E. S. Fedorov

1853-1919

Among the scientists who in various ways paved the way for Laue's discovery and for Bragg's determination of crystal structures, there is one who occupies the most important place: E. S. Fedorov (1853–1919), the eminent Russian crystallographer. His most outstanding achievement is the derivation of the 230 symmetry space groups which now serve as the mathematical basis of structural analysis.

Already in his first excellent book, *The Elements of Configurations*, Fedorov clearly outlines the idea of this derivation. From his autobiography it is known that he started writing this book in 1879, at the age of 26, prior to his enrollment as a student at the Mining Institute (Gorny Institute).*

During the years 1881–1882 Fedorov gave many of his papers on 'the theory of crystal structures' before the St. Petersburg Mineralogical Society.

In 1883 the finished book was accepted for printing on the recommendation of A. V. Gadolin, member of the Academy, the well-known author who derived the 32 crystal classes. Nevertheless, the book was published only in 1885 in the form of the 21st volume of *Transactions of the Mineralogical Society* (*Zapiski Mineralogicheskogo Obshchestva*).

An important point, underlying the future derivation of space groups, is found on page 240 of this book. Proof of the theorem that 'every real point system is a system of corresponding points of stereohedra' is substantiated by the following specific remark by Fedorov: 'In the past, the definition of real point systems has been taken from Sohncke. But equally, this term is applicable also to an aggregate of other real systems where one is symmetrical with the other... If, for the purpose of differentiating, systems of points with symmetry planes are

* Son of an Army Engineer, Fedorov lost his father at an early age and had to attend a complete course at a military school. At 18 years he was a combat officer in Kiev but resigned from military duty after two years to devote himself to the 'Sturm und Drang' [storm and stress] which was characteristic of the progressive Russian youth of the sixties and seventies [19th century]. He then tried two higher institutes of learning, belonged to the revolutionary underground, vigorously participated in the publishing of the newspaper of the Revolutionary Organization, and spent several years abroad on business, and finally his fascination with crystallography led him in 1880 to the Mining Institute (Gorny Institute).

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called real double systems, then it is seen that the theorem just proved is applicable to simple as well as double systems.'[1]

In the following years, E. S. Fedorov systematically developed the studies of symmetry, the outcome of which was his 'Symmetry of real systems of configurations' with the complete derivation of space groups. Separate preprints of this work were published in 1890 and were sent to all his friends, including A. Schoenflies, but the complete 28th volume of the Transactions of the Mineralogical Society, which contained Fedorov's paper, was published in 1891.[2]

E. S. Fedorov himself comments on his work in the following words: 'A complete derivation of real point systems is given and a derivation of the possible forms of crystal structures is outlined. The systems of Sohncke are included among the others only as a special case and are called simple systems. Every group is rigorously determined by an algebraic equation.' [3]

As is generally known, Fedorov's derivation is very closely interrelated with the derivation of the same space groups which were almost simultaneously derived by the German mathematician, A. Schoenflies.

The first two papers by Schoenflies were published in 1888 and Fedorov's comments were as follows: 'The papers by Schoenflies, published in Göttingische Gelehrte Anzeigen, have come to my attention recently. It is with pleasure that I see a repetition of the important underlying features of my theory of crystal structures presented in these papers, although in a less developed form.' [4]

A year later Schoenflies published his paper describing 227 space groups. At that time Federov had already submitted his 'Symmetry of real systems of configurations' for publication. However, the final 230 space groups were not represented yet. As a result of the publication of the paper by Schoenflies, Federov requested that his preliminary Table of the derived 228 groups be recorded in the Minutes of the Meeting of the Mineralogical Society, held on 21 November 1889, and that it be compared with the results obtained by Schoenflies. Referring to the overall similarity of the results of these two derivations Fedorov commented: 'Nevertheless, such concordance is accidental and is dependent on the circumstance that Schoenflies neglected as many possible groups as he repeated in the derivation of identical groups.' [5] From this moment on the authors enter into a lively correspondence which is preserved partially in the Archives of E. S. Fedorov and was published in 1951.[6] A study of this correspondence reveals, step-by-step, the details of the path which lead the authors to one and the same final result.

The following is an excerpt from the book by S. A. Bogomolov [7] which gives a brief résumé of these letters.

'In his first letter of 14 December 1889, Schoenflies acknowledges that the Russian scientist has the priority in time.' * In his third letter, of 29 October 1890, he raises an objection to Fedorov's statement that groups V_8^d and V_9^g are identical [these groups coincide with V_d^3 according to the later classification by Schoenflies, the first edition (page 622) erroneously speaks of V_d^4] and to the omission of a group from each pair (5s) and (6s), (1h) and (2h) †, and could not clarify the later problems completely owing to a difference in classification. In his letter of 10 November 1890, Schoenflies completely acknowledges the validity of Fedorov's statements and also mentions the disagreement in the numbers of groups of the following symmetries:

$$V^h, C_4^v, C_3^v.$$

In a post card, dated 17 November 1890, he states that he is investigating the latter problem. The ninth letter, of 7 January 1891, concerns the problem of group (103a) [in the final compilation in *Zeitschr. f. Kristal.*, Vol. 24, it has the number (93a) given by Fedorov; afterwards Schoenflies called it T_d^6]. Schoenflies does not admit its existence, but in the thirteenth letter, of 17 March 1891, fully admits his error. The truth is that even Fedorov omitted this system in his book; he records it, however, in the list of errata.

This, then, is the way in which our scientists arrived at the whole set of 230 space groups.[8]

The well-known book by A. Schoenflies, *Kristallsysteme und Kristallstruktur,* was published in 1891. The author repeatedly refers to E. S. Fedorov, indicating his priority in many problems concerning theoretical crystallography.

For example: 'Die Notwendigkeit die Sohncke'sche Theorie so auszubilden, wie es durch die reine Strukturtheorie im engeren Sinn geschieht, wurde wohl zuerst von E. Fedorow betont.' [The necessity to expand Sohncke's theory as it is done in the narrower sense of pure structure theory proper was emphasized first by E. Fedorov.]

And further: 'Eine Schrift von Fedorow, welche eine vollständige Ableitung aller Raumgruppen und ihre Beziehung zur Kristallsymmetrie enthält, ist 1890 unter dem Titel *Symmetrie der regelmässigen*

* 'Die Priorität gebe ich Ihnen gern zu' [I gladly acknowledge your priority].

† 5s, 6s(fifth and sixth symmorphous)—Fedorov's classification of groups P_m and C_m; 1h and 2h (first and second hemisymmorphous)—groups P_c and C_c.

Systeme von Figuren in russischer Sprache erschienen.' [A book by Fedorov which contains a complete derivation of all space groups and their relation to crystal symmetry has been published in 1890 in Russian under the title *Symmetry of regular systems of configurations*.]

A comparison of these two papers—the one by E. S. Fedorov and the other by A. Schoenflies—clearly shows two principally different approaches by the two scientists: for Schoenflies it is just an interesting case of representation in the theory of groups, in particular infinite groups, which were being developed at that time; for Fedorov it is a means of studying real systems of configurations, the underlying feature of a crystal.

Fedorov found his results by deriving the only possible 230 types of basic design which underlie all natural crystals; accordingly, the most important part of his book are the 230 diagrams compiled in amazingly compact Plates. In 1894 these diagrams, slightly revised by Fedorov himself, were re-published in *Zeitschrift für Kristallographie* and in 1900 presented by Hilton in his well-known *Mathematical Crystallography* in English and in 1919, with certain revisions, by Niggli in *Geometrische Kristallographie des Diskontinuums*.* Fedorov's name is mentioned every time Hilton uses any part of his diagrams, Niggli however, omits it completely. The same omission in the presentation of Fedorov's diagrams appears in the Atlas by Astbury and Yardley (Lonsdale) and then also in the first edition of the *Internationale Tabellen* (1935). This error was corrected at our request only in the revised edition of the *International Tables* (1952).

In 1892 E. S. Fedorov published 'A Comparison of the Crystallographic Results of Mr. Schoenflies with mine'. ('Zusammenstellung der kristallographischen Resultate des Herrn Schoenflies und der meinigen') in *Zeitschrift für Kristallographie*. From this time on he starts an extensive correspondence with the founder of this journal, the well-known P. Groth, who also played an active role in preparing the way for Laue's discovery.

The letters from Groth, preserved in Fedorov's archives, and drafts of his own letters, 30 in number, cover a period of 25 years from 1891 to 1915. These letters show how highly Groth valued the work of the Russian crystallographer and how widely he publicized Fedorov's achievements abroad. The great interest of the German scientist in Fedorov's theory of the structure of crystals deserves special mention. 'I have carefully studied your manuscript *Theory of the Structure of*

* The compact diagrams of E. S. Fedorov, in most instances, show only one quadrant of the elementary cell. Hilton and Niggli have drawn out the quadrants for the complete cell.

Crystals and have prepared it for publication. The results are astonishing. However, I cannot raise any contradictions whatsoever', writes P. Groth in one of his letters, dated 26 February 1902.[9]

Thus, the fundamental geometrical rules of the structure of crystals were established and only the crystals themselves remained to be analyzed, i.e., by determination of the concrete picture of the distribution of atoms. The only way to conduct such an analysis at that time was the optical method and geometrical analysis with the aid of a goniometer. Fedorov became and remained to the very end of his life the most prominent specialist in the field of petrographic (optical) analysis of minerals; at the same time he was also very interested in the goniometric analysis of minerals. At an amazing speed he brought forth inventions which in themselves would have made his name immortal, i.e., the two-circle goniometer and the Fedorov universal stage which are the basic instruments of crystallographers and petrographers the world over.*

Fedorov and the students close to him collected enormous quantities of data from the measurements of all possible crystals; this material was systematized and published only a year after the death of the author as the monumental volume *Das Kristallreich*. From the geometry of crystals Fedorov derives conclusions about their internal structure, an idea taken up by Harker, Donnay, and others 40 years later.

All of this was complicated work requiring long periods of time, a factor to which Fedorov's searching geometrical mind could not reconcile itself. He itemized the 230 groups and established the theory of *Stereohedra* and *planigons*, i.e., division of three- and two-dimensional space into geometrically identical cells which continuously and without gaps fill the space. Despite the importance of the purely geometrical results (for this work Fedorov was elected to the Bavarian Academy), they seem at the present time to be a deviation from the correct path, a deviation caused by the negative attitude of the Petersburg chemists whose authority Fedorov accepted and which led him to study electrolytic dissociation, ions and the coordination nature of matter. Fedorov passively accepted the concept of the molecule as the final stage of matter and considered, in principle, that the ultimate aim of crystallography should be the classification of all possible

* All of Fedorov's outstanding discoveries and inventions, including the derivation of the 230 groups, date to the years 1895–6, a time when he was in great financial difficulties. Although he was one of the best students graduating from the Gorny Institute, he was not permitted to remain there; for many years he worked in the office of the Committee of Geology, making field trips in the summer under rather strenuous conditions, so as to enable him to work more intensely in the winter.

'receptacles' for this finite unit. Desiring to accommodate the exact sciences, namely chemistry, he even attempted to consider the 103 asymmorphous groups, included among the 230 groups, as merely theoretical.

Fedorov acquires world-wide fame which he deserves. He is granted the chair at the St. Peter's (now Timiriazev) Academy in Moscow and triumphantly undertakes the journey to the center of western crystallography, which at that time was located in Munich, to meet Groth. Soon afterwards he combines his professorship in Moscow with a professorship in St. Petersburg, where he travels twice a week during the academic year. In 1905 Fedorov becomes the first elected director of his alma mater, the Gorny Institute (Mining Institute) and permanently moves to St. Petersburg. A large group of scientists gather around him, many from abroad (Barker, England; Duparc, Switzerland, and others). Fedorov is the founder of the *Zapiski Gornogo Instituta* (*Transactions of the Mining Institute*), where his numerous papers are published.

The impression of Laue's discovery on Fedorov is illustrated by his letter to the well known revolutionist and scientist N. A. Morozov (1854–1946) which describes this portentous scientific event.

2 October 1912

Dear Nikolai Aleksandrovich,

You conclude your letter by saying that the human eye shall never see atoms. You wrote this approximately at the time when people saw atoms with their own eyes; if not the atoms themselves, then the photographic images caused by them.

How does this come about? Very simply really. With a dividing machine we can draw a thousand parallel lines on glass within the range of a millimeter; this is a diffraction grating which gives a series of magnificent diffraction spectra and the number of divisions on glass is readily determined from these spectra.

A thin crystalline plate in itself represents two intersecting diffraction gratings where the lines are not a thousandth but a ten-millionth part of a millimeter apart.

Light waves are too coarse for obtaining diffraction spectra. But there are the X-rays with a wavelength millions of times shorter than that of light waves.

Several weeks ago in Röntgen's laboratory such diffraction spectra of atoms were photographed by means of X-rays. Indirectly people were able to see the immediate effect brought about by atoms, that is, in principle, they saw the atoms with their own eyes.

For us crystallographers this discovery is of prime importance because now, for the first time, we can have a clear picture of that on which we have but theoretically placed the structure of crystals and on which the analysis of crystals is based.

I am sure you will be very pleased about this news.

With the very best regards from me and the family.

E. Fedorov

(Archives of the Academy of Sciences USSR, Leningrad, 543, 4, No. 1952). [10]

Already Bragg's earliest work on the analysis of crystal structures by means of X-rays aroused Fedorov's lively response.

In his paper 'The first experimental demonstration of the asymmorphous real system' Fedorov emphasized that the determined structures belong to the systems of true point systems derived by him twenty-two years earlier. This paper starts with the following passages:

'The application of X-rays has enabled W. L. Bragg (and his father) to draw conclusions which are of the utmost importance to the theory of crystal structures. Some of these conclusions are unexpected, at least in the sense that in the points of real systems one expected to find centers of chemical particles, while the experiments of this scientist permit one to draw the conclusion that these are the centers of atoms. As a result, in substances of the simplest chemical composition special real point systems are obtained and the symmetry centers are occupied by separate atoms as though the atoms themselves have a high symmetry.' [11]

And it is stated further that 'the distribution of Fe and S atoms in pyrites confirms the asymmorphous real point group (25).'*

In conclusion Fedorov explains his derivation of the space groups and how the scientific circles of that era underestimated its value.

'Somehow I did not think that I would live to see the day when the distribution of atoms as I predicted it in my papers would actually be

* Group Pa 3 in the contemporary classification; this is one of the 103 which were previously considered as 'imaginary' Fedorov systems, in the same sense as $\sqrt{-1}$ is imaginary. Fedorov is very pleased to acknowledge this fact and soon afterwards, together with Groth, starts campaigning for the ionic-coordination-nature of crystalline substances rendering his imaginary systems more real than the non-imaginary symmorphous ones.

determined. In a letter to Prof. Groth I stated that a detailed analysis of the systems predicted in these papers could, perhaps, be realized only after 100 years.

'In 1891 I submitted the Russian work which predicted the possible atomic distribution or, rather, the laws of such distributions, to the St. Petersburg Academy of Sciences in competing for the Makarev prize of that year; neither did it receive the prize itself, nor was it found worthy of a mention, and was not even included in the lengthy official list of papers submitted on this occasion.' [12]

In addition to this first printed declaration E. S. Fedorov published a series of papers concerning Bragg's conclusions. In them the eminent crystallographer discusses the results obtained, attempting to bring them into harmony with his previously advanced views of crystal structure. The following is as complete a list as possible of these papers:

'On the structure of diamond crystals according to Bragg' (1914).

'The first steps on the path to the determination of the distribution of atoms in crystals' (1915).

'Results of the first stage in the experimental investigation of crystal structures' (1916).

'The basic law of crystal chemistry' (1916).

'The chemical aspect of crystal structures' (1916).

An interesting description of the acquaintance of E. S. Fedorov with Bragg's work can be found in the letters preserved in the Archives and in the now published letters of the well-known British crystallographer T. Barker (1881–1931). In 1908–1909 Barker came to St. Petersburg to study Fedorov's methods of analyzing crystals. E. S. Fedorov warmheartedly greeted the young scientist, installed him in his laboratory, and soon enlisted his services in the compilation of the Tables of Crystal Chemical Analysis *Das Kristallreich* (together with his students B. P. Orelkin, V. I. Sokolov, D. N. Artem'ev). After his return to England Barker continued his work on these Tables in Oxford, assisted Fedorov in proofreading the prints of *The Realm of Crystals,* and enthusiastically spread the word among the British scholars about the achievements of the Russian crystallographer.

His letters to Fedorov contain much interesting information about the scientific events of that era. An amusing misunderstanding which occurred among the British scientists is very vividly described in one of Barker's letters (15 November 1912): 'Sir Oliver Lodge in a lecture before the Chemical Society on recent developments of Natural Science stated some sentences which show that perusal of Tutton's second article had given him the impression that the Röntgen ray work and crystallochemical analysis were the same discovery!!

'On account of this I wrote my article in order to show that the credit of the method of 'crystallochemical analysis' belongs to you alone, and that no one else has taken any part in the matter.' [13]

Barker's letter of 7 January 1914 describes the impression left by Fedorov's paper 'The first experimental demonstration of the asymmorphous real system': *

'I have been busy for the last two months writing the annual report on Crystallography and Mineralogy for the Chemical Society... I have made a special feature in the report of your work on the correct setting—as far as it is possible to write about such a subject for chemists who have little knowledge of crystallography—and the Röntgen-ray work on crystals. The latter is causing somewhat of a sensation in the scientific world here.

'I do not know whether you are acquainted with the recent developments contributed by the two Braggs. If you are interested in the work I will ask them to send you copies of their papers.' [14]

E. S. Fedorov, after having received the reprints from W. L. Bragg, writes as follows: [15]

St. Petersburg, January 15/25, 1914

Dear Mr. Bragg,

Thank you for sending your valued papers. I hope that you will soon receive 'Reguläre Plan- und Raumtheilung' [The regular planar and spatial divisions].

Respectfully,
E. S. Fedorov

The Archives of Fedorov contain two short letters from W. L. Bragg. The first acknowledges the receipt of the monograph 'Reguläre Plan- und Raumtheilung'.

The text of the second letter is as follows: [16]

* This paper was sent to Barker, obviously, in the form of proofs or a manuscript (judging by the dates).

Trinity College, Cambridge
17 February 1914

Dear Sir,

Many thanks for your letter with the suggestions as to ways of depicting a space-arrangement of points. I have considered your method with great interest, because I find it so very difficult to describe a structure [in words] * when I have worked it out properly. If there is already a recognized way of denoting the situations of the atoms in the crystal, I would be very glad if you would tell me of it.

I will try to depict the great lot of crystals I do in your way, though they may be too complicated.

Yours sincerely,
W. L. Bragg

In conclusion we should like to quote the comments on E. S. Fedorov recently made by W. L. Bragg in his letter, dated 14 May 1958, to G. I. Kovan'ko, published in a paper by the latter:

'Fedorov was then to me an almost legendary being who had worked out the 230 crystal classes.

'Few people at that time were interested in crystallography. Such interest as did exist was in the outer forms of crystals, not in their inner structure. When I started analysing crystals with X-rays, I knew nothing at all about their geometry. It was wonderful for us to discover that great men like Fedorov and Barlow, whom I also got to know, had studied the inner geometry of crystals and provided a sure theoretical basis for our work.' [15]

I. I. Shafranovskii and N. V. Belov

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Artur Schoenflies

1853-1928

Schoenflies was born in the small district town of Landsberg an der Warte, then belonging to Brandenburg, now in Polish territory. He began studying mathematics in Berlin just after the war in 1870 and obtained his Ph. D. in March 1877. His main teacher was E. E. Kummer, famous for his research in geometry. The next six years Schoenflies spent as high-school teacher, the first two in Berlin, the others in Colmar in Alsace. He managed to continue research in this period along the lines begun in his thesis, combining in it geometrical inspection methods with those of analytical, synthetic and projective geometry. The success of his work led to his becoming Privatdozent

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