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# SIMPLY TRANSITIVE OPTIMAL BALL PACKINGS FOR THE ORIENTABLE CRYSTALLOGRAPHIC GROUPS OF THE CUBIC SYSTEM[1]

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## Abstract

In this paper we look for densest ball packings of Euclidean space $\mathbf{E}^3$ to given symmetry groups. We restrict our investigation to the 13 orientable (orientation preserving) crystallographic groups of cubic system, and we search for only those packings where the group acts simply transitively on the balls. In order to find the centre of a ball and its radius we will apply an algorithm and the corresponding computer program, which was developed by the second author [15, 10]. In the list of our results we will give the coordinates of the ball centre and the radius, moreover, we will compute the density of the optimal packing and display the corresponding D-V cell for each space group above (see also [9]).

*Keywords:* crystallographic groups, ball packings.

## 1. Introduction

In the first third of the twentieth century a lot of new results appeared in physics with respect to the material science. Applying X-ray diffraction method the crystal structures were investigated. Much earlier A. SCHOENFLIES [12], E. S. FEDOROV [4], [5] and L. BIEBERBACH [2, 3] had built the geometric theory of crystals.

In connection with a crystal and the corresponding crystallographic group it is an interesting and important problem to find the optimal (or densest) ball packing for this group. The question was raised by U. SINOGOWITZ [11] generalising the problem of densest lattice-like ball packing. He solved the corresponding problem in the Euclidean plane (see [11]), however, his three dimensional results (as we know) have not been published.

The symmetry group of the densest lattice-like ball packing is the crystallographic group $\mathbf{Fm\bar{3}m}$ (no. 225) (this is the complete symmetry group of the

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face centred cubic point lattice), the density is $\sqrt{2}\pi/6 \approx 0.74048$. The same density appears also in cases of some other regular and non-regular ball systems. Á. G. HORVÁTH and E. MOLNÁR in [7] proved that the density of the optimal ball packing is also $\sqrt{2}\pi/6$ for all the ten fixed point free crystallographic groups, and they determined their structure.

This work is related with a graphic software being in progress by our Department to the computer package CARAT, developed by colleagues in Aachen headed by W. PLESKEN. CARAT and many links to web sites in the topic of crystallographic groups is available via http://wwwb.math.rwth-aachen.de/carat/. A simple presentation of planar crystallographic groups and D-V cells can be found in the site http://www/math.bme.hu/ geom/Pattern2D/Pattern2D. html.

## 2. Crystallographic Groups and Ball Packings

Let Iso $\mathbb{E}^3$ denote the *group of isometries* of the Euclidean space $\mathbb{E}^3$.

**Definition 1** Let $\mathbf{G}$ be a subgroup of Iso $\mathbb{E}^3$, and let denote by

$$X^{\mathbf{G}} = \{X^{\mathbf{g}} : \mathbf{g} \in \mathbf{G}\} \subset \mathbb{E}^3$$

the orbit of a point $X \in \mathbb{E}^3$ under $\mathbf{G}$. We say that $\mathbf{G}$ is a *discrete transformation group* of $\mathbb{E}^3$ if $X^{\mathbf{G}}$ is a discrete point set (i.e. it does not contain any accumulation point) for all $X \in \mathbb{E}^3$.

**Definition 2** The point set $\mathcal{F}$ is said to be a *fundamental domain* of the discrete transformation group $\mathbf{G}$ if the following statements hold:

- $\mathcal{F} \subset \mathbb{E}^3$ is closed and simply connected;
- $\mathcal{F} \cap X^{\mathbf{G}} \neq \emptyset$ for all $X \in \mathbb{E}^3$;
- if $X, Y \in \operatorname{Int} \mathcal{F}$ and $Y \in X^{\mathbf{G}}$ then $Y = X$.

In this way the images of $\mathcal{F}$ under $\mathbf{G}$ tile the space $\mathbb{E}^3$ without gaps and overlaps.

**Definition 3** A discrete transformation group $\mathbf{G}$ is said to be a *crystallographic group* (or shortly *space group*) if it has a *compact* (bounded and closed) *fundamental domain* $\mathcal{F}$.

**Remark 1** Usually the shape of the fundamental domain of a crystallographic group is not determined uniquely. For example it is also possible that some fundamental domain of a group is not bounded, however, the group has also a bounded fundamental domain. The volume of the domain is finite and determined uniquely by the group.

In the following let $\mathbf{G}$ be a fixed crystallographic group of $\mathbb{E}^3$. We will denote by $\varrho(X, Y)$ the distance of two points $X, Y$.

**Definition 4** We say that the point set

$$\mathcal{D}(K) = \{X \in \mathbb{E}^3 \,:\, \varrho(K, X) \leq \varrho(K^{\mathbf{g}}, X) \text{ for all } \mathbf{g} \in \mathbf{G}\}$$

is the *Dirichlet–Voronoi cell* (D-V cell) to $\mathbf{G}$ around the kernel point $K \in \mathbb{E}^3$.

**Definition 5** We say that

$$\mathbf{G}_X = \{\mathbf{g} \in \mathbf{G} \,:\, X^{\mathbf{g}} = X\}$$

is the *stabiliser subgroup* of $X \in \mathbb{E}^3$ in $\mathbf{G}$.

**Remark 2** We can see that the D-V cell is always a convex domain bounded by finitely many planar faces. Moreover, if the stabiliser subgroup $\mathbf{G}_K$ of the kernel point $K$ is trivial, i.e. $\mathbf{G}_K = \mathbf{1}$ the identity, then $\mathcal{D}(\mathcal{K})$ is a fundamental domain of $\mathbf{G}$.

**Definition 6** We say that $\mathbf{N}(\mathbf{G}) \leq \text{Iso}\,\mathbb{E}^3$ is the metric normalizer of the crystallographic group $\mathbf{G}$ if

$$\mathbf{N}(\mathbf{G}) = \{\mathbf{h} \in \text{Iso}\,\mathbb{E}^3 \,:\, \mathbf{h}^{-1}\mathbf{G}\mathbf{h} = \mathbf{G}\}.$$

Namely, $\mathbf{h} \in \mathbf{N}(\mathbf{G})$ if and only if $(X^{\mathbf{G}})^{\mathbf{h}} = (X^{\mathbf{h}})^{\mathbf{G}}$ for each point $X \in \mathbb{E}^3$.

**Remark 3** It can be proved that $\mathbf{N}(\mathbf{G}) \geq \mathbf{G}$ is also a crystallographic group if $\mathbf{G}$ belongs to the cubic system, so its fundamental domain can be chosen as a part of a fundamental domain of $\mathbf{G}$:

$$\mathcal{F}_{\mathbf{N}(\mathbf{G})} \subseteq \mathcal{F}_{\mathbf{G}}.$$

**Definition 7** Assume that the stabiliser $\mathbf{G}_{\mathbf{K}} = \mathbf{1}$, i.e. $\mathbf{G}$ acts simply transitively on the orbit of a point $K$. Then let $\mathcal{B}(K)$ denote the *greatest ball* of centre $K$ inside the D-V cell $\mathcal{D}(K)$, moreover let $r(K)$ denote the *radius* of $\mathcal{B}(K)$. It is easy to see that

$$r(K) = \min_{\mathbf{g} \in \mathbf{G}-\mathbf{1}} \frac{1}{2}\varrho(K, K^{\mathbf{g}}).$$

The $\mathbf{G}$-images of $\mathcal{B}(K)$ form a ball packing $\mathcal{B}^{\mathbf{G}}(K)$ with centre points $K^{\mathbf{G}}$. The *density* of this packing is

$$\delta(K) = \frac{\text{Vol}\,\mathcal{B}(K)}{\text{Vol}\,\mathcal{D}(K)} = \frac{\frac{4}{3}\pi r^3(K)}{\text{Vol}\,\mathcal{D}(K)}.$$

It is clear that the orbit $K^{\mathbf{G}}$ and the ball packing $\mathcal{B}^{\mathbf{G}}(K)$ has the same symmetry group, moreover this group contains the starting crystallographic group $\mathbf{G}$:

$$\text{Sym}\,K^{\mathbf{G}} = \text{Sym}\,\mathcal{B}^{\mathbf{G}}(K) \geq \mathbf{G}.$$

**Definition 8** We say that the orbit $K^{\mathbf{G}}$ and the ball packing $\mathcal{B}^{\mathbf{G}}(K)$ is **characteristic** if $\text{Sym}\,K^{\mathbf{G}} = \mathbf{G}$, else the orbit is not characteristic (n. char).

## 3. Finding Optimal Ball Packings

Let **G** be one of 13 orientable (orientation preserving) crystallographic groups of the cubic system. The number and the short name of these groups in the International Tables [6] are as follows:

195. **P23**, 196. **F23**, 197. **I23**, 198. **P2$_1$3**, 199. **I2$_1$3**,
207. **P432**, 208. **P4$_2$32**, 209. **F432**, 210. **F4$_1$32**,
211. **I432**, 212. **P4$_3$32**, 213. **P4$_1$32**, 214. **I4$_1$32**.

We know that the groups **P4$_3$21** and **P4$_1$32** are isomorphic, forming an enantiomorphic pair. So their optimal ball packings will be congruent (by a plane reflection), moreover, the radius of balls and the density of packings will also be equal.

*Our problem is* to find a point $K \in \mathbb{E}^3$ and the orbit $K^{\mathbf{G}}$ for a fixed group **G** above such that $\mathbf{G_K} = \mathbf{1}$ and the density $\delta(K)$ of the corresponding ball packing $\mathcal{B}^{\mathbf{G}}(K)$ is maximal. In this case the ball packing $\mathcal{B}^{\mathbf{G}}G(K)$ is said to be *optimal.* We look for the coordinates of $K$ in the coordinate system of cubic lattice (fixed in the International Tables), the maximal radius $r(K)$ of the balls, and the density $\delta(K)$ of the packing.

We remark that in the general case when the lattice of the group has more affine parameters (not only one similarity factor as for the cubic system), the problem of optimal ball packing can be much more complicated. Then we have to find the densest ball packing for fixed parameters, and we have to vary them to get the optimal ball packing. However, the groups considered in this paper belong to the cubic system, so they have only a similarity parameter.

In earlier papers [13, 14] the second author examined some special groups, and determined the optimal ball packings without computer. The computations showed the difficulties of the problem. Having studied these instructive examples he developed an algorithm for finding the densest ball packing [15], and with Csilla MÁTÉ they implemented it for computer [10]. By remark 3, the program examines the points of the fundamental domain $\mathcal{F}_{\mathbf{N(G)}}$ of the metric normaliser of **G**, and it computes the coordinates of an optimal kernel point $K$ with arbitrary precision, giving also the radius $r(K)$ and the density $\delta(K)$.

With E. MOLNÁR we developed also a general D-V cell algorithm in [9], which is able to find the incidence structure of the D-V cell for a point set of a $d$-dimensional space of constant curvature. The first author implemented this algorithm for computer in the case of 3-dimensional Euclidean crystallographic groups. The program generates the orbit $K^{\mathbf{G}}$ of a point $K$ and forms the D-V cell around $K$ with the appropriate face pairing for a set of generators and the algebraic presentation of the group **G**. The program also displays the cell. Listing our results in section 4 we also publish the corresponding cell to each ball packing in our figures.

By the above algorithms in [8] we investigated the transitive (not only simply transitive) optimal ball packings for the crystallographic groups that can be derived

from Coxeter reflection groups by extension. Our method may be applicable to examine similar problems in higher dimensional spaces of constant curvature [1].

## 4. The List of Results with Figures

**G = P23** (No.195), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 8**;
$K$(0.207105, 0.207105, 0.5), n.char; $r \approx 0.207105$, $\delta \approx 0.4465$, *Fig. 1*.

**G = F23** (No.196), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 16**;
$K$(0, 0.128532, 0.208047), n.char; $r \approx 0.128531$, $\delta \approx 0.4269$, *Fig. 1*.

**G = I23** (No.197), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 4**;
$K$(0, 0.186016, 0.300938), n.char; $r \approx 0.186001$, $\delta \approx 0.6469$, *Fig. 1*.

**G = P$2_1$3** (No.198), **N(G) = Ia$\bar{3}$d**, **|N(G) : G| = 8**;
$K$(0, 0.25, 0.375), **characteristic**; $r \approx 0.233854$, $\delta \approx 0.6428$, *Fig. 1*.

**G = I$2_1$3** (No.199), **N(G) = Ia$\bar{3}$d**, **|N(G) : G| = 4**;
$K$(0.125, 0.125, 0.375), **characteristic**; $r \approx 0.176777$, $\delta \approx 0.5554$, *Fig. 1*.

**G = P432** (No.207), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 4**;
$K$(0.143086, 0.305938, 0.394492), **characteristic**; $r \approx 0.15618$, $\delta \approx 0.3830$, *Fig. 1*.

**G = P$4_2$32** (No.208), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 4**;
$K$(0, 0.25, 0.25), n.char; $r \approx 0.176777$, $\delta \approx 0.5554$, *Fig. 2*.

**G = F432** (No.209), **N(G) = Pm$\bar{3}$m**, **|N(G) : G| = 4**;
$K$(0.073906, 0.135937, 0.25), n.char; $r \approx 0.109398$, $\delta \approx 0.5265$, *Fig. 2*.

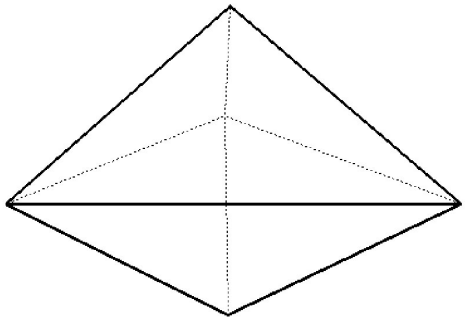
**G = F$4_1$32** (No.210), **N(G) = Pn$\bar{3}$m**, **|N(G) : G| = 4**;
$K$(0.068828, 0.206484, 0.431172), n.char; $r \approx 0.097310$, $\delta \approx 0.3705$, *Fig. 2*.

**G = I432** (No.211), **N(G) = Im$\bar{3}$m**, **|N(G) : G| = 2**;
$K$(0.128672, 0.128672, 0.310703), n.char; $r \approx 0.128672$, $\delta \approx 0.428332$, *Fig. 2*.

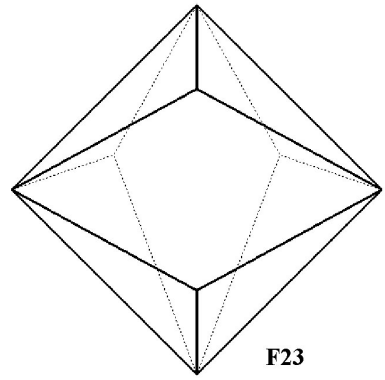
**G = P$4_3$32** (No.212), **N(G) = I$4_1$32**, **|N(G) : G| = 2**;
$K$(0.125, 0.125, 0.375), n.char; $r \approx 0.176777$, $\delta \approx 0.555360$, *Fig. 1*.

**G = P$4_1$32** (No.213), **N(G) = I$4_1$32**, **|N(G) : G| = 2**;
$K$(0.125, 0.375, 0.125), n.char; $r \approx 0.176777$, $\delta \approx 0.555360$, *Fig. 1*.

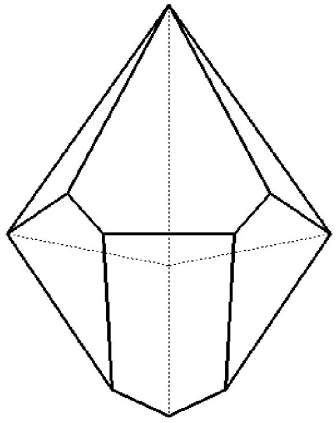
**G = I$4_1$32** (No.214), **N(G) = Ia$\bar{3}$d**, **|N(G) : G| = 2**;
$K$(0.172852, 0.374805, 0.245573), **characteristic**; $r \approx 0.125285$, $\delta \approx 0.395387$, *Fig. 2*.



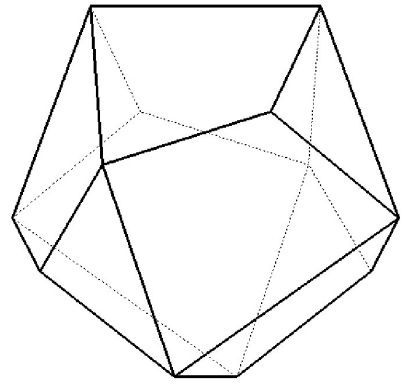
P23



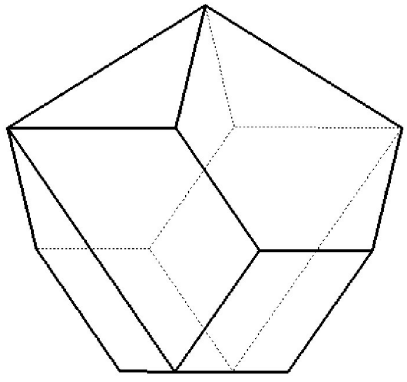
F23



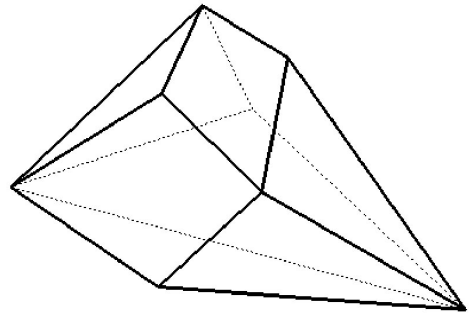
I23



$I2_13$, $P4_332$, $P4_132$

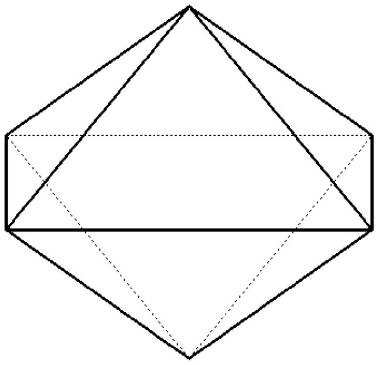


$P2_13$

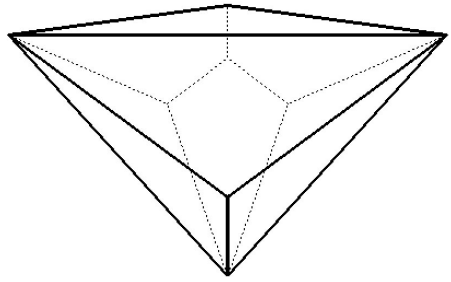


P432

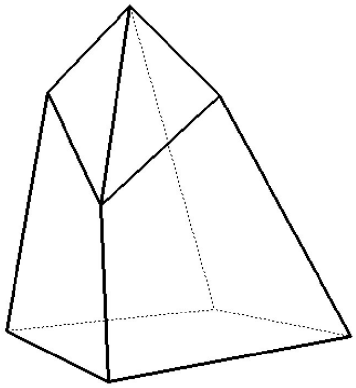
*Fig. 1.*



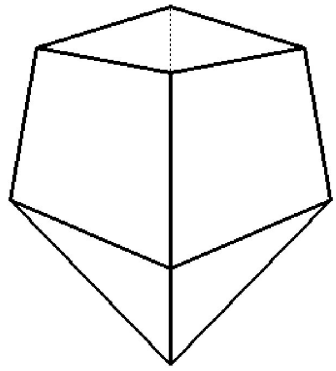
**$P4_232$**



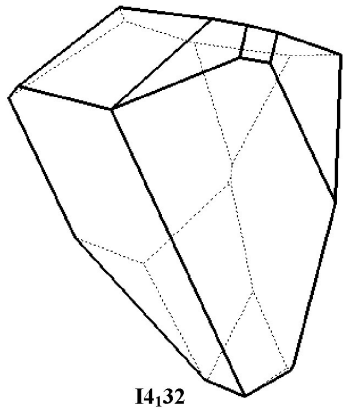
**F432**



**$F4_132$**



**I432**



**$I4_132$**

*Fig. 2.*

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