IUTAM Symposium on Growing solids
June 23-27, 2015, Moscow, Russia

Regularities Filling Coordination Spheres in the Crystal Lattice of the Cubic Symmetry

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An important characteristic of the crystal lattices is the law of distribution of atomic sites on the coordination spheres. In the traditional crystallography is not possible without the use of numerical methods to give a definite answer to the question of how many atomic sites contained in an arbitrary j-th neighborhood relative to the node selected as the starting point. There is no simple answer as to arbitrary geometry of the coordination sphere. For example, in the case of a simple cubic lattice for the first six spheres can write a single bond serial number of the coordination sphere $n_i=x_i^2+y_i^2+z_i^2$. Set $\{x_i, y_i, z_i\}$ indexes coordinates defines a basic polyhedron sphere and the number of nodes. However, the seventh sphere can not be represented as the sum of the squares of three integers. In [1-4] to determine the distribution of neighbors in the coordination spheres proposed a simple algorithm. According to this method numbers, such as 7,15,23,28 ... that cannot be represented as the sum of squares of numbers x_i, y_i, z_i determine the number of spheres of zero supplement. It was represented by a simple function of sample areas on an arbitrary number range from 1 to n_i. In [5], based on the methodology described the distribution of atoms and interstitials on the focal areas for the cubic symmetry of the crystal lattice: a simple cubic, body-centered cubic and face-centered cubic.

In [6-7], it was given to the distribution component of the focal areas for a number of alloy superstructures of the type oxide, perovskites and structures corresponding to the diamond lattice.

According to the ideas developed in this study, any coordination sphere can be represented as one of the 7 basis in the form of regular and semi-regular polyhedrons of Plato and Archimedes or their combinations for cubic crystals (Figure 1).

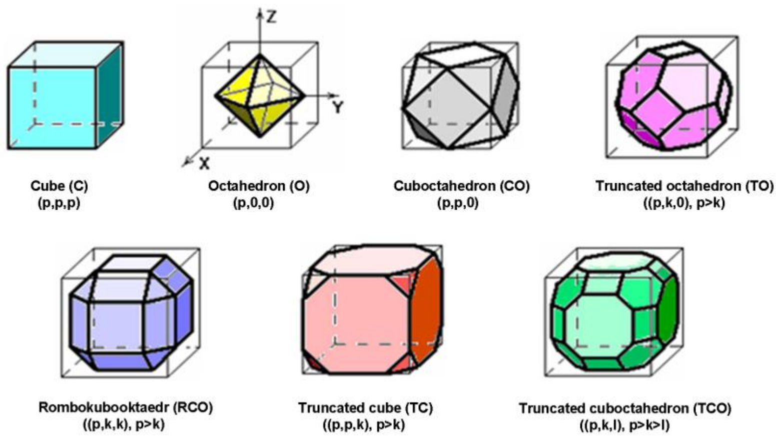

Figure 1: Polyhedrons of cubic symmetry.

In the case of the crystal lattice of the diamond type added to them another 4 types of spatial polyhedrons (Figure 2).

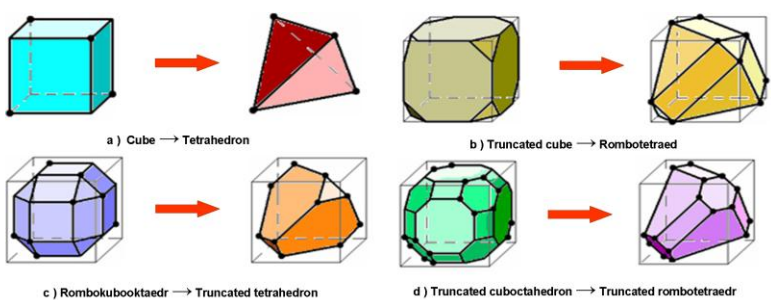

Figure 2: Tetrahedral transformations of polyhedrons.

This representation can be useful in the study design nanoparticles as sets of spatial figures presented here lead to design the most high symmetry packaging of nano-objects conforming to the magic numbers.

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