction can be expressed by applying the operator represented by +1. The pair of numbers (operators) –1, +1, in terms of the binary multiplication operation, forms a group, in this case called the spin inversion group and denoted by the symbol $R = \{1,\ -1\}$ or according to Shubnikov $R = \{1,\ 1'\}$. The comma (apostrophe) above the symbol represents the combination of the corresponding spatial operation with the magnetic moment flip, or more generally with the change of the value of the antisymmetry parameter. For example, the rotation by 90° about the fourfold axis of symmetry associated with the flipping of the magnetic moment is denoted by Shubnikov with the symbol 4′. In structures in which the atoms have doubly oriented magnetic moments, only some of the symmetry operations are combined with magnetic moment flipping, so they form only part of the relevant set of symmetry operations.

Shubnikov groups, often called magnetic groups, include three types of groups. The first kind are the so-called *colourless magnetic groups* M_0 , identical to the space, point or translation groups G, not containing combinations of space transformations with magnetic moment flipping, so that: $M_0 \equiv G$; thus, there are 230 colourless space groups, 32 colourless point groups, and 14 colourless translation groups.

The same calculus applies to the second kind - *paramagnetic groups P* also called *grey groups*, whose elements are both the operations of the space group (or point or translation group), but also all the operations of this group combined with the magnetic moment flip, which is expressed by notation: $M_\mathrm{P} \equiv G + G1'$. This essentially means that the probability of occurrence of one or the other orientation of the magnetic moment at a given location of the unit cell of the crystal is the same.

In the third kind, the *non-trivial* magnetic group M, i.e., the *black-white group*, there are two equally numerous sets of symmetry operations - space operations combined with magnetic moment flipping and space operations without this flipping; these two sets of space operations are disjunctive - the operations of the second set are not found in the first set, and vice versa. There are 1191 such space groups.

The sum of the number of *colourless*, *grey* and *black-white* space groups gives the number

$$230 + 230 + 1191 = 1651,$$

which is the total number of so-called Shubnikov space groups.

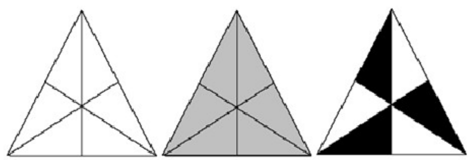
The formation of black-white M groups from the G group of space transformations is based on its subgroup H with an index of 2 (H has half of the elements of the G group). The elements of subgroup H are space transformations (rotations, reflections, translations) without a combination with a flip of the magnetic moment, while all other elements of the group G, i.e. elements of the coset $G - H$, are combined with flipping; they are written in the symbolic form $(G - H)1'$. The notation of the black-white group M thus has the form:

$$M = H + (G - H)1' .$$

Such a construction of black-white groups is directly applied to both point and translation groups, but for space groups, as shown below, there are two types of black- white groups. For the point groups, there are 32 colourless, 32 gray and 58 black-white, a total of 122 Shubnikov groups.

It should be noted that not all black-white groups are suitable for describing structures with ordered magnetic moments (ferromagnetics, antiferro-magnetics, and ferrimagnetics), because in some cases there is a mismatch between a dashed operation and an undashed one. Out of 58 black-white point groups, only 27 are feasible in this sense.

To illustrate the three types of Shubnikov point groups, the following figure will be used, which shows three plane objects. Their symmetries are described by a colourless, gray, and black-white point group.



The colourless point group G of the first object contains primarily rotations of 0°, 120° a 240° (symbols $e, 3, 3^2$) related to the threefold axis of symmetry perpendicular to the plane of the triangle and passing through its center, as well as three reflections m_{60}, m_{120} and m_{180} in three planes perpendicular to the plane of the triangle, which form angles of 120° to each other. In each of these transformations, the object identifies with itself. Thus, the colourless point group of symmetry G contains the following elements:

$$G \equiv \{e,\ \ 3,\ \ \ 3^2,\ m_{60},\ m_{120},\ m_{180}\}\,.$$

The third of the objects in the picture, in addition to the identical operation, identifies with itself even after rotations of 120° and 240° around the threefold axis, while this set of symmetry operations with the designations e, 3, 3^2 forms a subgroup with an index of 2 of group G. After reflection, however, the object gets into the same position only after the mutual swapping of black and white. Therefore, reflection must be combined with the inversion of colour, represented by an apostrophe. The black and white point group M then has the following elements:

$$M \equiv \{e, 3,\ 3^2,\ m'_{60},\ m'_{120},\ m'_{180}\,\}.$$

For the middle object – from the point of view of symmetry operations – the same applies as for the first object, while from the point of view of the arrangement of the magnetic moments of atoms, it is an image of the symmetry of the paramagnetic substance. According to what was mentioned above, the Shubnikov group describing the symmetry of this object contains all the elements of the colourless group and, in addition, all these elements associated with the inversion of colour (magnetic moment):

$$M \equiv \{e, 3, 3^2,\ m_{60},\ m_{120},\ m_{180},\\ e', 3', (3^2)',\ m'_{60},\ m'_{120},\ m'_{180}\}.$$

From this point of view, the symmetry of the first of the three objects would represent the symmetry of a substance containing atoms without a magnetic moment, and the symmetry of the third – the symmetry of an antiferromagnetic substance.

As an example of the construction of black-white point groups in three-dimensional space, we can mention groups formed from a point group marked in international tables with the symbol 4/m, which has eight elements:

- *identity* marked with the symbol 1, inversion (symbol $\overline{1}$),
- *rotations* around the fourfold axis by 90°, 180° and 270° (symbols 4, 4^2, 4^3),
- and these *rotations combined with inversion* (symbols $\overline{4}$, $\overline{4}^2$, $\overline{4}^3$).

The equivalences $4^2 \equiv 2$ apply, i.e. a double rotation of 90° around the fourfold axis is equivalent to one rotation of 180° around the twofold axis, and $\overline{4}^2 \equiv \overline{2} \equiv m$, i.e. a rotation of 180° with the following inversion is equivalent to the reflection m in a plane perpendicular to the rotation axis. Writing of the 4/m point group using the symbols of individual symmetry operations:

$$G_{4/m} \equiv \{1, 4, 4^2, 4^3, \overline{1}, \overline{4}, \overline{4}^2, \overline{4}^3\} \equiv \{1, 4, 2, 4^3, \overline{1}, \overline{4}, m, \overline{4}^3\}.$$

This group has 3 subgroups of index 2:

$$H_1 = 4 \equiv \{1, 4, 2, 4^3\}\ ,\ H_2 = \overline{4} \equiv \{1, \overline{4}, m, \overline{4}^3\}\ ,\ H_3 = 2/m \equiv \{1, 2, \overline{1}, m\}.$$

Based on them, the following three black-white groups can be constructed:

$$M_1 = 4/m' \equiv \{1, 4, 2, 4^3, \bar{1}', \bar{4}', m', \bar{4}^{3\prime}\}$$
$$M_2 = 4'/m' \equiv \{1, \bar{4}, 2, \bar{4}^3, \bar{1}', m', 4', 4^{3\prime}\}$$
$$M_3 = 4'/m \equiv \{1, 2, \bar{1}, m, 4', 4^{3\prime}, \bar{4}', \bar{4}^{3\prime}\}$$

The 4/m point group itself is considered to be a *colourless magnetic group* M_0within the Shubnikov groups:

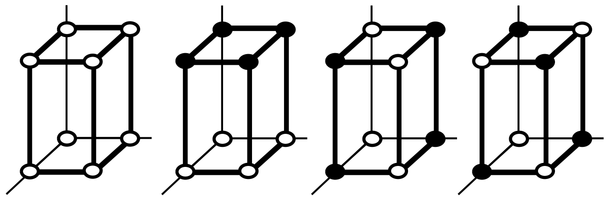
$$M_0 \equiv 4/m \equiv \{1, 4, 2, 4^3, \bar{1}, \bar{4}, m, \bar{4}^3\}$$

while the *paramagnetic group* M_{P} contains, in addition to the elements of the colourless group, its elements combined with magnetic moment flipping:

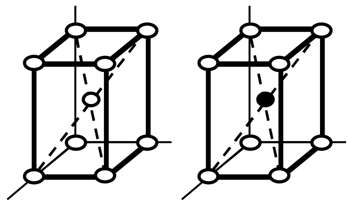
$$M_{\mathrm{P}} \equiv \{1, 4, 2, 4^3, \bar{1}, \bar{4}, m, \bar{4}^3, 1', 4', 2', 4^{3\prime}, \bar{1}', \bar{4}', m', \bar{4}^{3\prime}\}.$$

Here it is worth recalling again that not all the black-white point groups presented here are realizable in magnetically ordered structures, such as the group $M_3 = 4'/m$.

In a similar way to point black-white groups, the translation black-white groups are also constructed. That is, a subgroup with index 2, i.e., half of all possible translations, is selected from the translation group and the other half of the translations are combined with a magnetic moment flip (colour inversion). The translation groups contain an infinite number of elements (translations), but the corresponding procedure can be illustrated on a single unit cell. For example, in a primitive tetragonal lattice, half of the lattice points can be selected with the magnetic moment flipped in three ways, as indicated in the following figure, in which the "colourless" lattice is shown first:



The black rings represent lattice points, which are assigned magnetic moments of opposite orientation to those in the white rings. In a body centred tetragonal lattice, there is only one possible way of selection - when the translation directed to the center of the cell is coupled with a flip of the magnetic moment:



In the structures described by the black-white translation groups, positions with oppositely oriented magnetic moments alternate, and so the unit cell, if it is to respect the magnetic ordering as well, must in general become larger.

A similar procedure to that used for point and translation groups is also used in the construction of space black-white groups, but in this case two types are distinguished. Among the 1191 space black-white groups, there are 674 in which the translation subgroup H is the same as in the group G, i.e., its elements are not combined with a magnetic moment flip. Therefore, the magnetic unit cell is the same as the crystallographic one. These black-white space groups are referred to as the groups of the first kind. In the remaining 517 black-white space groups (groups of the second kind), the translation subgroup contains half of the translations combined with magnetic moment flipping (according to Shubnikov, these are *antitranslations*); the magnetic unit cell is then larger than the crystallographic one.

The construction of two-colour, i.e., black-white groups (point, translation, and space), is based on the decomposition of the colourless group into a subgroup with index 2 and the corresponding coset; the antisymmetry parameter *s* then takes only two values. All elements of the coset are combined with the antisymmetry operation, i.e. with the second value of the parameter *s*. In the construction of multicolour groups, when the parameter *s* can take *n* values (*n* - "colours"), the decomposition of the colourless group into an invariant subgroup with index *n* and the corresponding *n* - 1 cosets is used. The elements of the cosets are then successively combined with operators representing the individual values of the parameter *s*. This gives rise to a much more numerous set of symmetry types, which, however, does not have the same practical application as the set of black-white groups.

CRYSTALS WITH ANOTHER TYPE OF SYMMETRY

A crystal is commonly understood to be a solid in which the distribution of the constituent particles is characterized by a three-dimensional periodicity[1]. This periodicity is the reason for the existence of symmetry in both the structure of the crystals and their external shape. In real crystals, whether natural or synthetic, there is no perfect three-dimensional periodicity of the positions of the atoms; it is disturbed both by the oscillations of the atoms and by various types of point, line or plane defects. This can also break the symmetry of the crystal. If, nevertheless, the arrangement of the atoms can be regarded as periodic, or if there is at least a correlation between the positions of the atoms at a distance, such a crystal is said to be *ordered*; otherwise it is a *disordered* crystal. Disordered crystals include in particular *solid solutions* which are characterised by the non-periodic occupation of certain atomic positions by two or more atomic species. Crystals with partially broken or incomplete symmetry include *OD crystals*, the second group are *aperiodic crystals*, which include so-called *incommensurable modulated structures*, *incommensurable composite crystals* and *quasicrystals*.

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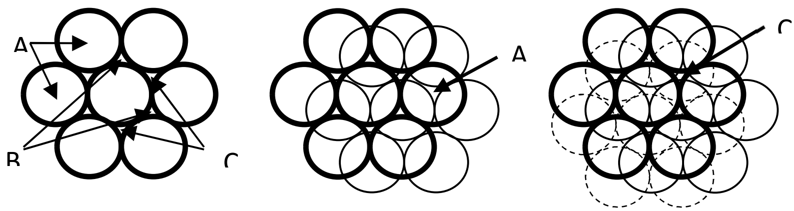
[1] According to the 1992 definition of the International Union of Crystallographers, a crystal is understood as a solid substance characterized by a diffraction diagram with sharp diffraction traces.

OD structures

A special type of crystals with disruption of strictly three-dimensional periodicity are OD crystals, whose structure is referred to as *OD structure* (*Order - Disorder*). This type of structure can be understood as composed of plates (layers) with intrinsic symmetry, while they are not layered structures in the chemical sense. The symmetry of the layers applies only within their framework and is described by two-dimensional symmetry groups. In terms of the overall crystal structure, these are partial symmetry operations, valid only in part of the whole crystal space. The existence of local symmetry, which is not part of the symmetry of the whole crystal, creates preconditions for ambiguity in the stacking of the layers. Whether the resulting structure will be ordered or disordered depends on the sequential stacking of the layers. The possible variability in the stacking of the layers leads to the formation of so-called ***polytypes***; these include, for example, SiC crystals or micas.



As a macroscopic example of polytypes, we can use the stacking of identically sized spheres. If they are to be stacked as tightly as possible, a layer with a hexagonal arrangement will appear in the plane (in the following figure the circles are drawn with a solid bold line). We denote the positions of these spheres as the "A" positions. When a second such layer of spheres is placed on top of the first layer so that the arrangement is as tight as possible (circles drawn with a solid thin line), the spheres of the second layer will fit into the wells between the spheres of the first layer, either in the positions marked 'B' or in the positions marked 'C'. Suppose that they occupied the B-type positions as shown in the figure. The spheres of the third layer (the circles drawn by the dashed line) sit in the holes in the second layer, and again they may take positions of two kinds - those above the spheres of the first layer - 'A-type' positions, or 'C-type' positions, which are positions above the other holes of the first layer. If such stacking is repeated regularly, in the first case (stacking of layers is referred to as ABABAB...) a hexagonal structure is formed, in the second case (referred to as ABCABCABC...) a cubic structure is formed. However, stacking can also take place in more complicated ways, which is the essence of the formation of polytypes. If even the more complex stacking is repeated periodically, an ordered structure is formed. It should be noted that such structures (polytypes) occur not only in hexagonal structures. It is noteworthy that the tightest stacking of spheres in plane and space was already addressed in the early 17th century by Johann Kepler, the author of the laws of planetary motion [4].

Disjunct (non-overlapping) parts of the OD structure characterized by two-dimensional periodicity are called *OD layers*. They do not have to match the layers selected on the basis of chemical identity or cleavage. The goal of selecting

OD layers is not to explain polytypism, but to describe it on the basis of symmetry. In OD structures, there are symmetry operations applied throughout the crystal volume, but also operations applied only within layers, the so-called local symmetry operations, the set of which forms a plane group (two-dimensional group). A set of symmetry operations valid in the entire volume of a crystal forms its space group, but the set that is created by adding local operations usually no longer meets all the criteria for the existence of a group, a more loosely defined mathematical structure is created – the so-called *grupoid*.

In the theory of OD structures, an important role is played by the *proximity condition*, which assesses the geometric equivalence of layers and thus the possibility of immediate overlapping. For example, geometrically equivalent layers, or layers whose translation groups are identical, or have at least a subgroup in common, satisfy the neighborhood condition. If the placement of the layer (both position and orientation) is unambiguous, determined by adjacent layers, and meets the neighborhood condition, the resulting structure is ordered. However, if there are multiple storage options complying with the neighborhood condition, then the resulting structure belongs to the OD structure. Therefore, structures that meet neighborhood conditions are either ordered or are OD structures. All OD structures belong to *polytypes*, but this does not have to be the other way around.

All OD structures, even those of different chemical compositions, if they are formed on the basis of the same type of symmetry, belong to the so-called *OD family of* *grupoids*. This concept has an analogous meaning to that of a space group: just as there is a finite number of space groups to describe an essentially infinite number of variations of structures, so there is also a finite number of families OD of groupoids to describe an infinite number of possible variations of OD structures. If we move from the abstract to the concrete level, the OD structures of a concrete substance formed on the basis of the same type of symmetry – differing only in the way the layers are deposited – belong to the same family: the members of the family are concrete real structures.

The theory of OD structures was developed in the fifties of the last century by the German crystallographer K. Dornberger-Schiff [22], and from the Slovak crystallographer, S. Ďurovič [23], who collaborated with her, participated in the completion of the theory. His share was accepted by the International Union of Crystallographers by commissioning him to write part of the relevant chapter in the International Tables for Crystallography [24].

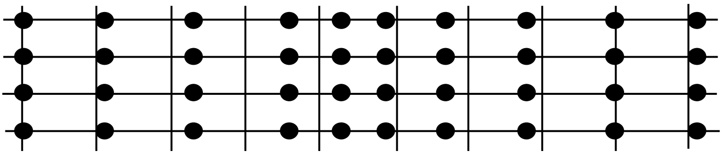
The terms order-disorder are also used outside of crystallography, in a similar, yet different meaning. In physics, it represents the presence or absence of a certain kind of symmetry or correlation in a system of many particles. From the point of view of condensed matter physics, systems of many particles are considered to be ordered near absolute zero temperature, their heating leads to a phase transition to a less ordered state. An example of such a phase transition is the melting of ice – the loss of the crystalline arrangement, or the demagnetization of iron by heating above the Curie temperature – the loss of the magnetic arrangement. When assessing orderliness, it can be not only about the positions of atoms or their groups, but also about the spatial arrangement of other parameters of atoms, such as their magnetic moments. Orderliness can also be assessed in terms of correlation between localities at different distances from each other – in this case, *short range order* and *long range order* are distinguished.

Aperiodic crystals

According to the definition of the International Union of Crystallographers from 1992, these are crystals that appear to be crystalline in terms of X-ray diffraction, because their diffraction image contains sharp diffractions, but in which there is no three-dimensional periodicity of atomic arragement. Such crystals include:

- incommensurable modulated structures,
- incommensurable composite crystals, and
- quasicrystals.

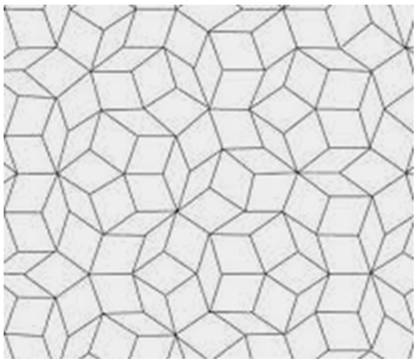
Modulated structures are divided into symmetrical and incommensurable, with their common feature being the additional periodicity of the positions of the atoms, superimposed to the basic periodicity determined by the lattice parameters. The superimposing periodicity — compared to the distances determined by the lattice parameters d — corresponds to a many times greater repetition distance λ. This is a similar phenomenon to radio waves, in which on the fundamental (carrier) frequency of the electromagnetic wave is superimposed a significantly lower frequency of the transmitted signal, i.e. a much longer wavelength. If the ratio d/λ cannot be expressed by the ratio of integers, the structure is referred to as *incommensurate* and is an aperiodic structure. Otherwise, the structure is referred to as *commensurate* and is not classified as aperiodic structures. Structures whose symmetry is judged by the arrangement of the magnetic moments of atoms can also be incommensurate.



The figure shows a structure in which modulation of the positions of atoms in the horizontal direction is applied, in the vertical direction the periodicity determined by the relevant lattice parameter is maintained. The number of atoms per unit length in the horizontal direction is not constant, but changes periodically. Such modulation is referred to as *positional modulation*, and the occupation of positions by various types of atoms can also be modulated – in this case, it is *occupation modulation*.

An **incommensurate composite crystal** consists of two or more sub-systems with modulated structures whose basic structures are incommensurate with each other. Crystals of this kind were first described by E. Makovický [26]. Examples of such crystals are various adherent crystals or adsorbed monolayers.

Quasicrystals represent a type of crystalline substance whose structure is somewhat ordered, but it is not periodic, lacking translational symmetry. A copy of a structure does not identify with its original by any of its displacements – it is aperiodic. Sharp diffraction records indicate their crystalline state, but also the presence of fivefold or tenfold axes of symmetry, not present in crystals. Quasicrystals were discovered in 1982 by D. Schechtman [25], for which he received the Nobel Prize in Chemistry in 2011.



Aperiodic surface coverage was discovered by mathematicians as early as the 1960s and was used to describe the structure of quasicrystals about 20 years later. It can consist of several shape units, while the stacked units fill the space perfectly, without gaps, without overlaps. An example of such a covering with the fewest number of shape units is Penrose tiling (Penrose tiling [32],[33]), It is created by laying tiles of only two types of diamond shape, with sides of the same length but different angles (pictured). Penrose paving is characterized by five-fold axes of symmetry, as well as mirroring.

From a mathematical point of view, an image of a three-dimensional aperiodic structure can be obtained by projecting a periodic hyperlattice, defined in multidimensional space, into three-dimensional space.

GLOSSARY

axis of symmetry – an element of symmetry – a line, by rotating around which the object can get to the position identical to the initial position. For crystals, only twofold, threefold, fourfold, and sixfold axes of symmetry are involved; other multiplicities are referred to as forbidden in the context of crystals.

centre of symmetry – an element of symmetry – a point with respect to which the inversion is performed.

column matrix – vector notation with a matrix that has only one column and, for vectors in three-dimensional space, three rows.

coset of a group - the set of elements of a group which is formed by "multiplying" all the elements of its subgroup by an element which does not belong to the subgroup. If the subgroup contains exactly half of the group elements, there is only one coset, otherwise there are more cosets. Due to the fact that the operations in the group may not be commutative - the result of the "product" depends on the order of operations - therefore left and right cosets of the group are distinguished, obtained by multiplying the elements of the subgroup from the left and right sides, respectively.

crystal class – one of the 32 types of external symmetry of crystals characterized by a set of rotational or inverse axes and mirror planes. In mathematical terms, described by one of the 32 point groups of symmetry.

crystal lattice, lattice – a set of periodically spaced points in crystal space. In three-dimensional space, the three basic directions of the distribution of points, as well as the distances between adjacent points in these directions, are represented by a triplet of basis vectors, their directions and length. The position vector of each lattice point can be expressed as an integral linear combination of the triplet of basis vectors. A lattice in real space is called a direct lattice. In physics, a crystal lattice is usually understood as a lattice including the filling of atoms.

cyclic group – a group that is formed by successive (multiple) application ("multiplication") of a single, so-called generating element - its "powers". After *n* - applications of the generating element, the object reaches the initial position, so that the *n*-th "power" of the generating element coincides with the neutral element of the group. For example, a cyclic group is the set of symmetry operations of a square, formed by successive rotations by 90° about an axis perpendicular to its plane passing through the centre of the square. After four rotations, the square is brought to its initial position, i.e., to the position as after "multiplication" by the neutral element, i.e., rotation by 0°.

determinant of the matrix – numerical value assigned to the matrix, which for matrices with three rows and three columns is obtained as the sum of six products of triplets of its elements, selected in the prescribed way. The determinants of matrices representing proper operations of symmetry have the value +1, for improper operations the value -1.

direct lattice – a lattice in real space ($\rightarrow$ crystal lattice).

factor group – group *F*, which is formed from the group *G* so that its neutral element is the invariant subgroup *H* of the group *G* (the so-called normal divisor of the group *G*) and the other elements are the cosets of the group *G* with respect to the subgroup *H*. The elements of a factor group are thus disjunctive sets of elements of the group *G* as a whole.

generating elements of a group – several elements of a group, the repetition and combination of which will produce all other elements of the group. Three generating elements are sufficient to create (generate) the largest point group of crystals (it contains 48 elements). If one generating element is sufficient to generate the whole group, the group is cyclic.

glide plane – an element of symmetry – a plane where the identification of the crystal structure is achieved by reflection in this plane combined with a non-lattice translation parallel to this plane.

group (definition) – a group *G* is a set of elements in which a binary operation is defined, i.e. an operation between two of its elements, which generally produces another element of the group; the operation must be associative, there must be a neutral element in the set, and there must be an inverse element to each element of the set. The name "element multiplication" is used for the operation between two elements of a group. "Multiplication" with a neutral element does not change the elements of the group. The result of "multiplying" an element with an inverse element is a neutral element. An example of a group is the set of integers with respect to the sum operation; the sum of the numbers is associative, the neutral element is zero, and each negative number is the inverse element of a positive number with the same absolute value.

group of symmetry operations – the set of symmetry operations satisfying the group existence conditions. Elements of this group can be rotations, reflections, inversions, translations and their combinations. A binary operation in this group is the successive execution of two symmetry operations, resulting in another symmetry operation.

grupoid – a set of elements between which a binary operation (operation between two elements) is defined; with respect to this operation the set is closed, but no other conditions are imposed. In the context of crystals, these are elements representing symmetry operations. A grupoid is a figure defined more loosely than a group.

holohedral group – point group, which in the respective crystallographic system describes the symmetry of the lattice; by filling the lattice with atoms, the point symmetry can only be reduced, it is then represented by subgroups of the holohedral group. The point symmetry of the primitive and the centred lattice, in so far as they belong to the same crystall system, is the same - described by the holohedral group.

improper rotation $\rightarrow$ improper symmetry operations.

improper symmetry operations – reflection and inversion, as well as their combinations with rotation; the determinant of the transformation matrix of such operations is equal to – 1. These operations cannot be performed on a real object, but there may be objects that are its mirror or inverse image.

invariant subgroup – a subgroup whose left cosets coincide with the right cosets; for an invariant subgroup the name *normal divisor of the group* is also used.

inverse group element – a group element whose "product" with the group element with respect to which it is inverse is equal to the neutral element. There are pairs of mutually inverse elements in groups, e.g. rotations about 90° and 270°, because their sequential application coincides with the rotation about 0°. Some elements of a group are inverse to themselves, e.g. rotation by 180°.

inversion – a point symmetry operation in which each point of an object with position vector $\boldsymbol{r}$ is transformed into a point with position vector $-\boldsymbol{r}$. This definition is valid when the centre of symmetry lies at the origin of the coordinate system. The term *reflection at the centre of symmetry* is also used for the inversion.

isomorphic groups – such groups, between the elements of which there is a simple, i.e. mutually unambiguous representation (assignment); therefore they have the same number of elements. For example, a group of matrices is isomorphic to a point group of symmetry operations if each element of the point group is assigned to a particular matrix representing the corresponding symmetry operation. The multiplication of the two matrices by each other is then consistent with the "multiplication" of the elements of the point group; the product of the two matrices produces a matrix representing the resulting symmetry operation.

lattice basis vectors - a triplet of vectors not lying in the same plane, whose integral linear combinations can be used to construct (describe) an entire space lattice. For a known lattice, they are chosen to be as short as possible and their arrangement is consistent with the symmetry of the lattice.

lattice postulate – the assumption of strict three-dimensional periodicity of the physical properties and distribution of atoms in crystals.

lattice translation – a translation that shifts the lattice to a congruent position; these are translations described by a vector that is an integral linear combination of the lattice basis vectors.

mirror plane → reflection plane

mirroring → reflection

neutral element of a group – an element whose combination ("multiplication") with other elements of the group does not change them. The neutral element in terms of summation is the number 0, in terms of multiplication the number 1, in terms of rotational symmetry operation the rotation by 0° respectively by 360°.

non-lattice translation – translation that cannot be expressed as an integral linear combination of the basis vectors of the lattice; instead of integers, multiples of one half, one third, one quarter or one sixth of the length of the lattice translation are applied, which is related to the multiplicity of rotational axes of symmetry.

normal divisor → invariant subgroup.

plane of symmetry → rerflection plane.

point group – a set of point operations of symmetry – rotations, reflections and inversions, which meets the conditions for the existence of a group, describing the symmetry of one of the 32 crystal classes.

point symmetry operations – symmetry operations in which the position of at least one point of the transformed object does not change. These are inversions, rotations and reflections.

proper symmetry operation – a symmetry operation representing only rotation about the axis, which does not combine with reflection or inversion; the determinant of its transformation matrix has the value +1.

reciprocal lattice – a lattice in → reciprocal space that is the transformed image of the direct lattice into reciprocal space. The distribution of points in a reciprocal lattice is also periodic and can be expressed by a linear combination of the basis vectors of the reciprocal lattice. There are unambiguous relationships between the basic vectors of the reciprocal lattice and the basis vectors of the direct lattice.

reciprocal space – virtual space, a mathematical transformation of direct space in which distances are measured in inverted units of length. It is used, for example, in determining the structure of crystals by X-ray diffraction methods. The position of points in this space is determined by reciprocal vectors.

reciprocal vectors – vectors in reciprocal space; they are important when a Cartesian coordinate system is not used, but a system based on basis vectors representing directions and distances corresponding to the crystal structure. They are expressed as a linear combination of the three basis vectors of the reciprocal lattice.

reflection – a point symmetry operation in which the points of space are moved to the opposite side of the symmetry plane along lines perpendicular to this plane, while maintaining the distance from it; the reflection matrix determinant has the value –1.

reflection plane, mirror plane – element of symmetry – plane with respect to which reflection is performed. It is always parallel to some lattice plane of the crystal.

rotation – a point symmetry operation by which a shape is brought to an identical position by rotating it about the axis of symmetry by a certain angle; for crystals, these are only the angles 60°, 90° and their integer multiples.

rotation axis $\rightarrow$ axis of symmetry.

scalar product of a vector with a tensor – a mathematical operation representing a transformation of the position of a point marked by the end point of the vector; the shape of the tensor depends on the type of operation, whether it is an inversion, rotation or reflection. The result of the transformation also depends on whether the tensor is multiplied by the vector from the right or from the left.

screw axis – an element of symmetry – a line at which the identification of the crystal structure is achieved by combining rotation about that line with non-lattice translation along that line.

space group – a group of symmetry operations whose elements are combinations of elements of the point group and the translation group. The point group and the translation group are its subgroups, the translation group is its invariant subgroup.

subgroup – any subset of a group whose elements satisfy the group's existence conditions.

symmetry (of crystal) – the property of a crystal, externally, of retaining its shape under rotations or reflections (corresponding to the point group of the crystal), in terms of the arrangement of the atoms in crystal also with respect to lattice translations, (i.e., operations belonging to the space group of the crystal) (→ symmetry operation)

symmetry element – a set of points (point, line, or plane) according to which symmetry operations are performed. Symmetry elements are symmetry centres, rotational axes, screw axes, reflection planes, glide planes.

symmetry operation – a transformation of an object after which the original and transformed objects are geometrically and physically equivalent. These are rotation, reflection, inversion, and, for crystal structures, lattice translation, as well as combinations of these.

transformation matrix – a mathematical tool allowing to calculate the position coordinates of a point after transformation (rotation, reflection) when the coordinates of the initial position are known; in three-dimensional space it is a table (scheme) of nine members (elements, numbers) arranged in three rows and three columns related to three space coordinates. The numerical values of the members and their arrangement in the matrix can be used to express whether a given transformation is an inversion, a reflection or a rotation; the position of the reflection plane or rotation axis and, in the case of a rotation axis, the angle of rotation can be expressed.

transformation tensor – a mathematical tool derived from the transformation matrix. In contrast to it, for each element of the tensor, in addition to the numerical value, there is also a pair of vectors expressing the belonging to the coordinate axes in accordance with the rows and columns of the matrix.

translation group – the set of translation symmetry operations satisfying the group existence conditions. In lattices, these are translations that are, in vector form, integral linear combinations of the triple of basis vectors of the lattice.

translation, displacement – a transformation in which all points of an object are displaced equally.

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C. J. Bradley – A. P. Cracknell: *Mathematical theory of symmetry in solids*, Clarendon Press, Oxford 1972 and a factually complete list in the tables [34]