SHORT COMMUNICATIONS

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On the uniformity of crystallographic orbits

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Abstract

The uniformity characteristics R of crystallographic orbits are studied by the geometrical analysis of the fundamental regions for the corresponding space groups. It is shown that R is no more than the diameter of a fundamental region. On this basis, the upper bounds for R values of the orbits of cubic space groups are determined with respect to the parameter **a** of the cubic lattice.

Let E^n be an n-dimensional Euclidean space with metric $d(x, y) = [\sum(x_i - y_i)^2]^{1/2}$, where $x = (x_1, \ldots, x_n)$, $y = (y_1, \ldots, y_n)$ and $\mathbf{E}(n)$ is a group of all isometries in E^n.

Definition 1. Subgroup $\mathbf{G}$ of $\mathbf{E}(n)$ is called a space group if it acts in E^n discontinuously and has a compact fundamental region $F_\mathbf{G}$.

Definition 2. Let $\mathbf{G}$ be a space group in E^n. A point set $\{x | x \in E^n\}$ is called a crystallographic orbit $O(\mathbf{G}, x_0)$ if for any point $x \in \{x\}$ there exists an isometry g, $g \in \mathbf{G}$, such that $x = g \cdot x_0$:

$$O(\mathbf{G}, x_0) := \{x_i | x_i = g \cdot x_0, \quad g \in \mathbf{G}\}.$$

Definition 3. A point set $\{x\}$ in R^n is called an (r, R) set if it fulfils the following conditions:

(i) there exists a fixed real r, $r > 0$, such that for any two points $x_i, x_j \in \{x\}$, $i \neq j$, it is fulfilled that $d(x_i, x_j) \geq r$;

(ii) there exists a fixed real R, $R = \sup\{R'\}$, $R' > 0$, where R' is the radius of a sphere that can be embedded in E^n and contains no points from $\{x\}$ in the interior. We call R the uniformity characteristic of $\{x\}$.

(r, R) sets are also called Delone sets in honour of B. N. Delone (Galiulin, 1980).

Because $\mathbf{G}$ is discontinuous, each crystallographic orbit $O(\mathbf{G}, x_0)$ is a discrete point set. Its r characteristic is equal to the minimal distance between its points: $r = \inf\{d(x_i, x_j)\}$, $x_i, x_j \in O(\mathbf{G}, x_0)$, $i \neq j$. For general orbits of most space groups, we can choose the point x_0 such that r will be as small as desired and, therefore, in this case r characteristic of $O(\mathbf{G}, x_0)$ does not depend on the type of group $\mathbf{G}$.

It may be shown that each crystallographic orbit also has a uniformity characteristic R, *i.e.* it is uniformly distributed in E^n. In accordance with Schoenflies–Bieberbach's theorem, each space group $\mathbf{G}$ in E^n has a normal translational subgroup $\mathbf{T}$ of finite index and hence each crystallographic orbit $O(\mathbf{G}, x_0)$ may be described as the union of a finite number of equivalent lattices, *i.e.* as a multilattice. Since each lattice is an (r, R) set, $O(\mathbf{G}, x_0)$ is also an (r, R) set. The uniformity characteristics R_L of a single lattice are usually used in calculating the Dirichlet domain partitions on the whole crystallographic orbit (Engel, 1986). The goal of this paper is to show that these estimates may be reduced by the geometrical analysis of the corresponding space group.

Let $\mathbf{G}$ be a space group and $F_\mathbf{G}$ be one of its fundamental regions. There are two important properties of $F_\mathbf{G}$:

(i) there is no isometry g, $g \in \mathbf{G}$, such that $y_i = g \cdot y_j$ for any two points $y_i, y_j \in F_\mathbf{G}$, $i \neq j$;

(ii) for any point $y_i \in E^n$, there is a point $y_j \in F_\mathbf{G}$ such that $y_i = g \cdot y_j$, $g \in \mathbf{G}$.

The application of all the isometries of $\mathbf{G}$ to $F_\mathbf{G}$ produces an orbit $O(\mathbf{G}, F_\mathbf{G})$, which is a space partition because, for each point y, $y \in E^n$, there exists a region $F'_\mathbf{G}$ and an isometry g from $\mathbf{G}$ such that $y \in F'_\mathbf{G}$, $F'_\mathbf{G} = g \cdot F_\mathbf{G}$. Otherwise, the condition (ii) mentioned above is not fulfilled.

We define a diameter $\operatorname{diam} F_\mathbf{G}$ of fundamental region $F_\mathbf{G}$ as a least upper bound for the distances between their points:

$$\operatorname{diam} F_\mathbf{G} := \sup\{d(y_i, y_j)\}, \quad y_i, y_j \in F_\mathbf{G}.$$

Theorem 1. The uniformity characteristic R of crystallographic orbit $O(\mathbf{G}, x_0)$ is no more than the diameter $\operatorname{diam} F_\mathbf{G}$ of the corresponding space group $\mathbf{G}$:

$$R \leq \operatorname{diam} F_\mathbf{G}.$$

Proof. Let $R > \operatorname{diam} F_\mathbf{G}$, that is, $R = \operatorname{diam} F_\mathbf{G} + \varepsilon$, $\varepsilon > 0$. We consider a sphere $S(y, R)$ in E^n. For any centre y of the sphere $S(y, R)$, there exists a fundamental region $F'_\mathbf{G}$, $F'_\mathbf{G} = g \cdot F_\mathbf{G}$, $g \in \mathbf{G}$, such that $y \in F'_\mathbf{G}$. Since $R > \operatorname{diam} F_\mathbf{G} \Rightarrow R > \operatorname{diam} F'_\mathbf{G} \Rightarrow F'_\mathbf{G} \subset S(y, R)$. That is, the sphere $S(y, R)$ contains in the interior at least one fundamental region $F'_\mathbf{G}$ from the orbit $O(\mathbf{G}, F_\mathbf{G})$ and therefore it contains inside at least one point x_k from any orbit $O(\mathbf{G}, x_0)$. Hence, $R > d(x_k, y)$ for any y, which is in contradiction with condition (ii) of definition 3. For $R = \operatorname{diam} F_\mathbf{G}$ (or $R < \operatorname{diam} F_\mathbf{G}$), we can choose y and x_k such that $d(x_k, y) = \operatorname{diam} F_\mathbf{G}$ $[d(x_k, y) < \operatorname{diam} F_\mathbf{G}]$ and therefore it may appear that the sphere $S(y, R)$ is empty with respect to the points from $O(\mathbf{G}, x_0)$. The theorem is proved.

The uniformity characteristic $R_{\max}$ of each cubic space group in E^3 is determined relative to the value of the parameter **a** of the cubic lattice. The fundamental regions for cubic groups were found by Koch & Fischer (1974). These types are shown in Fig. 1 in which their diameters are drawn as thick lines. The designations of $F_\mathbf{G}$ types are taken from Koch & Fischer (1974). Near each vertex of $F_\mathbf{G}$, its coordinates are indicated as integers n, $n \times \mathbf{a}/8$. The lengths of $\operatorname{diam} F_\mathbf{G}$ are given in Table. 1. It must be noted that the fundamental regions $4/4/a$, $4/4/d$, $5/5/c$ and $8/6/a$ may have different coordinates of the same corners for different space groups. For these types of $F_\mathbf{G}$, the second variant of vertices is given in square brackets and denoted by * in Fig. 1 and Table 1. For most cubic groups,

Koch & Fischer (1974) determined different possible variants of F_G to be chosen. In Table 1, the upper bounds R_{max} for R values are given, which are calculated from the minimal diam F_G. If theorem 1 gives an estimate of R that is greater than R_L for a single lattice, in Table 1 the latter is given.

It can be seen from Table 1 that only for 15 cubic space groups the upper bounds R_{max} determined from theorem 1 are smaller than R_L. The minimal bounds R_{max} are obtained for space groups $Ia\bar{3}d$ [$R_{max} = \mathbf{a}3^{1/2}/(4 \times 2^{1/2})$], $Fd\bar{3}c$ [$R_{max} = \mathbf{a}/(2 \times 2^{1/2})$] and $Fm\bar{3}c$ ($R_{max} = \mathbf{a}3^{1/2}/4$). The following values are for a single F lattice ($R_{max} = \mathbf{a}/2$) and for a single I lattice ($R_{max} = \mathbf{a}5^{1/2}/4$). The maximal R_{max} is for a single P lattice ($R_{max} = \mathbf{a}3^{1/2}/2$).

The upper bounds R_{max} for R values of $O(\mathbf{G}, x_0)$ are exploited in the theory of Dirichlet domain partitions on crystallographic orbits (Engel, 1986). For this purpose, the R characteristics for

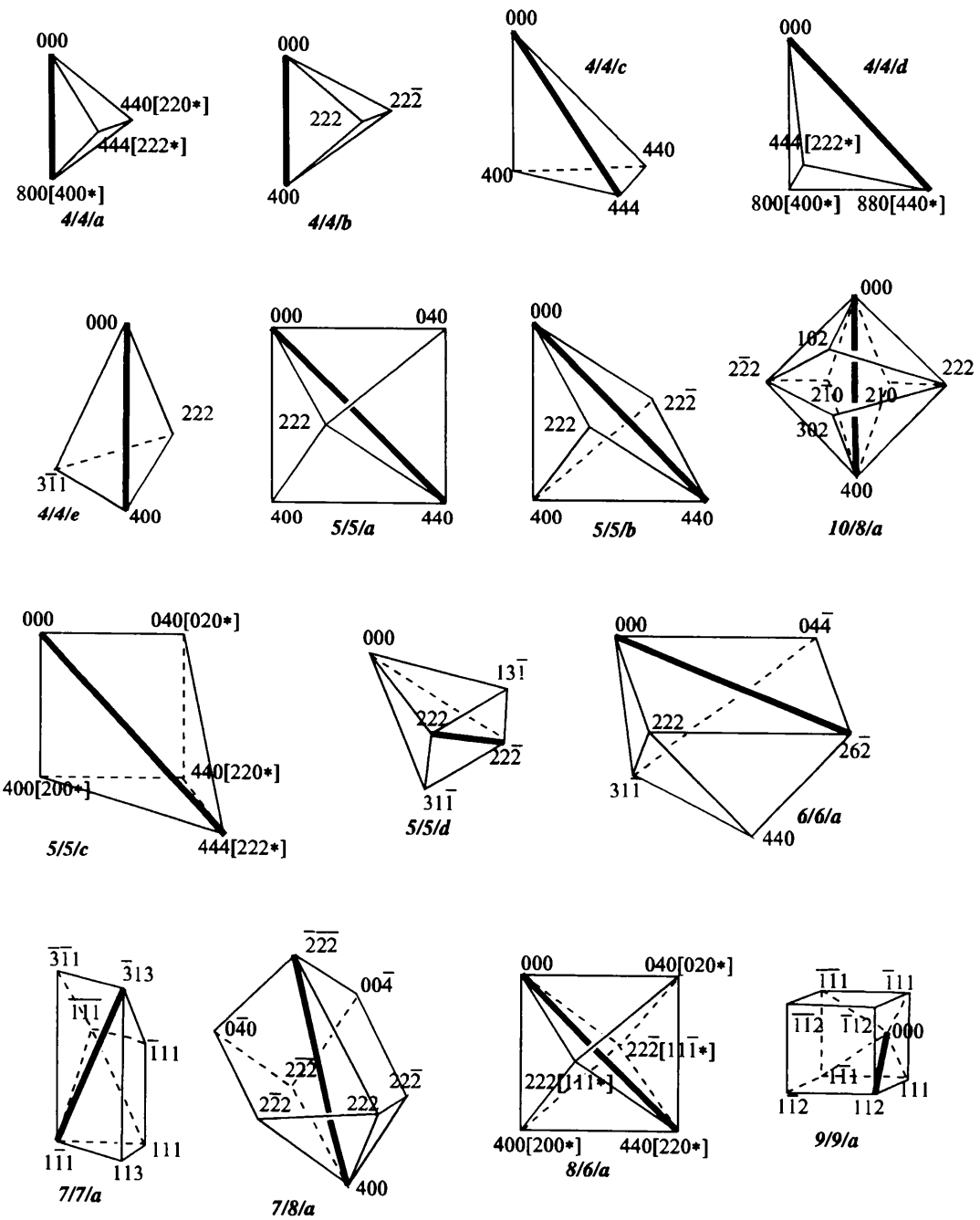

Fig. 1. Fundamental regions of the cubic space groups with diameters drawn as thick lines.

Table 1. *Fundamental regions F_G, their diameters and the upper bounds R_{max} for R values of the crystallographic orbits of cubic space groups*

Space group	F_G	diam $F_G \times \mathbf{a}$	$R_{max} \times \mathbf{a}$	Space group	F_G	diam $F_G \times \mathbf{a}$	$R_{max} \times \mathbf{a}$
$P23$	$4/4/d$	$2^{1/2}$	$3^{1/2}/2$	$P4_132$	$6/6/a$	$(11)^{1/2}/4$	$(11)^{1/2}/4$
$F23$	$10/8/a$	$1/2$	$1/2$	$I4_132$	$7/7/a$	$3^{1/2}/(2\times 2^{1/2})$	$5^{1/2}/4$
	$5/5/b$	$1/2^{1/2}$					
$I23$	$4/4/a$	1	$5^{1/2}/4$	$P\bar{4}3m$	$4/4/a^*$	$1/2$	$3^{1/2}/2$
	$5/5/c$	$3^{1/2}/2$					
	$8/6/a$	$1/2^{1/2}$					
$P2_13$	$7/8/a$	$(11)^{1/2}/4$	$(11)^{1/2}/4$	$F\bar{4}3m$	$4/4/b$	$1/2$	$1/2$
$I2_13$	$5/5/c$	$3^{1/2}/2$	$5^{1/2}/4$	$I\bar{4}3m$	$4/4/c$	$3^{1/2}/2$	$5^{1/2}/4$
					$5/5/b$	$1/2^{1/2}$	
$Pm\bar{3}$	$5/5/c$	$3^{1/2}/2$	$3^{1/2}/2$	$P\bar{4}3n$	$5/5/c$	$3^{1/2}/2$	$1/2^{1/2}$
					$8/6/a$	$1/2^{1/2}$	
$Pn\bar{3}$	$4/4/a$	1	$1/2^{1/2}$	$F\bar{4}3c$	$4/4/b$	$1/2$	$1/2$
	$8/6/a$	$1/2^{1/2}$			$4/4/d^*$	$1/2^{1/2}$	
$Fm\bar{3}$	$4/4/d^*$	$1/2^{1/2}$	$1/2$	$I\bar{4}3d$	$10/8/a$	$1/2$	$1/2$
$Fd\bar{3}$	$4/4/b$	$1/2$	$1/2$	$Pm\bar{3}m$	$4/4/c$	$3^{1/2}/2$	$3^{1/2}/2$
	$5/5/d$	$1/2$					
$Im\bar{3}$	$4/4/c$	$3^{1/2}/2$	$5^{1/2}/4$	$Pn\bar{3}n$	$4/4/c$	$3^{1/2}/2$	$1/2^{1/2}$
	$5/5/a$	$1/2^{1/2}$			$5/5/a$	$1/2^{1/2}$	
					$5/5/b$	$1/2^{1/2}$	
$Pa\bar{3}$	$5/5/c$	$3^{1/2}/2$	$1/2^{1/2}$	$Pm\bar{3}n$	$5/5/a$	$1/2^{1/2}$	$1/2^{1/2}$
	$8/6/a$	$1/2^{1/2}$					
$Ia\bar{3}$	$5/5/a$	$1/2^{1/2}$	$1/2$	$Pn\bar{3}m$	$5/5/b$	$1/2^{1/2}$	$1/2^{1/2}$
	$10/8/a$	$1/2$					
$P432$	$4/4/a$	$1/2$	$3^{1/2}/2$	$Fm\bar{3}m$	$4/4/a^*$	$1/2$	$1/2$
	$5/5/c$	$3^{1/2}/2$					
$P4_232$	$8/6/a$	$1/2^{1/2}$	$1/2^{1/2}$	$Fm\bar{3}c$	$4/4/a^*$	$1/2$	$3^{1/2}/4$
					$5/5/c^*$	$3^{1/2}/4$	
$F432$	$4/4/b$	$1/2$	$1/2$	$Fd\bar{3}m$	$4/4/e$	$1/2$	$1/2$
	$4/4/d^*$	$1/2^{1/2}$					
$F4_132$	$5/5/d$	$1/2$	$1/2$	$Fd\bar{3}c$	$4/4/e$	$1/2$	$1/(2\times 2^{1/2})$
					$8/6/a^*$	$1/(2\times 2^{1/2})$	
$I432$	$5/5/a$	$1/2^{1/2}$	$5^{1/2}/4$	$Im\bar{3}m$	$4/4/d^*$	$1/2^{1/2}$	$5^{1/2}/4$
	$5/5/b$	$1/2^{1/2}$					
$P4_332$	$6/6/a$	$(11)^{1/2}/4$	$(11)^{1/2}/4$	$Ia\bar{3}d$	$9/9/a$	$3^{1/2}/(4\times 2^{1/2})$	$3^{1/2}/(4\times 2^{1/2})$

single lattices are usually used. The use of smaller R_{max} may be favourable to obtain new theoretical and experimental results.

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