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GENERALIZED ANTISYMMETRY

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Abstract—A. V. Shubnikov introduced the antisymmetry concept as the essential extension of the classical symmetry. For the later decades antisymmetry found numerous applications in the practice of natural sciences and it was generalized in the form of the multiple antisymmetry, colour symmetry, colour antisymmetry, cryptosymmetry, *P*-symmetry, etc. It is given the reveiw of the developement of antisymmetry and its generalizations.

SECTION 1

Drawing attention to the rich and varied contribution made by A. V. Shubnikov to extending the Fedorov theory of symmetry, the present-day crystallographers are fair in their judgements that the discovery of antisymmetry is the height of his scientific work in this field (see, for example, Ref. [1, p. 2]). It does not really matter at this point who was the first to introduce the concept of antisymmetry (rather too much prominence was given to the truth about this problem in the sixties). But it is of importance that it was Shubnikov who was the first to pay attention to the applied value of the idea itself consisting in enriching the geometric symmetry by adding changes in a physical property. The head of the Soviet school of crystallography always believed that further improvement in the theory of symmetry is worth while only in cases when it works or will work in practice of natural sciences in future [1, p. 76]. He has created a fundamentally new trend to the knowledge of which in our time is necessary for every research crystallographer (the concepts of the Shubnikov antisymmetry [2] and the Belov colour symmetry [3] have become chrestomathic: they have formed a part of the Master's degree examination program and have been covered in the encyclopedic book [4]). The development of antisymmetry, its generalizations and applications are presented in monographs [5–9], review articles [10–14], in Chap. 9 of the noteworthy book [15] and the author does not quote these below.

The paper suggested cannot claim to cover all the literature on antisymmetry, its extensions or, for example, its geometrical applications as the Kishinev geometricians alone, apart from the other authors, were written on these problems, more than 100 works cited in the above-mentioned books and articles [5–15].

SECTION 2

The Shubnikov centenary coincides with the sixtieth anniversary of the origin of the antisymmetry conception in the depths of the classical symmetry. The discovery of the X-ray diffraction early in the twentieth century and the generation of structural analysis of crystals gave wide practical vent to the Fedorov theory almost concurrent with the development of the general theory of the n-dimensional space groups G_n by the German mathematicians. Hence it was not by chance that in the twenties crystallographers markedly put more emphasis on detailed elaboration of the symmetry theory stimulating the emergence of a number of works (mostly by German and Swiss scientists) containing the description of "small" crystallograph groups: 31 band groups G_{321}, 80 layer groups G_{32} and 75 cylinder (rod) groups G_{31} derived as subgroups of 230 Fedorov groups G_3 characterized by the presence of specific (invariant) planes and straight lines.† Heesch and

†Bohm's symbols [16] used here for characterizing different categories of crystallographic symmetry groups are the following: G_r—Fedorov r-dimensional groups (infinite in r dimensions); G_{rt}—their subgroups with the invariant t-dimensional subspace; $G_{rs\ldots t}$— their subgroups with a set of inserted into one another invariant subspaces of $s, \ldots, t$ $(r > s > \cdots > t)$ dimensionalities; the symbols $G^l_{r\ldots}$, $G^p_{r\ldots}$ and $G^{l,p}_{r\ldots}$ used for generalizing the $G_{r\ldots}$ category with l-fold antisymmetry, with p-colour symmetry and so on were suggested by Koptsik [10].

Shubnikov were deeply impressed by the idea proposed in 1927 by Speiser for interpreting the G_{321} group and practically realized in two years by Weber in relation to the G_{32} group to represent the figure (band, layer) being plane from two sides on the one-side plane of the drawing using black and white colours. As a result they both in different ways and at different times, but independently of each other, arrived at the distinct definition of the antisymmetry concept.

In 1930 mathematician Heesch passed immediately from the derivation of 80 layer groups G_{32} (as black–white two-dimensional groups G_2^1) starting directly from 17 two-dimensional Fedorov groups G_2 to the derivation of four-dimensional "hyperlayer" groups G_{43} (in the form of black–white three-dimensional groups G_3^1) from 230 Fedorov groups G_3; concurrently he derived 122 four-dimensional point goups G_{430} (as black–white three-dimensional groups G_{30}^1) from 32 classes of G_{30}. Unlike Heesch who was interested basically in the problem of multidimensional generalization of classical groups (owing to which fact his work was not noted by crystallographers in proper time), Shubnikov was able to formulate the antisymmetry concept *only as basic extension* of the classical symmetry (due to the addition of changes of physical property) and thereby essentially proceeded with the development of the idea (though in 15 years time): Heesch had solved the particular case of the problem, going back to Bieberbach and Frobenius, but Shubnikov had formed the basis for radically new range of problems.

As is known the essence of antisymmetry consists in ascribing the sing "+" or "−" (in an arbitrary physical meaning it may be a sign of a charge, black or white colour, etc.) to any point of the figure, following which the isometric transformation of the figure is defined as the transformation of symmetry or antisymmetry when it transfers the figure points to the points with the same sign or to the points with the opposite sign respectively. The symmetry transformations of sign bearing figures do not differ from classical ones and every antisymmetry transformation is the product of the symmetry transformation by anti-identical one (operation of a sign change).

Symmetry and antisymmetry groups fall into three types depending on the presence of antisymmetry transformations in them: (1) polar (single-coloured) or generating groups (Π), that is the same classical symmetry groups; (2) neutral (grey) or senior groups (C) obtained by doubling the classical ones due to the addition of the anti-identical transformation; (3) groups of mixed polarity (black–white) or junior ones (M) containing antisymmetry transformations without the anti-identical one. The derivation of the groups of the last type was non-trivial. Shubnikov found them by replacing in turns formative elements of a classical group with the corresponding antisymmetry transformations. After revealing similar groups and removing unnecessary ones (there can be senior groups among them as well), 58 different junior groups are obtained from 32 crystal classes G_{30}, and all in all the generalized groups G_{30}^1 are found to be $32\Pi + 32C + 58M = 122$, as also are the findings of Heesch.

The Shubnikov method for the derivation of junior groups from the generating ones was theoretically substantiated by the present author in 1953 and was significantly supplemented by Belov in 1954 and by Indenbom and Niggli in 1959 [17–20]. In 1953–1954 the present author and Belov with their followers using fundamentally different (approaching) ways made two independent derivations of Shubnikov space groups G_3^1; they obtained $230\Pi + 230C + 1191M = 1651$ groups G_3^1 from 230 Fedorov groups G_3 (methodically new derivation of Shubnikov groups was made later on by Koptsik [5]).

Similarly from 17 groups G_2 one derives $17 + 17 + 46 = 80$ two-dimensional Shubnikov groups G_2^1 (describing 80 layer groups G_{32} when giving an interpretation of the signs "+" and "−" from the standpoint of geometry), from 75 groups G_{31} and 80 groups G_{32} one derives, respectively 394 $(= 75 + 75 + 244)$ groups G_{31}^1 and 528 $(= 80 + 80 + 368)$ groups G_{32}^1, etc. (see Tables 1 and 2).

The appearance of antisymmetry applications in X-ray structural analysis [21] and in crystal physics [22] in 1952–1956 started its triumphal procession and stimulated its further extensions, such as multiple antisymmetry and colour symmetry in the first place. Let us follow their genesis and development which proved to be particularly intensive over the last 15 years of Shubnikov's life.

SECTION 3

The idea of multiple antisymmetry (ascribing some qualitatively different signs to the figure points) appeared naturally from a wide variety of sign interpretations in terms of physics; such

Table 1. Values of N_l for different categories

l	G^l_o	G^l_{10}	G^l_{210}	G^l_{3210}	G^l_{20}	G^l_{320}	G^l_{30}	G^l_1	G^l_{21}	G^l_{321}	G^l_{31}	G^l_2	G^l_{32}	G^l_3
0	1	2	5	16	10	31	32	2	7	31	75	17	80	230
1	0	1	6	35	11	63	58	3	17	117	244	46	368	1191
2	0	0	6	84	9	138	116	3	42	522	945	167	2312	9511
3	0	0	0	168	0	252	196	0	84	2520	4074	700	18396	109139
4	0	0	0	0	0	0	0	0	0	10080	15120	2520	164640	1640955
5	0	0	0	0	0	0	0	0	0	0	0	0	1249920	28331520
6	0	0	0	0	0	0	0	0	0	0	0	0	0	419973120

Table 2. Values of P_l for different categories

l	G^l_o	G^l_{10}	G^l_{210}	G^l_{3210}	G^l_{20}	G^l_{320}	G^l_{30}	G^l_1	G^l_{21}	G^l_{321}	G^l_{31}	G^l_2	G^l_{32}	G^l_3
0	1	2	5	16	10	31	32	2	7	31	75	17	80	230
1	2	5	16	67	31	125	122	7	31	179	394	80	528	1651
2	5	16	67	374	125	671	624	31	179	1379	2784	528	4920	17807
3	16	67	374	2825	671	4885	4362	179	1379	14419	27044	4920	64924	287658
4	67	374	2825	29212	4885	48907	42244	1379	14419	207187	366300	64924	1214800	6880800
5	374	2825	29212	417199	48907	679985	572014	14419	207187	4127123	6973228	1214800	32242516	240900462

conception was expressed by Shubnikov in his report as early as 1944 (but he did not return to it in his 1951 monograph). Ten years later under the influence of the appearance of the first applications of antisymmetry the Kishinev geometricians independently started developing that concept known by the name antisymmetry of different kinds [23].

The essence of this extension of the antisymmetry consists in ascribing to the figure points the signs "+" or "−" in different meanings and in introducing the antisymmetry of the kind 1, the kind 2, the kind (1, 2), etc. according to the change of only the first sign, only the second sign, the first and the second signs simultaneously etc., at isometric transformations of the figure; altogether at l signs there are $2^l - 1$ kinds of the antisymmetry. The classification of groups becomes rather complicated: according to the presence of transformation of the antisymmetry of either kind (anti-identical ones, specifically) in the group the groups are divided into types and forms, i.e. they can be senior or junior of the same kind [of the kind 1, of the kind 2, of the kind (1, 2)—this is denoted by a symbol C_1 or M_1, C_2 or M_2, C_{12} or M_{12}], senior of two or more kinds, (for instance, C_1C_2), junior of two or more kinds (M_1M_2 etc.) or senior of one and junior of other kinds (C_1M_2, C_2M_1, etc.). Thus at $l = 2$ there are 6 types of the groups (Π, C, M, C^2, M^2, CM) subdivided into 12 forms (they are interpreted by figures in Ref. [7, 11]); when $l > 2$ the classification becomes even more cumbersome. The Kishinev geometricians have produced a full scheme of "small" crystallographic groups $G^l_{r\ldots}$ and developed various techniques for deriving radically new, i.e. non-trivially found groups (of the M^m type at $m > 1$). The derivation of groups of C^k types ($1 \leqslant k \leqslant l$) is trivial, and it is easy to derive the groups C^kM^m ($1 \leqslant k \leqslant l - m$) if the groups of the m-fold symmetry have already been found for $m < l$. Denoting a number of radically new groups (of the M^l type at $l \geqslant 1$) by N_l (Table 1), and a number of various groups $G^l_{r\ldots}$ of the given category by P_l (Table 2) ($P_0 = N_0$ is the number of various classical groups $G_{r\ldots}$) we express the number P_l in the terms of known N_0, $N_1, \ldots, N_l$ using a simple formula: $P_1 = 2N_0 + N_1$, $P_2 = 7N_0 + 6N_1 + N_2$, etc. (for more detail see Ref. [7 Chap. II]); for every category $N_l = 0$ at rather high values of l and hence the problem is totally surveyed if all $N_m > 0$ have already been found.

The interpretation of signs "+" or "−" in different meanings can be both physical (for example, the first sign is black or white colour and the second one is the charge sign) as well as geometrical (l signs "+" or "−" are interpreted as coordinate signs in l additional dimensions) or can be partially physical, partially geometrical (say, for the two-dimensional figure the first sign is the sign of a coordinate in the third dimension and the others have physical meaning). It gives the possibility by extending the idea of Weber and Heesch to consider the two-dimensional two-fold Shubnikov groups G^2_2 both as models of layer groups G^1_{32} with simple antisymmetry and as models of four-dimensional ornament symmetry groups G_{432} (in each of three cases 528 groups are distinguished); in the same manner the one-dimensional three-fold Shubnikov groups G^3_1 serve as models of border G^2_{21}, band G^1_{321} and hyperband G_{4321} groups (all four cases yield 179 groups each). Such comparison between the categories $G^l_{2\ldots}$ and $G^{l-1}_{32\ldots}$ served as a check on the solution and helped to complete the scheme of "small" groups $G^l_{r\ldots}$ for non-trivial cases; at the same time until recently, the non-trivial derivation of multiple Shubnikov space groups G^l_3 yielded results only up to $l = 2$ [7–13].

Let us note that a peculiar version of multiple antisymmetry was suggested in 1957 by Mackay [24] who stopped his investigations in connection with the publication of the work of the present author on the antisymmetry of different kinds (see Refs [7, 11, 12] for comments).

The theory of simple and multiple antisymmetry is actually completed, the only thing left is to develop new methodical techniques for the purpose of its further incorporation into natural sciences. Such new techniques were developed recently by Yugoslav mathematician Jablan [25] who introduced the concept of "antisymmetry characteristic" which gave his the possibility to complete the scheme of groups G^l_3 (being non-trivial up to $l = 6$) not accomplished by the present author in the seventies.

In Tables 1 and 2 composed according to the scheme of Table 1 and 2 of paper [11] and Tables III_8 and III_9 of book [7] the values of $N_l (0 \leqslant l \leqslant 6)$ and $P_l (0 \leqslant l \leqslant 5)$ are given for all the categories of the crystallographic groups $G^l_{r\ldots}$. At this point the numbers N_3, N_4, N_5 for G^l_3 were brought to the author's attention by Jablan, and the numbers P_3, P_4 and P_5 were found by Palistrant (the other numbers are in conformity with those from work [7] other than that of P_4 obtained when correcting its calculations for the cylinder groups G^l_{31}).

SECTION 4

If in the antisymmetry theory the emphasis is layed not on the contrast of two features (as it was done by Shubnikov comparing them with the right side and the left side of figures, with the face side and the back side of a fabric, etc.), but on special reference to their distinction and alternation within the scope of nature generality, it is not difficult to be led to the p-phase symmetry extending the antisymmetry due to ascribing to the points any number of p different homogeneous features (for example, colours) transforming one into another according to certain law (say, alternating cyclically) at isometric transformations of the figure. Just this involves the pithiness of Belov's transfer from two-colour interpretation of the antisymmetry to the multi-colour symmetry expressed in the year 1955 [17] and developed then in his subsequent papers.

Belov and Tarkhova [3] presented the two-dimensional groups G_2^p $(p > 2)$ of p-colour symmetry by using colour mosaics interpreting them as the "generalized projections" of some Fedorov space groups G_3 (retaining the invariant vector of the main translation **c**: different colours correspond to the levels alternating every other $(1/p)\mathbf{c}$ over the projection plane and recurring every other **c**). Separating the groups G_3 with vertical screw axes we obtain 15 groups $G_2^p (p = 3, 4, 6)$ denoted in Ref. [3] by international symbols of the projecting groups.

The method of the derivation of Belov colour symmetry groups from the classical ones geometrically coinciding with the former was suggested by Indenbom and Niggli who independently of each other noticed the connection of the colour groups with one-dimensional complex representations of the symmetry groups [19, 20]. Using this connection Indenbom, Belov and Neronova derived from the point groups G_{30} all the 18 eigencolour groups G_{30}^p $(p = 3, 4, 6)$ or Belov classes interpreting them by colour figures [26].

The synthesis of the concepts of the colour symmetry and the multiple antisymmetry has resulted in the concept of the colour antisymmetry introduced in different ways by Pawley and by Neronova with Belov [27, 28]. Pawley received two-dimensional groups $G_2^{p'}$ of the colour antisymmetry by the "generalized projecting" of the Fedorov groups G_3 converting the translation vector **c** into itself or into $-\mathbf{c}$). The Neronova–Belov groups $G_2^{1,p}$ of the colour antisymmetry appeared as "generalized projections" of the Shubnikov group G_3^1 with the invariant vector **c**; here unlike the Pawley groups colours and signs can be heterogeneous from the point of view of physics.

Palistrant specified the concept of the colour symmetry and the Neronova–Belov colour antisymmetry having extended the latter to the colour antisymmetry of different kinds [29]. Using for checking the connection between the layer groups $G_{32}^{l-1,p}$ and the two-dimensional groups $G_2^{l,p}$, between the band groups $G_{321}^{l-1,p}$ and the border groups $G_{21}^{l,p}$ and the like via the geometric interpretation of the first sign in the two-dimensional groups (cf. the connection between G_{32}^{l-1} and G_2^l and the like above) the Kishinev geometricians accomplished the scheme of "small" crystallographic groups $G_{r\ldots}^{l,p}$ and derived the Belov space groups G_3^p (basically by means of the Shubnikov method of formative elements substitution). The summary of all eigencolour three-dimensional groups according to the categories at $p = 3, 4, 6$ is as follows: 817 G_3^p, 203 G_{32}^p, 196 G_{31}^p, 18G_{30}^p, 60 G_{321}^p and 15 G_{320}^p (G_{310}^p) [8, 13].

The works of foreign scientists on cryptosymmetry connected with the Indenbom–Niggli method of representations play an impressive part in further extension of the concepts of Shubnikov and Belov. Thus, Niggli and Wondratschek distinguish between the groups of the simple cryptosymmetry derived through irreducible representations of the classical (generating) groups [30] and the groups of the multiple cryptosymmetry derived by superposing some irreducible representations on the generating group. This restriction of the simple cryptosymmetry (apparently for purely methodical reasons) used to reduce slightly the scope for its applications: statement of the problem from the point of view of physics (for example, the Naish techniques for the symmetry of non-collinear magnetics [31]) demands quite often wider interpretation of the cryptosymmetry. Such an interpretation is presented by Wittke in Ref. [32] where the cryptosymmetry groups are obtained by searching for all the representations of the generating group and thus the problem is reduced to revealing its normal subgroups. A more delicate approach to the presentation of the cryptosymmetry groups (the derivation of colour groups by revealing all the subgroups of the generating group) was suggested by Van der Waerden and Burckhardt [33].

SECTION 5

While in investigations on the simple and multiple antisymmetry methodical attention was given to the classification of groups according to their forms and types, all first works on the colour symmetry and the cryptosymmetry were dedicated to eigencolour (junior) groups. The "colour" language and predilection for the method of representations and characters prevented to notice that even the Belov p-colour (cyclic) symmetry at the composite number p provided examples of "partially grey" groups being intermediate between "grey" (senior) and eigencolour groups. General theory and complete classification of groups of the colour symmetry and the cryptosymmetry are kept in the scheme for P-symmetry. The P-symmetry coinciding essentially with the cryptosymmetry by Wittke differs from it in community of the problem statement and encloses all the group types in the previous generalizations of the antisymmetry (its scheme does not include the Wittke–Garrido polychromatic symmetry [34] and the Bienenstock–Ewald complex symmetry [35]).

Let us state briefly the essence of the P-symmetry. We ascribe at least one of indexes $i = 1, 2, \ldots, p$ to each point of the figure and then fix some group P of permutations of these indexes. The isometric transformation of the figure mapping any point with the index i onto the point with the index k_i in such a way that the permutation

$$\begin{pmatrix} 1, 2 \ldots p \\ k_1 k_2 \ldots k_p \end{pmatrix}$$

belongs to P, is termed the P-symmetry transformation; the P-symmetry transformations decompose naturally into the symmetry transformations and the permutations from P. The P-symmetry transformations of the figure form the G group, the symmetry transformations entering into them form its generating groups, and the indexes permutations form the P_1 group; at $P_1 = P$ the group G is defined as the group of complete P-symmetry. Every such group can be derived from the generating group S by searching in S and P for normal subgroups H and Q for which there is isomorphism of factor-groups S/H and P/Q, by paired multiplication of the cosets adequate in isomorphism and by joining the products received (for the primary theorem see Refs [8–12]). The cases when $Q = P$, $Q = e$ and $e \subset Q \subset P$ make it possible to divide the groups into senior, junior and middle ones; at $Q = e$ (the group G is junior, i.e. eigencolour) the isomorphism of S/H to P results in homomorphism of S to P with H nucleus or the representation of the S group (cf. the Indenbom–Niggli method).

In the scheme of the P-symmetry the Belov colour symmetry (p-symmetry) corresponds to the cyclic group $P = \{(1, 2, \ldots, p)\}$, the Shubnikov antisymmetry is the 2-symmetry, the antisymmetry of different kinds is the $(2, \ldots, 2)$-symmetry, the Neronova–Belov colour antisymmetry is the $(p, 2)$-symmetry, and the Pawley colour antisymmetry is defined as the (p')-symmetry and corresponds to a dihedron group $P = \{(1 \ldots p)\ (\bar{p} \ldots \bar{1}),\ (1\bar{1}) \ldots (p\bar{p})\}$ with $2p$ transformed features (p "positive" i and p "negative" $\bar{i}$). The P group is clearly interpreted by vertices permutations at the symmetry of an oriented regular p-gon in the case of the p-symmetry and of a non-oriented equiangular-semiregular $2p$-gon in the case of the (p')-symmetry.

Three main principles of the classification are developed for crystallographic P-symmetries (18 groups P isomorphic to 32 point groups G_{30}): (1) group-abstract principle reflected in the Wittke cryptosymmetry and making it possible to distinguish between 18 P-symmetries, 139 junior point groups; (2) group-concrete principle (as to the structure of permutation groups) reflecting the Van der Waerden–Burckhardt method and making it possible to distinguish between 45 P-symmetries, 212 junior point groups and (3) geometric principle induced by the Naish techniques of magnetic symmetry making it possible to distinguish between 32 crystallographic P-symmetries (geometrically interpreted exactly as 32 G_{30}) and 566 junior point groups [36].

The number summary of the three-dimensional crystallographic groups (the Belov junior groups) of the p-symmetry at $p = 3, 4, 6$ is given above [at the end of item (4)], the similar summary of the junior (Pawley) groups of the (p')-symmetry made by Palistrant is as follows: 2212 $G_3^{p'}$, 471 $G_{32}^{p'}$, 290 $G_{31}^{p'}$, 23 $G_{30}^{p'}$, 96 $G_{321}^{p'}$ and 19 $G_{320}^{p'}$ ($G_{310}^{p'}$) [9].

The other extensions of the colour symmetry not included into the scheme of the P-symmetry (including the Q-symmetry and the W-symmetry) are interpreted in the article [37] and the monographs [8, 9]. Let us say some words about them.

The Koptsik–Kotsev W-symmetry [38] reflecting the symmetry of a real crystal in which (unlike the P-symmetry) the law of feature variation combines with the geometric transformation depending on points selection has covered the Wittke–Garrido and the Bienenstock–Ewald generalizations [34, 35] but it requires more complicated mathematical techniques—groups wreath product. The general theory is not yet accomplished; the attempt to classify completed the W-symmetry groups is given in Ref. [9].

On the other hand, the Q-symmetry techniques suggested by Koptsik and his followers under the influence of the Tavger–Zaitsev magnetic symmetry description [22] in which (also unlike the P-symmetry techniques) the geometric transformation component acts both on the points and on the features bearing not scalar but vector or tensor nature) was developed in detail by Lungu and defined as $\bar{P}$-symmetry [40, 9].

SECTION 6

There is no possibility in the present paper to dwell either upon geometrical applications of the antisymmetry and its generalizations—investigations of the similarity symmetry, the multidimensional symmetry, etc. or upon the examination of non-crystallographic P-symmetries—they are covered in special surveys and monographs of the author [8, 9, 13, 14]. There is even less possibility here to dwell upon large physical and crystalographic applications of the generalized antisymmetry. It is of delight to point out that all the new ideas in the symmetry investigations arising in our century from the requirements of natural sciences and the curiosity of pure mathematicians are closely interwoven and encourage the development of each other.

How deeply right Shubnikov was having said more than forty years ago [1, p. 91]: "It is clear for us that the symmetry theory is far from being considered as an accomplished field of knowledge; it will live and develop together with science as a whole, with natural sciences and their constituent, the crystallography"!

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