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Regularities of coordination spheres in the crystal lattice of the cubic symmetry

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Abstract

A procedure that allows us to describe the distribution patterns of atomic sites of the diamond type structure over the coordination spheres is presented. The spatial packing of the coordination spheres is formed by the vertices of the seven base polyhedra with cubic symmetry and the four polyhedra with tetrahedral symmetry. The former is given by a set of the seven regular or semi-regular polyhedra of Platonic and Archimedean solids such as the cube, the truncated cube, the octahedron, the cubic-, truncated-, rhomboidal-, and truncated cubic octahedrons. The latter is given by a set of four other shapes such as the tetrahedron, the rhombohedral-, truncated-, and truncated rhombohedral tetrahedrons.

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1. Introduction

An important characteristic of crystal lattices is the distribution law of atomic sites over the coordination spheres. It is impossible in the traditional crystallography to give a definite answer to the question of how many atomic nodes are contained in an arbitrary j^{th} neighbourhood relative to the node selected as a starting point without the use of some numerical techniques. There is no simple answer about the geometry of an arbitrary coordination sphere. For example, in the case of a simple cubic lattice we can only write down a simple relationship for the first six spheres $n_i = x_i^2 + y_i^2 + z_i^2$, to describe the sequential number of the coordination sphere. A set of focal indices $\{x_i, y_i, z_i\}$ defines the base polyhedron of the sphere as well as the number of nodes. However, the seventh sphere cannot be represented as the sum of the squares of three numbers. The sequence becomes broken.

This study is original and based on earlier publications by Starostenkov[1,2] and Starostenkov and Dmitriev[3,4], where a simple algorithm to determine the distribution of neighbours over the coordination spheres was proposed. Otherwise, there is not much literature available on the subject. According to this methodology such numbers as

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$7, 15, 23, 28, \ldots$, which cannot be represented as the sum of the squares by x_i, y_i, z_i, define the sequential numbers of "zero" spheres. It is given a simple sample function of such spheres on the arbitrary interval from 1 to n_i. Based on the proposed methodology the distribution of atoms and interstitials over the coordination spheres for the crystal lattices of cubic symmetry is described in Starostenkov et al.[5], particularly, simple cubic (SC), body-centred cubic (BCC) and face-centred (FCC) symmetries. These and other abbreviations can be found in Table 1.

The distribution of components over the coordination spheres for a number of alloy superstructures, oxides and perovskites is given in Dmitriev et al.[6]. On the basis of a new approach, this study presents the algorithm which allows us to describe the distribution of nodes for the diamond crystal lattice.

2. Key provisions of the algorithm

2.1. Formulation of the algorithm

The foundation of the algorithm for filling the coordination spheres can be illustrated by the example of a simple cubic lattice. The relationship between the radius of the coordination sphere and its number n_i is given as

$$z_i = a_{lp}(n_i)^{1/2} \tag{1}$$

where a_{lp} is a lattice parameter. Here we introduce the following notation: $R_i = z_i/a_{lp}$. The filling order of the first few coordination spheres is shown in Table 2.

As may be seen from Table 2, all the values R^2 are positive integers which form a set of focal indices. However, some natural numbers cannot be represented as the sum of the squares of three focal numbers. These numbers form "zero" coordination spheres as described in Dmitriev *ea al.*[6]. The general rule for finding such numbers satisfies the following expression

$$N = (8\mu - 1)4\nu^2 \tag{2}$$

where $\mu \in \mathcal{N}$ is the set of natural numbers, $\nu = 1, 2, 4, 6, \ldots$. The actual number of the coordination sphere is related to R^2 as

$$n_i = R^2 - f_i\{(8\mu - 1)\nu^2\}$$

Here R^2 accounts for the number of omitted coordination spheres. Thus, in the case of filling the coordination spheres of a simple cubic lattice the seventh sphere corresponds to the sum of the squares of three integers equal to eight, $n_7 = 8 - 1 = 7$. In such a case $n_{15} = 16 - 2 = 14$ is associated with the fourteenth coordination sphere in the SC lattice (see Table 2.).

There is one more regularity: the number of possible polyhedra is finite and consists of the seven bodies (see Fig. 1).

In the case shown in Table 2, the ninth sphere is filled with the two polyhedra, the octahedron and the truncated cube with a number of nodes 6 and 24, respectively. Thus, the ninth sphere is packed by the two polyhedra with a total of 30 nodes. From the rules obtained it may be deduced that the filling of any coordination sphere is defined in the crystallography of cubic symmetry by one of the seven basic polyhedra or their combinations.

The allocation rules for polyhedra over the coordination spheres can be divided into the following classes: $f(8\mu - m)$, where $m = 0, 2, 3, 7$.

Here the number 8 has a certain meaning. An ideal primitive cell SC has 8 nodes in total. Accordingly, the sampling functions are determined by possible fillings of one or more of the 8 nodes of the primitive cell in a three-dimensional Cartesian coordinate system. The filling procedure of these classes is described by the following algorithm (see Starostenkov et al.[7,8]):

$$f(8\mu - 7) : \begin{cases} (2l \pm 1, 0, 0) \longrightarrow \text{O} \\ (2l \pm 1, 4p, 0) \longrightarrow \text{TO} \\ (2l \pm 1, 2p, 2k) \longrightarrow \text{TC, TCO, RCO} \end{cases}$$

$$f(8\mu - 6) : \begin{cases} (2l \pm 1, 2p \pm 1, 0) \longrightarrow \text{CO, TO} \\ (4l, 2p \pm 1, 2k \pm 1) \longrightarrow \text{TCO, TC, RCO} \end{cases}$$