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GROUP-THEORETICAL APPROACH TO REDUCED ORIENTATION SPACES FOR CRYSTALLOGRAPHIC TEXTURES

V. P. YASHNIKOV and H. J. BUNGE

Institute of Solid State Physics Russian Academy of Science, Russia
Department of Physical Metallurgy TU Clausthal, FRG

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A unified group-theoretical approach to the reduction problem for the orientation space of a crystallographic texture is developed. After preliminary considerations of the three-dimensional rotation group SO(3) the concept of the invariant inner distance function in the group space has been introduced. Left and right group translations, inner auto-morphisms, motions of general form, and inversion transforms in the space SO(3) are analysed. The concept of Dirichlet-Voronoi partition dual to an arbitrary finite set of rotations has been considered. It is shown that the Dirichlet-Voronoi partition, dual to the proper point group for the grain lattice of original orientation, is regular with respect to the group of motions generated by elements of proper point group.
It is demonstrated that the true orientation space of a texture (at the absence of specimen symmetry) may be obtained by passing to the topological closure of any Dirichlet-Voronoi domain with the next, identifying crystallographically equivalent rotations belonging to its topological boundary. Thus an invariant derivation for the reduced (true) orientation space is given that does not require using any particular parametrization for the group space SO(3).
Symmetry properties of Dirichlet-Voronoi domains are studied in conclusion. It is shown that any domain of such kind admits a finite group of symmetries generated by elements of a proper point group and by an appropriate inversion of the group space SO(3). It is proved that only part of them may be extended onto the true orientation space.

KEY WORDS: Crystal structures, lattices, grain orientations, point groups, rotation group, reduction, Dirichlet-Voronoi partitions, Dirichlet-Voronoi domains, true orientation space, symmetries.

INTRODUCTION

The mathematical apparatus of three-dimensional rotations has numerous applications in modern investigations of crystallographic texture as a convenient tool for quantitative characterization of grain (crystallite) orientation in polycrystalline materials (Bunge, 1982). The description of grain (crystallite) orientation by rotations does not find any difficulties in the case of a material with triclinic crystal symmetry, since in this case there is a one-to-one correspondence between geometrically possible orientations of a grain lattice and rotation operations of the three-dimensional specimen space. If, however, the grain lattice posesses certain proper rotational symmetry axes, the one-to-one correspondence of grain orientations and rotation operations is broken so that, as a consequence, the ODF data interpretation may be essentially complicated especially for materials with high symmetry.

In connection with the above, the problem arises to construct a maximal connected subdomain in the group SO(3), interior points of which are in one-to-one correspondence

with grain orientation, and the shape of which is simplest in certain geometrical sense. The problem will be called the reduction problem for the orientation space of a crystallographic texture. A natural and comparatively easy numerially realizable method to construct a fundamental domain of such kind may be obtained if, instead of the set of all possible rotations describing an arbitrary grain orientation, we use the rotation of minimal possible angle.

The geometrical form of the fundamental domain was studied recently in a series of papers both for different ways of parametrization of the rotation group and in its dependence on the crystal class as well as on the specimen symmetry group of the crystallographic texture under investigation. In particular, the problem was solved by Frank (1987, 1988, 1992) and by Heinz and Neumann (1991) using Rodrigues parameters introduced earlier in the context of texture analysis by Bonnet (1980). Matthies et al. (1990) analyzed the problem in terms of Eulerian angles. The problem was considered also by Gertsman (1989) using computer methods and recently by Ibe (1993), both on the basis of the quaternion formalism which was first proposed for description of grain orientations by Grimmer (1974).

It is the main purpose of the paper to develop a unified group-theoretical approach to the reduction problem of the orientation space for crystallographic textures. We introduce the so called angular distance function in the space of all three-dimensional rotations and further we obtain, using the natural group structure in the totality of all rotations, a simple description for related group space motions in terms of left and right shifts (or group translations). We analyse, after that, the reduction problem interpreting it as the problem of constructing the partition of the group space SO(3) into domains which are mutually equivalent with respect to the transforms of right shifts generated by the elements of the proper point group of the grain lattice of original orientation. By this approach, there is no necessity to use a parametrization of the group SO(3). Besides that, it is evident, in the frame of the approach, that the possibility to construct the reduced orientation space is a consequence of the intrinsic geometric structure of the group space SO(3) which does not depend on the choice of a parametrization.

We construct, using domains of the regular partition, the so called true orientation space and we show further that its topology and, as a consequence, its geometry in the whole, both are essentially distinct from those for the domains of partition. However, the symmetry group for any domain of partition as well as for the true orientation space may be characterized as the group of inner automorphisms generated by all proper crystallographic rotations for the grain lattice of original orientation. Thus, we distinguish consequently the following geometrical objects which are naturally connected with an arbitrary crystallographic texture:

1) the whole (unreduced) orientation space, i.e. the group space SO(3) with a prescribed group of motions which play the role of symmetry group for the texture under consideration;
2) the topologically open domains of regular partition associated with the symmetry group of a texture (or in other words the fundamental domains with respect to the texture symmetry group);
3) the topologically closed domains of regular partition obtained after joining to any open domain of partition its topological boundary;
4) the true orientation space having the topology and inner geometry which takes into account the existence of classes of crystallographically equivalent rotations on the topological boundary of any fundamental domain.

A geometrical characterization of the domains of a regular partition as well as a geometrical description of a reduction procedure in terms of geodesic lines and geodesic surfaces in the space SO(3) will be given in the second part of the paper. A series of important examples corresponding to different crystal classes using the concept of inner geometry will be considered in the third part. A preliminary anouncment concerning the group-theoretical and inner-geometry approach to the reduction problem was given in an unpublished report (Yashnikov, 1989). See also further communications (Yashnikov 1990,1991, 1993).

In the present paper our consideration have been restricted to the case of an arbitrary texture without any specimen (statistical) symmetry. However, the group-theoretical approach and the technique of regular partitions are also applicable to the case of a non-trivial specimen symmetry group. Besides that, the approach, in combination with some inner-geometrical and topological considerations, is applicable for constructing the true grain misorientation space. A brief account of the last topics is contained in (Yashnikov, 1991, 1992). These questions will be considered in details in further publications.

The three-dimensional rotation group SO(3) in texture analysis

It is the purpose of this section to give a brief account of two different methods of description of grain (crystallite) orientations in polycrystals in a form which is suitable for further exposition. Both methods are mathematically equivalent, therefore the choice of any of them may be motivated only by reasons of convenience.

In three-dimensional texture analysis one starts usually from the choice and fixing of a certain (as a rule cartesian) specimen reference system which is rigidly connected with the volume of the polycrystalline material under investigation. The reference system is necessary for representation of quantitative data of orientations of individual grains, and also to visualize a statistical information concerning the crystallographic texture (for instance ODF data). An other technical but important reason to fix a specimen reference system is the following: the majority of computations with geometrical quantities in texture analysis may not be performed up to the end in a coordinateless way owing to their complexity.

In principle, any Cartesian reference system rigidly connected with the specimen is suitable for that. Any physical sense can, however, only be attributed to a description of the crystallographic texture, which does not depend on the choice of the original reference system. However, in many cases certain exceptional systems may be preferred to all other ones, since the geometrical quantities of interest or their interrelations have simpler form with respect to the exceptional reference system. If, for instance, a polycrystalline material was treated by plastic deformation and thereby the related external strain field posessed three mutually perpendicular symmetry axes, it is natural to choose these axes as a specimen reference system, since, in this case, the specimen symmetry group is reduced to the simplest matrix form. If a privileged reference system of such kind exists, but its position with respect to the geometrical form of specimen is unknown, the very important problem arises to determine the system from pole density data. The situation of so called "oblique" texture, typical for geological materials and related problem, is not solved satisfactory at present time.

We will denote the axes of an arbitrary reference system (which is, however, fixed in further considerations) by OX_s; OY_s; OZ_s. It is convenient also to fix a crystallite (grain) of "original orientation", the angular position of which is unchangeable in all

further considerations. If the crystal lattice of the material under investigation posesses an inversion center (i.e. infinitely many different inversion centers, which may be obtained one from another by all possible lattice translations) we will additionally suppose, for the grain lattice of original orientation, that one of its inversion centers coincides with the origin O of the specimen reference system.

Any geometrically possible orientation of the grain lattice may be obtained from the above fixed original one by means of an appropriate (clockwise) rotation through an angle $0 \leq j \leq \pi$ about an appropriate axis $C^- = (c_1, c_2, c_3)$ having c_1, c_2, c_3 as directional cosin'es refered to the specimen coordinate system OX_s, OY_s, OZ_s. Any rotation will be denoted, as a rule, as $g(C^-; j) = g(c_1, c_2, c_3, j)$. Two arbitrary rotations such as $g(C^-; j)$ and $g(D^-; y)$ are distinct if either $C^- \neq D^-$ or $j \neq y$ except the case of rotations with $j = p$ since the rotations $g(C^-; p)$ and $g(-C^-; p)$ are identical for any axis C^-.

Thus, the ball of radius $R = p$ with its center at the origin O of the specimen reference system is a topological model for the totality SO(3) of all possible three-dimensional rotations, however, antipodal points of the sphere $R = p$ should be identified, i.e. each pair of antipodal points should be considered as one point of a new topological space. That means, topologically the totality SO(3) is essentially distinct from the three-dimensional Euclidean space and, as a consequence, it may not be realized (modelled) as any closed subdomain of this space, so that any attempt to introduce in the space SO(3) a global three-dimensional parametrization will be unsuccesful. An obstacle to that is the boundary $R = p$ of the sphere which becomes, after the above mentioned identifying, topologically equivalent to the two-dimensional projective space. As it will be seen from further considerations, also the inner geometry of the space SO(3) is non-euclidean.

Since any rotation $g(\bar{C}\ ; \varphi)$ is a linear transformation of the (euclidean) specimen space it may be represented as a 3 * 3 matrix

$$g = \begin{vmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{vmatrix} = |g_{i,j}| \tag{1}$$

the components of which must obey the orthogonality relations

$$g_{i1}g_{i1} + g_{i2}g_{i2} + g_{i3}g_{j3} = \delta_{i,j} \qquad i,j = 1, 2, 3 \tag{2}$$

as well as the additional determinant condition

$$\det |g_{i,j}| = 1 \tag{3}$$

whereby $\delta_{i,j}$ is the Kronecker's symbol. The equations eq(2) combined with the condition eq(3) furnish a realization of the totality SO(3) in the form of a topologically connected and bounded surface in the nine-dimensional Euclidean space of the matrix coefficients. Thereby eq(2), at the absence of condition eq(3), give an unconnected three-dimensional surface that is composed of two connected pieces, the first of which is the totality SO(3), the second is the totality of all possible improper rotations which satisfy, instead of eq(3), the condition

$$\det |g_{i,j}| = -1 \tag{4}$$

It is easy to prove, using the matrix representation for rotations, that the product of any two rotations $g(\bar{C}\ ;\ \varphi)$. $g(\bar{D};\ \varphi)$ *is* also a rotation $g(\bar{E};\ \Theta)$ having the matrix which is the product of the matrices of the two factor-rotations.

$$|g_{i,j}(\bar{E};\ \Theta)| = |g_{i,k}(\bar{C};\ \varphi)| \cdot |g_{k,j}(\bar{D}\ \psi)| \tag{5}$$

There is also, in the totality SO(3), an inversion operation which can be written in the form

$$[g(\bar{C};\ \varphi)]^{-1} = g(-\bar{C};\ \varphi) \tag{6}$$

The operation is identical with the conventional matrix transposition in the representation eq(l) so that we have for the related matrix elements

$$g_{i,j}(-\bar{C};\ \varphi) = g_{j,i}(\bar{C};\ \varphi) \qquad i,j = 1,\ 2,\ 3 \tag{7}$$

It may be verified that all standard axioms of a group are satisfied, thereby the matrix

$$e = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \tag{8}$$

which represents the identity transform of the specimen space, plays the role of the unit element in the totality SO(3). The group structure in SO(3) will be essentially used in further considerations.
The matrix elements $g_{i,j}(\bar{C};\ \varphi)$ may be expressed in the form

$$\begin{aligned}
g_{11} &= \cos\varphi + (1 - \cos\varphi) \cdot c_1^2 \\
g_{12} &= (1 - \cos\varphi) \cdot c_1 \cdot c_2 - c_3 \cdot \sin\varphi \\
g_{13} &= (1 - \cos\varphi) \cdot c_1 \cdot c_3 - c_2 \cdot \sin\varphi \\
g_{21} &= (1 - \cos\varphi) \cdot c_1 \cdot c_2 + c_3 \cdot \sin\varphi \\
g_{22} &= \cos\varphi + (1 - \cos\varphi) \cdot c_2^2 \\
g_{23} &= (1 - \cos\varphi) \cdot c_2 \cdot c_3 - c_1 \cdot \sin\varphi \\
g_{31} &= (1 - \cos\varphi) \cdot c_3 \cdot c_1 - c_2 \cdot \sin\varphi \\
g_{32} &= (1 - \cos\varphi) \cdot c_3 \cdot c_2 + c_1 \cdot \sin\varphi \\
g_{33} &= \cos\varphi + (1 - \cos\varphi) \cdot c_3^2
\end{aligned} \tag{9}$$

The inverse functional dependence of the geometrical parameters $\bar{C};\ \varphi$ on the matrix components is given by the expression

$$\cos\ \varphi = \frac{1}{2} \cdot (Tr\ |g_{ij}| - 1) \tag{10}$$

$$c_1 = \frac{g_{32} - g_{23}}{2 \cdot \sin\varphi}; \qquad c_2 = \frac{g_{13} - g_{31}}{2 \cdot \sin\varphi}; \qquad c_3 = \frac{g_{21} - g_{12}}{2 \cdot \sin\varphi} \tag{11}$$

Thereby the trace of an arbitrary 3 * 3 matrix is defined by

$$Tr|g_{ij}| = g_{11} + g_{22} + g_{33} \tag{12}$$

The expressions eq(11) have singularities of topological nature at $\varphi = \pi$. The singularities reflect the above mentioned fact that the rotation group SO(3) may not be realized with the help of any appropriate parametrization as a closed subdomaine of the three-dimensional Euclidean space. It should be mentioned, in conclusion of this section, that the totality $G(\bar{C})$ of all possible rotations about the axis $\bar{C} = (c_1, c_2, c_3)$ constitutes a one-parametric subgroup of the group SO(3). The subgroup is the union of two families of mutually inverse rotations

$$G^{+}(\bar{C}) = [g(\bar{C};\ \varphi) : \qquad 0 = \leq \varphi \leq \pi] \tag{13}$$

and

$$G^{-}(\bar{C}) = [g(-\bar{C};\ \varphi) : \qquad 0 = \leq \psi \leq \pi] \tag{14}$$

It is easy to verify immediately that the union $G(\bar{C}) = G^{+}(\bar{C}) \cup G^{-}(\bar{C})$ *is* a subgroup. The multiplication rules for the rotations of the totality $G(\bar{C})$ may be described in terms of rotation axis and angle in the form

$$g(\bar{C};\ \varphi) \cdot g(\bar{C};\ \psi) = g(\bar{C};\ \varphi + \psi) \qquad \text{if } \varphi + \psi \leq \pi \tag{15}$$

$$g(\bar{C};\ \varphi) \cdot g(\bar{C};\ \psi) = g(-\bar{C};\ \varphi + \psi - \pi) \qquad \text{if } \varphi + \psi < \pi \tag{16}$$

$$g(-\bar{C};\ \varphi) \cdot g(-\bar{C};\ \psi) = g(-\bar{C};\ \varphi + \psi) \qquad \text{if } \varphi + \psi \leq \pi \tag{17}$$

$$g(-\bar{C};\ \varphi) \cdot g(-\bar{C};\ \psi) = g(-\bar{C};\ \varphi + \psi - \pi) \qquad \text{if } \varphi + \psi > \pi \tag{18}$$

$$g(-\bar{C};\ \varphi) \cdot g(\bar{C};\ \psi) = g(-\bar{C};\ \varphi - \psi) \qquad \text{if } \psi \geq \varphi \tag{19}$$

$$g(\bar{C};\ \varphi) \cdot g(-\bar{C};\ \psi) = g(-\bar{C};\ \varphi - \psi) \qquad \text{if } \psi \geq \varphi \tag{20}$$

Thus, any subgroup $G(\bar{C})$ *is* commutative (abelian), and geometrically it may be represented as the diameter of the ball $R = \pi$ that passes through the vector $\bar{C}$. Since any pair of antipodal points $g(\bar{C};\ \pi)$ and $g(-\bar{C};\ \pi)$ represents one and the same rotation the subgroup $G(\bar{C})$ is a closed curve in the space SO(3). Any subgroup $G(\bar{C})$ is topologically equivalent to a circle. One can show, in addition, that the group SO(3) has no other closed subgroups except $G(\bar{C})$ for all possible directional vectors $\bar{C}$, thereby $G(\bar{C}) = G(-\bar{C})$ for any $\bar{C}$, so that the antipodal vectors $\bar{C}$ and $-\bar{C}$ generate one and the same one-parametric subgroup of the rotation group.

Grain orientations. Unreduced (multivalued) description

We suppose for further considerations that the grain lattice posesses an inverion center. At the absence of this, analogous considerations may be carried out for the totality O(3) of all proper and improper rotations. More detailed treatment of this subject will be presented in an other paper.

The description of grain (crystallite) orientations does not find any difficulties in the case of the triclinic crystal class. In this case, the grain lattice does not possess any proper rotational symmetry axes. That means, with the help of different rotations, we obtain from the grain lattice of original orientation the lattices of strictly different orientations, so that the orientation space, for a lattice of the triclinic class, is identical with the whole three-dimensional rotation group SO(3).

For materials of other crystal classes the one-to-one correspondence between the elements of SO(3) and the orientations of the grain lattice has been lost, so that in these cases any orientation of a grain may be described by an appropriate finite family of crystallographically equivalent rotations. Let us denote, for further considerations,

by $M(K_o)$ the space group at the grain K_o of original orientation. Any transformation of the group may be represented in the form

$$m(g;\bar{t}) = g\bar{x} + \bar{t} \tag{21}$$

whereby $\bar{x}$ is any vector of the crystal space of the grain of original orientation; $\bar{t}$ is a translation of the crystal space K_o; g is a rotation of the space. Thereby the transformations of the group $M(K_o)$ may be characterized by the property to transform the crystal lattice of K_o onto itself.

As it is well known, all admissible translations of K_o constitute the Bravais lattice $T(K_o)$ which is generated by three linearly independent primitive translation vectors $\bar{\tau}_1$; $\bar{\tau}_2$; $\bar{\tau}_3$; so that any translation $\bar{t}$ belonging to $T(K_o)$ may be expressed in the form

$$\bar{t} = n_1 \cdot \bar{\tau}_1 + n_2 \cdot \bar{\tau}_2 + n_3 \cdot \bar{\tau}_3 \tag{22}$$

whereby n_1, n_2, n_3 are any integers. Besides that, the totality $T(K_o)$ is an abelian subgroup (and even normal subgroup) of the space group $M(K_o)$. Also it is well known that the totality of all admissible rotations $g = g(\bar{C}; \varphi)$ in eq(21) constitutes a finite subgroup of SO(3) which will be denoted in further considerations by $SO(K_o)$ or P_O^+.
The list of all possible elements of the group will be denoted as

$$SO(K_o) = \{k_o = e;\ k_1;\ \ldots\ k_N;\} \tag{23}$$

whereby $k_o = e$ is the identiy transformation eq(8).

It has been shown in mathematical crystallography that the algebraic form of the lincage between the translation group $T(K_o)$ and the related proper group $P_O^+ = SO(K_o)$ depends on the crystallographic structure of K_o and, as a consequence, two different cases are possible

1) for each spatial transformation $m(g;\ \bar{t})$ which is an element of the group $M(K_o)$ the transformation $m(g;\ \bar{0})$ belongs to $M(K_o)$;
2) there is at least one transformation m(g; $\bar{t}$) in the group $M(K_o)$ such that the rotation $m(g;\ \bar{0})$ does not belongs to $M(K_o)$.

The first of these cases corresponds to the so called class of symmorphic crystal structures. The space group $M(K_o)$ in this case is the algebraic direct sum of the translation subgroup $T(K_o)$ and the so called full point group $O(K_o)$ which is equal, in the presence of an inversion center, to the set-theoretical union of the form $O(K_o) = P_O^+ \cup P_O^-$, whereby P_O^- *is* the totality of all possible improper rotations $\hat{g} = g \cdot i = i \cdot g = -g$ which are obtained by multiplying; any element g of the group P_O^+ by the inversion transform i of the crystal space K_o.

A crystal structure of the second case has been called non-symmorphic. This case can be realized only in crystal structures having several atoms per primitive cell. The space group $M(K_o)$ of any non-symmorphic crystal K_o may not be represented as the algebraic direct sum of its point group $O(K_o)$ and the translation group $T(K_o)$. That means, geometrically the inversion center $\bar{0}$ of K_o does not coincide with any of the centers of rotational symmetry of K_o. Thereby we define the center of rotational symmetry as the point of crystal space at which the total number of proper rotational symmetry axes, being incident to the point, is the maximal possible. Because of the non-coincidence of centers of the two different kinds the space group $M(K_o)$ of a non-

symmorphic crystal may be constructed only as a non-trivial extension of its translation group $T(K_o)$. The diamond-type structure may be considered as an example for K_o of such kind.

However, the essential distinction between symmorphic structures and non-symmorphic ones disappears in three-dimensional texture analysis if we restrict ourself to the analysis of individual or statistical data concerning grain orientations. Any rotation k that belongs to the group $M(K_o)$, in the form of a combination eq(21), but with an appropriate fractional translation leeds, after its application to K_o, to the crystal pattern $k \cdot K_o$ which also may be obtained from K_o by this fractional translation. Consequently, both crystals K_o and $k \cdot K_o$ posses one and the same orientation.

If $g = g(\bar{C}; \varphi)$ is an arbitrary proper rotation and k_i belongs to the proper point group P_O^+ then any rotation of the form $g \cdot k_i$ describes the same orientation as that which has been occupied by the lattice $g \cdot K_o$. Thus, in the presence of a non-trivial proper point group $P_O^+ \neq \{e\}$ any orientation of the crystal lattice may be described by an appropriate co-set

$$g \cdot P_O^+ = \{g, g \cdot k_1, \ldots, g \cdot k_N\} \tag{24}$$

of the subgroup P_O^+. One can verify, using simplest group-theoretical techniques, that any two co-stes $g_1 \cdot P_O^+$ and $g_2 \cdot P_O^+$ are identical if $g_2 = g_1 \cdot k_j$ for an appropriate element k_j of the group P_O^+. In the opposite case, the two co-sets have no common elements. That means, there is a one-to-one correspondence between the totality of all possible orientations of a crystal lattice (i.e. the orientation space) and the totality of all possible co-sets of the subgroup P_O^+. The last totality has been denoted usually as $SO(3)\backslash P_O^+$.

In spite of the fact that the above accounted multivalued description of orientations by co-sets may be consequently used for formulating as well as for solving of all problems in three-dimensional texture analysis, the approach is unconvenient and non-optimal for texture (ODF) data visualization. Therefore, the necessity appears not only to construct a minimal connected subdomain in the group space SO(3), the rotations of which may represent all possible grain orientations, but also to give a more detailed analysis of the topological and geometrical distinctions between the subdomain and the true orientation space $SO(3)\backslash P_O^+$.

ANGULAR DISTANCE IN THE GROUP SPACE SO(3)

The concept of angular distance plays an important role in further considerations. If $g(\bar{C}; \varphi)$ and $g(\bar{D}; \psi)$ are two arbitrary rotations of the specimen space, the product of the form

$$g(\bar{D}; \psi) \cdot g(\bar{C}; \varphi) = g(\bar{E}; \Theta) \tag{25}$$

is also a rotation with a certain angle Θ. The magnitude of the angle Θ (measured in radians or in other units) will be called the angular distance between the rotations $g(\bar{C}; \varphi)$ and $g(\bar{D}; \psi)$. It will be denoted as

$$dist\ [g(\bar{C}; \varphi); g(\bar{D}; \psi)] = \Theta \tag{26}$$

The explicit expression of the function in its dependence both on the directional vectors $\bar{C}$, $\bar{D}$ and on the rotation angles φ, ψ is too complicated. However, some simpler analytical form for the function may be obtained by using the matrix representation. In fact, we have, according to the formula eq(10), the expression

$$\begin{aligned} dist\ [g(\bar{C};\ \varphi);\ g(\bar{D};\ \psi)] = \\ \arccos\frac{1}{2} \cdot [g_{11}(\bar{C};\ \varphi) \cdot g_{11}(\bar{D};\ \psi) + g_{12}(\bar{C};\ \varphi) \cdot g_{12}(\bar{D};\ \psi) \\ +g_{13}(\bar{C};\ \varphi) \cdot g_{13}(\bar{D};\ \psi) + g_{21}(\bar{C};\ \varphi) \cdot g_{21}(\bar{D};\ \psi) + g_{22}(\bar{C};\ \varphi) \\ \cdot g_{22}(\bar{D};\ \psi) + g_{23}(\bar{C};\ \varphi) \cdot g_{23}(\bar{D};\ \psi) + g_{31}(\bar{C};\ \varphi) \cdot g_{31}(\bar{D};\ \psi) + \\ g_{32}(\bar{C};\ \varphi) \cdot g_{32}(\bar{D};\ \psi) + g_{33}(\bar{C};\ \varphi) \cdot g_{33}(\bar{D};\ \psi) - 1] \end{aligned} \tag{27}$$

One can verify, using eq(27), that the angular distance function eq(26) satisfies all usual axioms of an abstract distance function (i.e. the so called metric axioms) as following

1) Non-negativity and non-degeneracy:

   $dist(g_1;\ g_2) \geq 0$ for any two rotations g_1 and g_2;
   $dist(g_1;\ g_2) = 0$ is equivalent to the condition $g_1 = g_2$.

2) Symmetry property:

$$dist(g_1;\ g_2) = \text{dist}(g_2;\ g_1) \tag{28}$$

   for any two rotations g_1, g_2.

3) Triangle inequality:
   if g_1, g_2, g_3 are any three rotations the inequality

$$dist(g_1;\ g_3) \leq dist(g_1;\ g_2) + dist(g_2;\ g_3) \tag{29}$$

   is valid

Besides that, the above defined angular distance is intrinsic in the sense that there exists, for any two rotations g_1 and g_2, a third rotation $\tilde{g}$ "in the middle" between g_1 and g_2 so that

$$dist(g_1;\ g_2) = dist(g_1;\ \tilde{g}) + dist(\tilde{g};\ g_2) \tag{30}$$

Right and left translations of the group space SO(3). Motions

The presence of a certain group structure in the totality of all possible three-dimensional rotations gives a possiblity to introduce some analogies to the so called "solid transformations" or "motions" in the space SO(3). The motions play the same role as the ones of the Euclidean space, however, in consequence of the more complicated topological and geometrical structure of the group space SO(3), its motions must be described in a more complicated way. We will start with the consideration of two important particular cases.

Any rotation τ generates the "right translations" $R(\tau)$ under the action of which each point g of the space SO(3) transforms according to

$$R(\tau)g = g \cdot \tau^{-1} \tag{31}$$

It may be immediately verified that the angular distance between rotations is invariant under the acting of right translations

$$dist(R(\tau)g_1;\ R(\tau)g_2) = dist(g_1;\ g_2) \tag{32}$$

In order to verify this property we write

$$\begin{aligned} dist[R(\tau)g_1;\ R(\tau)g_2] &= dist[g \cdot \tau^{-1};\ g \cdot \tau^{-1}] \\ &= \arccos \frac{1}{2} \cdot [Tr\ \{g_2 \cdot \tau^{-1} \cdot (g_1 \cdot \tau^{-1})^{-1}\} - 1] \\ &= \arccos \frac{1}{2} \cdot [Tr\ (g_2 \cdot \tau^{-1} \cdot \tau \cdot g_1^{-1}) - 1] \\ &= \arccos \frac{1}{2} \cdot [Tr\ (g_2 \cdot g_1^{-1}) - 1] \\ &= dist(g_1;\ g_2) \end{aligned} \tag{33}$$

One can analogously consider the "left translation" $L(\tau)$ by the element τ defined by

$$L(\tau)g = \tau \cdot g \tag{34}$$

The angular distance between rotations is also invariant by transformations of this kind as may be demonstrated in the same way

$$\begin{aligned} dist[L(\tau)g_1;\ L(\tau)g_2] &= dist[\tau \cdot g_1;\ \tau \cdot g_2] \\ &= \arccos \frac{1}{2} \cdot [Tr\ \{\tau \cdot g_2 \cdot (\tau \cdot g_1)^{-1}\} - 1] \\ &= \arccos \frac{1}{2} \cdot [Tr\ (\tau \cdot g_2 \cdot g_1^{-1} \cdot \tau^{-1}) - 1] \\ &= \arccos \frac{1}{2} \cdot [Tr\ (g_2 \cdot g_1^{-1}) - 1] \\ &= dist(g_1;\ g_2) \end{aligned} \tag{35}$$

Thereby we have used the invariance property of the trace of a matrix with respect to the so called similarity transformation. This property may be expressed by

$$Tr\ (\tau \cdot g \cdot \tau^{-1}) = Tr \cdot g \tag{36}$$

which is valid for any two rotations g and τ.
General motion of the group space SO(3) has been defined by an arbitrary pair of rotations τ and σ. It transforms any rotation g according to

$$M(\tau,\ \sigma)g = \tau \cdot g \cdot \sigma^{-1} \tag{37}$$

so that we have the representation

$$M(\tau;\ \sigma) = L(\tau) \cdot R(\sigma) = R(\sigma) \cdot L(\tau) \tag{38}$$

The relation eq(38) shows, in particular, that left and right translations are permutable (commuting). Therefore we obtain, as a consequence, that the angular distance between any rotations g_1, g_2 is invariant under transformations $M(\tau;\ \sigma)$. It should be noted, in addition to the above, that the totality of all possible motions of the space SO(3) constitutes a group which will be denoted as M[SO(3)]. The related group multiplication rules have the form

$$M(\tau_1;\ \sigma_1) \cdot M(\tau_2;\ \sigma_2) = M(\tau_1 \cdot \tau_2;\ \sigma_1 \cdot \sigma_2) \tag{39}$$

for any four rotations τ_1, τ_2, σ_1, σ_2 The group inversion is given by

$$[M(\tau;\ \sigma)]^{-1} = M(\tau^{-1};\ \sigma^{-1}) \tag{40}$$

and the identity transformation may be written in the form

$$E = M(e;\ e) \tag{41}$$

The group of motions M[SO(3)] includes as subgroups both the totality L[SO(3)] of all possible left translations $M(\tau;\ e) = L(\tau)$ and the totality R[SO(3)] of all possible right translations $M(e;\ \sigma) = R(\tau)$. The subgroups are elementwise permutable. The group M[SO(3)] is the algebraic direct sum of its subgroups L[SO(3)] and R[SO(3)].

Another important subgroup of motions is constituted by all possible inner automorphisms $A(\tau) = M(\tau;\ \tau)$. An arbitrary inner automorphism $A(\tau)$ transforms any rotation g according to

$$A(\tau)\mathrm{g} = \tau \cdot \mathrm{g} \cdot \tau^{-1} \tag{42}$$

so that we have the representation

$$A(\tau) = R(\tau) \cdot L(\tau) \tag{43}$$

As it follows from eq(42), the identity rotation e *is* a unique common fixed point for all possible transformation $A(\tau)$

$$A(\tau)e = e \tag{44}$$

Therefore, transformations of this kind may be interpreted as certain analogies of rotations in Euclidean space. In addition to eq(44) we have

$$\mathrm{A}(\tau)(g_1 \cdot g_2) = [A(\tau)\mathrm{g}_1] \cdot [A(\tau)g_2] \tag{45}$$

for any rotations g_1 and g_2. That means, algebraically, each transformation $A(\tau)$ is an isomorphism of the group SO(3) onto itself or in other words $A(\tau)$ *is* an automorphism of SO(3)

Any motion $M(\tau; \sigma)$ of the space SO(3) may be represented in a unique way as the product of an appropriate inner automorphism and a left translation. The decomposition has the form

$$M(\tau; \sigma) = R(\sigma \cdot \tau^{-1}) \cdot A(\tau) \tag{46}$$

In fact, we have the following sequence of equalities

$$\begin{aligned} &[R(\sigma \cdot \tau^{-1}) \cdot A(\tau)]g = (\tau \cdot g \cdot \tau^{-1}) \cdot (\sigma \cdot \tau^{-1})^{-1} \\ &= \tau \cdot g \cdot \tau^{-1} \cdot \tau \cdot \sigma^{-1} = \tau \cdot g \cdot \sigma^{-1} \\ &= M(\tau; \sigma)g \end{aligned} \tag{47}$$

Any motion $M(\tau; \sigma)$ may also be decomposed in the following manner

$$M(\tau; \sigma) = A(\tau) \cdot R(\tau^{-1} \cdot \sigma) \tag{48}$$

Thus, the group of motions M[SO(3)] has been decomposed into the algebraic direct sum of its subgroup A[SO(3)] of all possible inner automorphisms and the subgroup R[SO(3)] of right tranlations. It is seen, after comparison of eq(46) and eq(48), that the right translations and the inner automorphisms are not permutable in contrast with the above considered case of left and right translations. In an analogous way we obtain the representations

$$M(\tau; \sigma) = L(\tau \cdot \sigma^{-1}) \cdot A(\sigma) \tag{49}$$

$$M(\tau; \sigma) = A(\sigma) \cdot L(\sigma^{-1} \cdot \tau) \tag{50}$$

so that any motion may be expressed as a combination of an appropriate left translation and an inner automorphism. In accordance to that, the group of motions M[SO(3)] has been decomposed into the algebraic direct sum of its subgroups L[SO(3)] and A[SO(3)] which are elementwise unpermutable by virtue of the equalities eq(49) and eq(50).

Regular partitions of the group space SO(3).

We may now realize a procedure in the group space SO(3) which is analogous, in some extent, to constructing the Wigner-Seitz cell of a crystal space or the Brillouin zone in the reciprocal space. Let

$$T = \{\tau_1, \ldots, \tau_N\} \tag{51}$$

be an arbitrary finite set of rotations. We may further introduce, for any τ_i, the subdomain $D(\tau_i)$ that includes all possible rotations which are nearer (in the sense of angular distance) to the rotation τ_i than to any other rotation τ_j ($j = 1, \ldots, N$; $j \neq i$) of the set T. So, a rotation g belongs to the domain $D(\tau_i)$ if and only if the following inequality is satisfied

$$dist(g; \tau_i) < \min_{\substack{j = 1, \ldots, N \\ j \neq i}} dist(g; \tau_j) \tag{52}$$

As it follows from the definition, any rotation g either belongs to one of the domains $D(\tau_1)$, ..., $D(\tau_N)$ or it lies on the topological boundary between neighboring domains of the family, so that the family of domains $D(\tau_1)$, ..., $D(\tau_N)$ constitutes a partition of the whole group space SO(3). The partition will be called the Dirichlet-Voronoi partition dual to the finite set of rotations eq(51).

Dirichlet-Voronoi partitions of general form are the subject of potential interest as a base for further development of the so-called discrete methods in three-dimensional texture analysis. However, in the frame of the present paper only a special class of partitions will be considered which corresponds to the case when the finite set of rotations eq(51) is identical to the totality P_O^+ of all possible elements of the proper point group for the crystallite K_O of original orientation. In this case the related Dirichlet-Voronoi partition

$$D(e),\ D(k_1),\ ...,\ D(k_N) \tag{53}$$

is *regular* with respect to the finite group of motions (right translations)

$$M(e;\ e) = R(e),\ M(e;\ k_1) = R(k_1),\ ...,\ M(e,\ k_N) = R(k_N) \tag{54}$$

which is generated by elements of P_O^+, that means the domains eq(53) are mutually congruent and the congruence has been realized with the help of the transformations eq(54) .

In fact, one can immediately verify, using the invariance property of the angular distance function $dist(g_1;\ g_2)$ with respect to motions, that the right translation $M(e;\ k_j^{-1} \cdot k_j) = R(k_j^{-1} \cdot k_i)$ transforms the domain $D(k_i)$ into the domain $D(k_j)$

$$R(k_j^{-1} \cdot k_i)\ D(k_i) = D(k_j) \tag{55}$$

The congruence property eq(55) implies particularly that all domains of the partition eq(53) have one and the same group invariant volume so that we obtain the following interrelation

$$volD(k_i) = \frac{vol[\mathrm{SO}(3)]}{ordP_O^+} \tag{56}$$

whereby $ordP_O^+ = N + 1$ denotes the total number of elements of the proper point group and $vol(D)$ *is* the group invariant volume of an arbitrary subdomain D in the group space SO(3). Concerning the concept of group invariant volume see for example in (Bunge, 1982).

The topological boundary $B(k_i)$ of the domain $D(k_i)$ includes all those and only those rotations which obey the following equality

$$dist(k_i;\ g) = \min_{\substack{j = 0,\ 1,\ ...,\ N \\ j \neq i}} dist(k_j;\ g) \tag{57}$$

After joining of the boundary $B(k_i)$ to the open domain $D(k_i)$ we obtain the so-called closed domain

$$\bar{D}(k_i) = D(k_i)\ \cup\ B(k_i) \tag{58}$$

Any of the closed Dirichlet-Voronoi domains may be used to construct the whole orientation space of a crystallographic texture, since the rotations of the domain $\bar{D}(k_i)$ (but not of the open domain $D(k_i)$) contain all possible orientations of the crystallites. Thereby any two different rotations g_1, g_2 which belong to the interior of $\bar{D}(k_i)$ represent respectively two different orientations of the lattice. The last statement follows immediately from the inequality eq(52).

In contrast with that, any rotation g which belongs to the topological boundary $B(k_i)$ corresponds to at least one (or in some exceptional cases more) additional crystallographically equivalent rotations that lie on the boundary $B(k_i)$, too. The total number of rotations on $B(k_i)$ which are equivalent to any rotation g depends on the position of g with respect to the domains $\bar{D}(k_j)$ neighboring to the domain $\bar{D}(k_i)$ under consideration. If a rotation g is a common point both for $\bar{D}(k_i)$ and for $\bar{D}(k_j)$ then the right translation $R(k_i \cdot k_j)$ transforms it into the rotation $\tilde{g} = g \cdot k_j^{-1} \cdot k_i$ which also belongs to the boundary $B(k_i)$ as follows from the eq(57). In general, one can show, using the characterization of the boundary $B(k_i)$ in terms of the extremal condition eq(57), that the interrelation

$$R(k_i^{-1} \cdot k_j)B(k_j) = B(k_i) \tag{59}$$

must be satisfied for any $i, j = 0, 1, ..., N$. The boundary invariance principle is similar to eq(55). It may be obtained also by consideration of arbitrary small neighborhoods for any boundary rotation g (i.e. by purely topological argumentation). Thus, for any rotation g on the boundary $B(k_i)$, the condition is fulfilled for $k \geq 1$ different rotations on the boundary which are crystallographically equivalent to g. This is equivalent to the condition that g belongs to k different closed domains of partition which are neighboring to $\bar{D}(k_i)$. The number $\mu(g) = k + 1$ for the maximal value k which is possible for a given rotation g will be defined as the multiplicity of g. More detailed analysis of possible values which may be taken by $\mu = \mu(g)$ for all particular proper point groups, as well as a completed geometrical description of equivalent rotations on the boundary of Dirichlet-Voronoi domains will be given in the next parts of the paper.

The so-called true orientation space of a crystal lattice may be obtained from any closed Dirichlet-Voronoi domain $\bar{D}(k_i)$ by identifying the crystallographically equivalent rotations on its boundary $B(k_i)$. By this operation we transpose the closed domain $\bar{D}(k_i)$ onto a new topological space which will be denoted as $\hat{D}(k_i)$. Any point of this space is either a rotation g which belongs to the interior of $D(k_i)$ or (if g lies on $B(k_i)$) it is the total class of all possible boundary rotations

$$g,\ g \cdot k_{j(i)},\ ...,\ g \cdot k_{j(\mu(g))} \tag{60}$$

which are equivalent to g. So, the totality eq(60) should be considered as images which represent, in $\bar{D}(k_i)$, one and the same point of the space $\hat{D}(k_i)$. One can show, using standard argumentation, that the spaces $\hat{D}(k_i)$ for different values $i = 0, 1, ..., N$ are topological equivalent. Therefore, our further considerations will be confined to the space $\hat{D}(e)$ which is associated with the *principal* Dirichlet-Voronoi domain $\bar{D}(e)$.

It should be emphasized that the topological structure of $\bar{D}(e)$ and that of the true orientation space $\hat{D}(e)$ are essentially distinct. Only the part (open subset) $D(e)$ of $\hat{D}(e)$ may be realized as a subdomain of a three-dimensional Euclidean space. The boundary $B(e)$ transforms, after identifying the crystallographically equivalent rotations, into a new two-dimensional topological object $\hat{B}(e)$ which can not be realized as a two-

dimensional closed surface in a three-dimensional Euclidean space. This implies, in particular, the impossibility to introduce a global three-dimensional coordinate system in the true orientation space $\hat{D}(e)$ i.e. a one-to-one correspondence between the space of all possible orientations of a crystallite and the totality of all possible points of a closed subdomain in the Euclidean space. In addition to the above, any point of the true orientation space $\hat{D}(e)$ *is* an interior point i.e. it belongs to the space, together with an open neighborhood. Thus, the space $\hat{D}(e)$ does not possess a boundary, i.e. it is closed in itself. The Poincaré group of the space $\hat{D}(e)$ *is* identical with the original proper point group P_O^+.

Another important consequence of the particular topological structure of the true orientation space $\hat{D}(e)$ must be mentioned. Not every continuous function $f(g)$ defined on the closed principal Dirichlet-Voronoi domain $\bar{D}(e)$ may be considered as a continuous function on the true orientation space. The necessary and sufficient condition for a continuous function $f(g)$ on $\bar{D}(e)$ to be continuous also on the true orientation space $\hat{D}(e)$ *is*

$$f(g_1) = f(g_2) \tag{61}$$

where g_1 and g_2 are two arbitrary, crystallographically equivalent, rotations which belong to the boundary $B(e)$.

The additional "boundary" condition eq(61) must be taken into account for example in analytical and numerical model distributions on the true orientation space $\hat{D}(e)$, since a distribution that depends continuously on the rotation parameters such as rotation axis and rotation angle, on the closed Dirichlet-Voronoi domain $\bar{D}(e)$ may prove to be discontinuous (multivalued) in the true orientation space $\hat{D}(e)$. The continuity condition eq(61) must also be taken into account in discrete methods in order to obtain a "good" approximation for a continuous ODF by "step" distributions on the space $\hat{D}(e)$.

Symmetry properties of Dirichlet-Voronoi domains and of the true orientation space

It is purpose of this section to show the existence of a symmetry center in each Dirichlet-Voronoi domain $\bar{D}(k_i)$ $i = 0, 1, ..., N$. Also, it will be shown that the principal Dirichlet-Voronoi domain $D(e)$ posseses the group of inner automorphisms, generated by the elements of the proper point group P_O^+, as a symmetry group of the domain. The same is valid for an arbitrary Dirichlet-Voronoi domain $D(k_i)$ $i = 1,...,$ N. The related symmetry group may be characterized as the finite group of motions generated by the elements of P_o^+, and also motions of the group admit the rotation k_i as common fixed point. It will be demonstrated on this basis that similar symmetry properties take place in the true orientation space $\hat{D}(e)$. The group inversion transformation

$$I(e)g = g^{-1} \tag{62}$$

will be called the inversion of the group space SO(3) with respect to the center $g = e$. It should be noted that the identity element is a fixed point which is unique for the transformation $I(e)$ so that we have

$$I(e)e = e \tag{63}$$

Since the inverse rotation g^{-1} for any g *is* identical with the transposed rotation g^* we may write

$$Tr(g) = Tr(g^*) = Tr(g^{-1}) \tag{64}$$

This implies for the angular distance

$$dist(g;\ e) = dist(g^{-1};\ e) \tag{65}$$

On the other hand, the rotations belonging to the domain $\bar{D}(e)$ may be characterized by

$$dist(g;\ e) \leq \min_{i=1,\ ...,\ N} dist(g;\ k_i) \tag{66}$$

That means that the rotation g^{-1} belongs to $\bar{D}(e)$ if and only if g belongs to it. Thus, the point $g = e$ is the center of symmetry for the principal domain $\bar{D}(e)$ with respect to the inversion $I(e)$.

Analogously to the inversion eq(62) one can introduce the inversion transformation in the group space SO(3) with respect to an arbitrary point τ of this space by the definition

$$I(\tau)g = \tau \cdot g^{-1} \cdot \tau \tag{67}$$

for any rotation g. It is seen immediately that the rotation $g = \tau$ is an invariant point under the transformation eq(67)

$$I(\tau)\tau = \tau \tag{68}$$

Being repeated twice, the inversion $I(\tau)$ recovers any rotation g at its original position so that we have

$$I(\tau)\{I(\tau)g\} = g \tag{69}$$

Besides that, the angular distance between rotations is invariant under any inversion transformation $I(\tau)$

$$dist(I(\tau)g_1;\ I(\tau)g_2) = dist(g_1;\ g_2) \tag{70}$$

In particular we have

$$dist(I(\tau)g;\ \tau) = dist(g;\ \tau) \tag{71}$$

for any rotation g.

The above formulated properties of inversions $I(\tau)$ may be applied to the special case $\tau = k_i$ $i = 0, 1, ..., N$; when we deal with the inversion $I(k_i)$ of the whole group space SO(3) with respect to an arbitrary element k_i of the proper point group P_O^+. The characterization of the Dirichlet-Voronoi domain $\bar{D}(k_i)$ as the totality of all possible rotations satisfying the inequality

$$dist(g;\ k_i) \leq \min_{\substack{j=0,\ 1,\ ...,\ N \\ j \neq i}} dist(g;\ k_j) \tag{72}$$

in combination with the invariance property eq(71) shows that the domain $\bar{D}(k_i)$ is invariant under the inversion transformation $I(k_i)$. Thus, the point $g = k_i$ plays the role of a symmetry center for $\bar{D}(k_i)$ with respect to the inversion $I(k_i)$. The same result is naturally valid for any open Dirichlet-Voronoi domain $D(k_i)$.

Now it will be demonstrated that each Dirichlet-Voronoi domains $\bar{D}(k_i)$ $i = 0, 1, ..., N$ possesses some additional symmetry transforms generated by elements of the proper point group P_O^+. First of all, symmetry properties of such kind will be obtained for the principal Dirichlet-Voronoi domain $\bar{D}(e)$. Let

$$A(e) = E, A(k_1), ..., A(k_N) \tag{73}$$

be the group of all possible inner automorphisms eq(42), generated by the elements of P_O^+. By virtue of the general congruence interrelations eq(55) and eq(59) any right translation $R(k_i)$ transforms the principal domain $\bar{D}(e)$ onto the domain $\bar{D}(k_i^{-1})$. Analogously, the corresponding left translation $L(k_i)$ maps this latter domain back onto $\bar{D}(e)$. Therefore, we may conclude, taking into account the representation eq(43) that, any inner automorphism eq(73) maps the principal domain $\bar{D}(e)$ onto itself. Thus, the totality eq(73) may be considered as a symmetry group for the principal Dirichlet-Voronoi domain. It may be observed, in addition to the above, that the group inversion $I(e)$ and any inner automorphism $A(k_i)$ are permutable as transformations of the group space SO(3)

$$I(e) \cdot A(k_i) = A(k_i) \cdot I(e) \quad i = 0, 1, ..., N \tag{74}$$

Besides that, any transformation eq(74) preserves the angular distance and it maps the domain $\bar{D}(e)$ onto itself. That means, the principal Dirichlet-Voronoi domain $\bar{D}(e)$ admits the extended group of symmetries (i.e. the group of reflections) as following

$$A(e) = E, A(k_1), ..., A(k_N); \tag{75}$$

$$I(e), I(e) \cdot A(k_i), ...; I(e) \cdot A(k_i). \tag{76}$$

Multiplication rules (i.e. the group table) for the extended group eq(75, 76) are completely determined by the general relations eq(39) for motions and by the constitutive relation eq(74). This latter relation permits to multiply inner automorphisms eq(75) and inner automorphisms "with inversion" eq(76).

The symmetry group generated by the elements of P_O^+ and by the inversion $I(k_i)$ for an arbitrary Dirichlet-Voronoi domain $\bar{D}(k_i)$ $i = 1, ..., N$ may be obtained from the transformations eq(75, 76) by the operation of conjugation with the help of the corresponding right translation $R(k_i)$. So that the list of symmetry transformations for the domain $\bar{D}(k_i)$ has the following form

$$A(e) = E, R(k_i^{-1}) \cdot A(k_1) \cdot R(k_i), ..., R(k_i^{-1}) \cdot A(k_N) \cdot R(k_i) \tag{77}$$

$$I(k_i) = R(k_i^{-1}) \cdot I(e) \cdot R(k_i), R(k_i^{-1}) \cdot I(e) \cdot A(k_i) \cdot R(k_i), ... \\ ..., R(k_i^{-1}) \cdot I(e) \cdot A(k_N) \cdot R(k_i) \tag{78}$$

The symmetry center k_i of the domain $\bar{D}(k_i)$*is* a common fixed point both for "proper" symmetries eq(77) and for "symmetries with inverion" eq(78).

It will be shown, in conclusion of this section, that any symmetry transform eq(75, 76) of the principal Dirichlet-Voronoi domain $\bar{D}(e)$ may also be considered as a

symmetry transform of the true orientation space $\hat{D}(e)$. In fact, any symmetry eq(75, 76) transforms the open domain $D(e)$ continuously and in one-to-one correspondence onto itself. The same is valid for its topological boundary $B(e)$. In addition to that, if τ_1 and τ_2 are arbitrary crystallographically equivalent rotations on $B(e)$

$$\tau_2 = R(k_j)\tau_1 \tag{79}$$

then the boundary rotations $A(k_i)\tau_1$ and $A(k_i)\tau_2$ are also crystallograpgically equivalent. In fact we may write

$$A(k_i)\tau_2 = R(k_i \cdot k_j \cdot k_i^{-1})A(k_i)\tau_1 \tag{80}$$

for any transform $A(k_i)$ of the subgroup eq(75). That means, any transform eq(75) is correctly defined not only on the closed Dirichlet-Voronoi domain $\bar{D}(e)$ but also on the true orientation space $\hat{D}(e)$. In contrast with the above, the group inversion $I(e)$ cannot preserve the crystallographic equivalence relations between rotations. Therefore, the transforms eq(76) cannot be extended from the open principal domain $D(e)$ onto the true orientation space $\hat{D}(e)$. However, the relative multiplicity $\mu(\tau)$ of any boundary rotation τ is invariant under the transformations eq(76).

Concluding remarks

The above described reduction procedure for the group space SO(3) with respect to the proper point group P_O^+ in purely metric terms is analogous, to certain extent, with the partition of a crystal space into Wigner-Seitz cells or with the one of the reciprocal space into Brillouin zones. However, the analogy extends not too far. In contrast with the case of Euclidean space, any "regular" partition of the space SO(3) admits only a finite number of congruent cells (i.e. Dirichlet-Voronoi domains in our terms). Moreover, there exists only a finite number of different (i.e. mutually non-congruent) regular partitions of the group space SO(3). That implies, in particular, the impossibility to construct a regular partition of SO(3), the domains of which have arbitrarily small size (for instance angular diameter or group invariant volume). The obstacle for that is the more complicated topological structure of the space SO(3) (in comparison with the euclidean case).

In the paper, the angular distance function eq(26) was used in order to define the Dirichlet-Voronoi partition of SO(3) dual to the proper point group P_O^+. The same partition eq(53) may be obtained by using the so-called "trace distance" function defined by the expression

$$dist_{tr}(g_1;\ g_2) = Tr\ [(g_2^* - g_1^*) \cdot (g_2 - g_1)] \tag{81}$$

whereby g_1 and g_2 are two arbitrary rotations; $g^* = g^{-1}$ is the rotation transposed to g. The distance eq(81) as well as the angular distance eq(26) satisfy the metric axioms 1), 2), 3), and also the trace distance is invariant under left and right translations of the space SO(3). However, in contrast with eq(26), the trace distance is not inner. The use of the trace distance in order to construct Dirichlet-Voronoi domains $\bar{D}(k_i)$ was proposed in the unpublished paper (Yashnikov, 1982). It should be mentioned that any translation invariant distance function on the group of rotations furnishes the same domains of partition $\bar{D}(k_i)$ as the angular distance. Thus, the resultant reduction procedure does not depend on the choice of translation invariant distance of the space SO(3).

A geometrical characterization of any Dirichlet-Voronoi domain $\bar{D}(k)$ as a polyhedron of the group sapce SO(3), as well as a general geometric form of the reduction procedure suitable for any proper crystallographic point group, will be given in the second part of the paper.

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