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Junior spatial groups of (22$\underline{1}$)-symmetry

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Abstract. The connection between junior groups of three independent kinds of antisymmetry transformations and junior groups of (22$\underline{1}$)-symmetry, derived from space Fedorov groups was established. This connection allowed us to find all these groups.

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I. The problem of generalization of 230 space Fedorov groups with 32 crystallographic P-symmetries has a great theoretic and applied significance when receiving junior groups of these P-symmetries we assign indices to points of the space. By means of adequate physical explanation of these indices the junior groups of these P-symmetries coincide with the space groups of magnetic symmetry of crystals. On other hand, by these groups it is possible to model all various symmetry groups of the six-dimensional Euclidean space which keep invariant a three-dimensional plane in this space, i.e. groups of the category G_{63} [1].

The most point of the problem of derivation of junior groups from 230 space Fedorov groups for 32 crystallographic P-symmetries was solved by Kishinev geometricians [1, 2]. To finish this problem it remains to receive only junior space groups of (22$\underline{1}$)-symmetry. This article is devoted to the resolving of this extensive problem.

II. The symbol 22$\underline{1}$ is the symbol of thesenior space point group of symmetry and antisymmetry generated by rotations around three pairwise orthogonal two-fold rotational axes and by antiidentical transformation $\underline{1}$. One of the 32 crystallographic P-symmetries, modeling the symmetry group of a rectangular parallelepiped, i.e. the symmetry group mmm, generated by reflections in three pairwise orthogonal planes, is denoted by this symbol ($\underline{1}$ is interpreted as the reflection in a point, i.e. as an inversion) [3].

The groups mmm and $E_3 = \{\underline{1}\} \times \{1'\} \times \{^*1\}$ are isomorphic, where the group E_3 is the direct product of three groups of order 2, generated by antiidentical transformations of the kind 1, kind 2 and kind 3, respectively. The existence of such isomorphism between groups 22$\underline{1}$ and E_3 makes it possible to reduce the problem of searching for junior space groups of (22$\underline{1}$)-symmetry to the problem of searching for junior space groups of three-fold antisymmetry. Thus, to resolve the problem we need only junior groups of three independent kinds (i.e. groups of the type M^3), isomorphic to Fedorov groups.

To find these groups it is enough to know the number q of independent generators of Fedorov group by the change of which for respective transformations of antisymmetry of one kind we receive only junior groups. Then the initial group generates groups of the type M^l only when $l \leq q$. Such groups are derived from classic ones by means of the Shubnikov–Zamorzaev method: l or more symmetry transformations in the system of generators of Fedorov group are replaced with respective transformations of antisymmetry of different kinds, among which l kinds are independent [4].

To apply this method it is convenient to use the catalogue of Fedorov groups in Zamorzaev symbolism, which reflects the full system of generators of these groups. However if first we derive from each Fedorov group $(2^q - 1) \times ... \times (2^q - 2^{l-1})$ groups of type M^l and then we compare them in order to find identical and to eliminate extra ones, it is not quite relevant. That's why it is rational to divide the main problem into more simple problems. To receive groups of the type M^l it is convenient to proceed as follows:

a) to derive all possible point groups $M^m (m \leq l)$ from 32 generating groups G_{30} which are subgroups of 230 groups G_3;

b) to make the same procedure with 14 translation subgroups of groups G_3;

c) to finish the derivation of space groups of the type M^l, using the results of a) and b) [4].

However, to different junior space groups of the type M^3 obtained from one family identical groups of (22$\underline{1}$)-symmetry may correspond, as the group $E_3 = (e,\ \underline{1},\ 1',\ {}^*1,\ \underline{1}',\ {}^*\underline{1},\ {}^*1',\ {}^*\underline{1}')$ contains 7 different kinds of antisymmetry transformations, and in the group $mmm = m_1 m_2 m_3 = (e, m_1, m_2, m_3, m_1 m_2 = 2_{12}, m_1 m_3 = 2_{13}, m_2 m_3 = 2_{23}, m_1 m_2 m_3 = i_{123})$ only three transformations are essentially different, for example, $m_1, 2_{12}, i_{123}$, as the transformations m_1, m_2, m_3 and $2_{12}, 2_{13}, 2_{23}$ play the same geometrical role, respectively.

Consequently, for example, to the group $\{a, b, c\}(2' \cdot {}^*m : 2)$ and to five groups, obtained from this group by all permutations of signs –, /, * (which mean transformations of antisymmetry of kind 1, kind 2 and kind 3, respectively),

$\{\underline{a}, b, c\}({}^*2 \cdot m' : 2)$; $\{a', b, c\}(\underline{2} \cdot {}^*m : 2)$;
$\{a', b, c\}({}^*2 \cdot \underline{m} : 2)$; $\{{}^*a, b, c\}(\underline{2} \cdot m' : 2)$; $\{{}^*a, b, c\}(2' \cdot \underline{m} : 2)$,

i.e. to six different junior groups of three-fold antisymmetry of the family $18s$ correspond the following six identical groups of (22$\underline{1}$)-symmetry:

$\{a^1, b, c\}(2^2 \cdot {}^3m : 2)$; $\{a^1, b, c\}(2^3 \cdot {}^2m : 2)$; $\{a^2, b, c\}(2^1 \cdot {}^3m : 2)$;
$\{a^2, b, c\}(2^3 \cdot {}^1m : 2)$; $\{a^3, b, c\}(2^1 \cdot {}^2m : 2)$; $\{a^3, b, c\}(2^2 \cdot {}^1m : 2)$.

Thus, only one group of (22$\underline{1}$)-symmetry corresponds to six different groups of the type M^3.

Consequently, to obtain all different junior groups of (22$\underline{1}$)-symmetry one needs to obtain all different junior groups of three-fold antisymmetry, to unite them in nests and to examine only representatives of these nests.

At the same time it is convenient to use the distribution of 230 space Fedorov groups in 34 different equivalence classes [5]:

1. $1s$; **2.** $2s$; **3.** $3s, 2a$; **4.** $4s, 26s, 1h, 33h, 3a, 7a, 42a$; **5.** $5s$;

6. $6s, 16s, 22s, 35s, 47s, 48s, 53s, 54s, 55s, 56s, 57s, 71s, 4h, 7h, 9h, 10h, 15h, 25h, 29h, 30h, 31h, 32h, 34h, 5a, 10a, 11a, 25a, 27a, 33a, 36a, 37a, 38a, 41a, 43a, 44a, 45a, 50a, 52a, 84a, 85a, 103a$; **7.** $7s$; **8.** $8s, 10s, 32s, 62a$; **9.** $9s$; **10.** $11s, 24h, 6a$; **11.** $12s$; **12.** $13s, 17h$; **13.** $14s, 15s, 24s, 58s, 6h, 11h, 20h, 23h, 35h, 36h, 15a, 16a, 23a, 54a, 55a, 60a, 61a$; **14.** $17s, 22h, 20a$; **15.** $18s$; **16.** $19s, 36s, 14a$; **17.** $20s$; **18.** $21s$; **19.** $23s, 40s, 41s, 42s, 49s, 63s, 65s, 66s, 69s, 73s, 27h, 42h, 43h, 44h, 45h, 46h, 47h, 53h, 54h, 12a, 32a, 34a, 35a, 39a, 40a, 48a, 49a, 51a, 53a, 76a, 77a, 79a, 80a, 81a, 82a, 83a, 86a, 96a, 99a, 100a, 101a, 102a$; **20.** $25s, 29s, 31s, 34s, 50s, 72s, 12h, 13h, 14h, 26h, 28h, 37h, 48h$; **21.** $27s$; **22.** $28s$; **23.** $37s$; **24.** $38s$; **25.** $61s$; **26.** $3h$; **27.** $5h$; **28.** $8h$; **29.** $19h$; **30.** $21h$; **31.** $1a$; **32.** $8a$; **33.** $21a$; **34.** $29a$.

Groups of one class have isomorphic so called antisymmetric characteristics and as a result generate the same quantity of groups of the type M^3. That's why it is enough to study only representatives of these classes: $1s, 2s, 3s, 4s, 5s, 6s, 7s, 8s, 9s, 11s, 12s, 13s, 14s, 17s, 18s, 19s, 20s, 21s, 23s, 25s, 27s, 28s, 37s, 38s, 61s, 3h, 5h, 8h, 19h, 21h, 1a, 8a, 21a, 29a$.

As in the groups $23s, 27s, 38s, 61s, 8a$ the number q of generators which we may replace by transformations of antisymmetry at the same time is smaller than 3, then we exclude these groups. Consequently, we have to examine 29 Fedorov groups, but not 34: $1s, 2s, 3s, 4s, 5s, 6s, 7s, 8s, 9s, 11s, 12s, 13s, 14s, 17s, 18s, 19s, 20s, 21s, 25s, 28s, 37s, 3h, 5h, 8h, 19h, 21h, 1a, 21a, 29a$.

So, only 141 Fedorov groups generate junior groups of three-fold antisymmetry.

III. By means of the above method all possible junior groups of three-fold antisymmetry were derived from each of the enumerated group. These groups were unibed in nests, which contain six, three, two or one group.

The obtained results were reduced in the following table:

Representatives of the equivalence classes in Fedorov symbolism	Quantity of the groups in the given equivalence class (including the group representative)	Quantity of the groups of type M^3, derived from the given group representative	Quantity of the groups of type M^3 derived from the groups from given equivalence class (including the group representative)	Quantity of the nests (junior groups of (22$\underline{1}$)-symmetry) derived from the given group representative	Quantity of the nests (junior groups of (22$\underline{1}$)-symmetry), derived from the groups from given equivalence class (including the group representative)
1	2	3	4	5	6
$1s$	1	$1 \times 1 = 1$	1	1	1
$2s$	1	$2 \times 3 + 2 \times 1 = 8$	8	2+2=4	4
$3s$	2	$19 \times 6 + 17 \times 3+$ $+3 \times 1 = 168$	336	19+17+3=39	78
$4s$	7	$4 \times 6 + 6 \times 3 = 42$	294	4+6=10	70
$5s$	1	$34 \times 6 + 20 \times 3+$ $+2 \times 1 = 266$	266	34+20+2=56	56
$6s$	41	$12 \times 6 + 4 \times 3 = 84$	3444	12+4=16	656
$7s$	1	$151 \times 6 + 79 \times 3+$ $+5 \times 1 = 1148$	1148	151+79+5=235	235

1	2	3	4	5	6
$8s$	4	$108 \times 6 + 36 \times 3 = 756$	3024	108+36=144	576
$9s$	1	$95 \times 6 + 61 \times 3 +$ $+3 \times 1 = 756$	756	95+61+3=159	159
$11s$	3	$3 \times 6 + 3 \times 3 +$ $+1 \times 1 = 28$	84	3+3+1=7	21
$12s$	1	$28 \times 6 + 14 \times 3 = 210$	210	28+14=42	42
$13s$	2	$602 \times 6 + 112 \times 3 = 3948$	7896	602+112=714	1428
$14s$	17	$212 \times 6 + 24 \times 3 = 1344$	22848	212+24=236	4012
$17s$	3	$204 \times 6 + 12 \times 3 = 1260$	3780	204+12=216	648
$18s$	1	$1051 \times 6 + 238 \times 3 +$ $+1 \times 2 + 6 \times 1 = 7028$	7028	1051+238+ +1+6=1296	1296
$19s$	3	$1228 \times 6 + 148 \times 3 = 7812$	23436	1228+148=1376	4128
$20s$	1	$73 \times 6 + 21 \times 3 +$ $+3 \times 1 = 504$	504	73+21+3=97	97
$21s$	1	$702 \times 6 + 69 \times 3 +$ $+1 \times 2 + 3 \times 1 = 4424$	4424	702+69+1+3=775	775
$25s$	29	$28 \times 6 = 168$	4872	28	812
$28s$	8	$104 \times 6 + 30 \times 3 = 714$	5712	104+30=134	1072
$37s$	4	$420 \times 6 = 2520$	10080	420	1680
$3h$	1	$52 \times 6 + 36 \times 3 = 420$	420	52+36=88	88
$5h$	2	$49 \times 6 + 21 \times 3 = 357$	714	49+21=70	140
$8h$	1	$1 \times 6 + 5 \times 3 = 21$	21	1+5=6	6
$19h$	1	$8 \times 6 + 16 \times 3 +$ $+2 \times 1 = 98$	98	8+16+2=26	26
$21h$	1	$1140 \times 6 + 128 \times 3 = 7224$	7224	1140+128=1268	1268
$1a$	1	$2 \times 3 + 1 \times 1 = 7$	7	2+1=3	3
$21a$	1	$68 \times 6 + 12 \times 3 +$ $+2 \times 2 = 448$	448	68+12+2=82	82
$29a$	1	$9 \times 6 + 1 \times 2 = 56$	56	9+1=10	10
Σ	141	41820	109139	7556	19469

Thus, the full number of junior groups of three independent kinds, derived from 141 space Fedorov groups G_3, is equal to 109139, and the full number of junior groups of the $(22\underline{1})$-symmetry, generated by these 141 space Fedorov groups G_3, is equal to 19469.

References

[1] Shenesheutskaia A., Palistrant A. *On space groups of crystallographic P-symmetries in the geometrical classification.* Analele stiintifice ale USM. Seria "Stiinte fizico-matematice". Chişinău, USM, 2002, p. 207–210 (in Russian)

[2] Palistrant A.F., Shenesheutskaia A.A. *Spatial groups of crystallographic P-symmetries in geometric classification.* Second Conference of the Mathematical Society of the Republic of Moldova. Communications, Chişinău, 2004, p. 241–244.

[3] Zamorzaev A.M., Palistrant A.F. *Geometrical classification of P-symmetries.* DAN USSR, 1981, **256**, N 4, p. 865–859 (in Russian)

[4] Zamorzaev A.M. *Theory of simple and multiple antisymmetry.* Kishinev: Shtiintsa, 1976

[5] Jablan S.V. *Generalized space Shubnikov groups.* Publications de l'institut mathematique. Nouvelle serie, 1986, **40(54)**, p. 33–48 (in Russian)

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