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ATOMIC STRUCTURE OF MONOELEMENT NANOCRYSTALS

V. Liopo, A. Nikitin, E. Ovchinnikov, A.Sabuts, A. Sitkevich
Yanka Kupala State University of Grodno, Grodno, Belarus

The distribution of atoms in nanocrystals should be analyzed taking into account the structure of the macroscopic analogue [1]. The aim of the study was to develop a method for calculating the crystallographic orbits for single-element spherical nanocrystalline particles with different sizes.

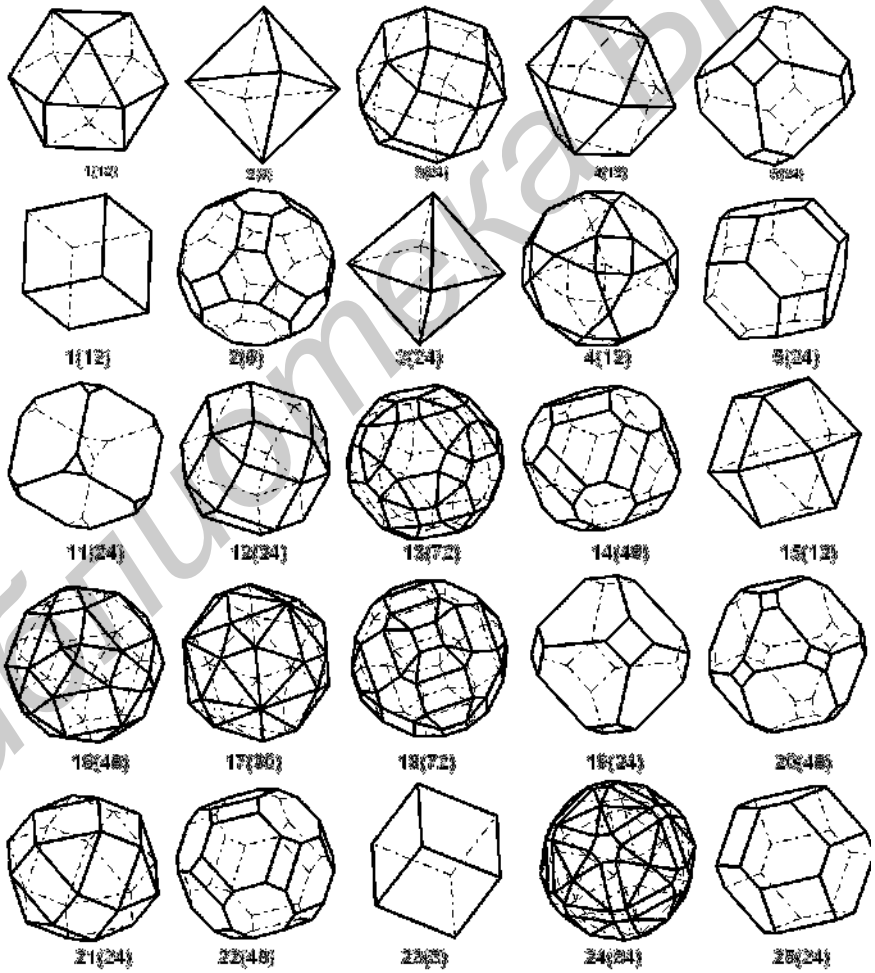

Figure 1 – Fm3m. Face centered cubic

The computer program gives possibility to determine the parameters of coordination polyhedron. There are the radius-vectors of every external atoms (R), atoms quantity of the surface (N) and in volume particle (S) and coordinates of all atoms in it.

The coordination polyhedra of different point groups of nanocrystals are shown in Figures 1 ± 5:FCC (face centered cubic, figure 1), ICC (Inter centered cubic, figure 2), PC (Primitive cubic, figure 3), D (Diamond Figure 4).

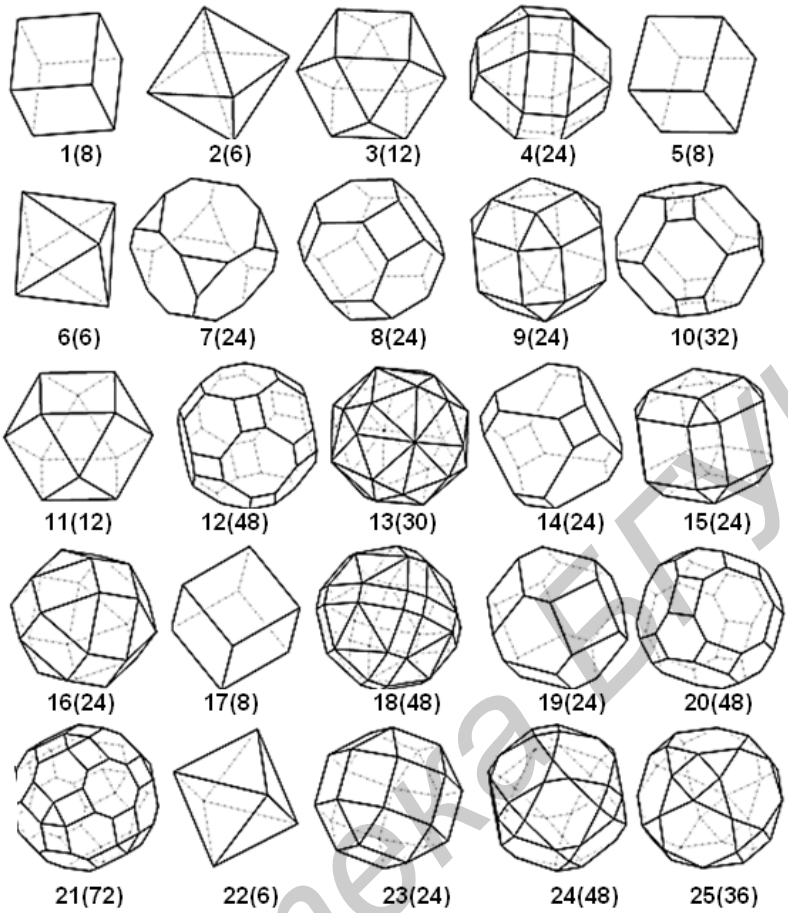

Figure 2 – Im3m. Inter centered cubic

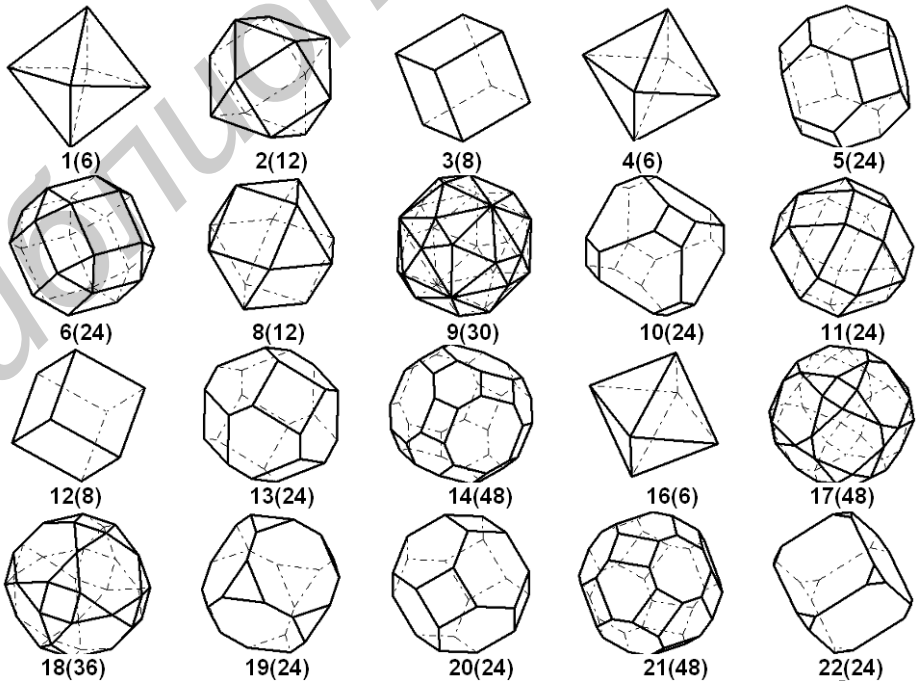

Figure 3 – Pm3m. Primitive cubic

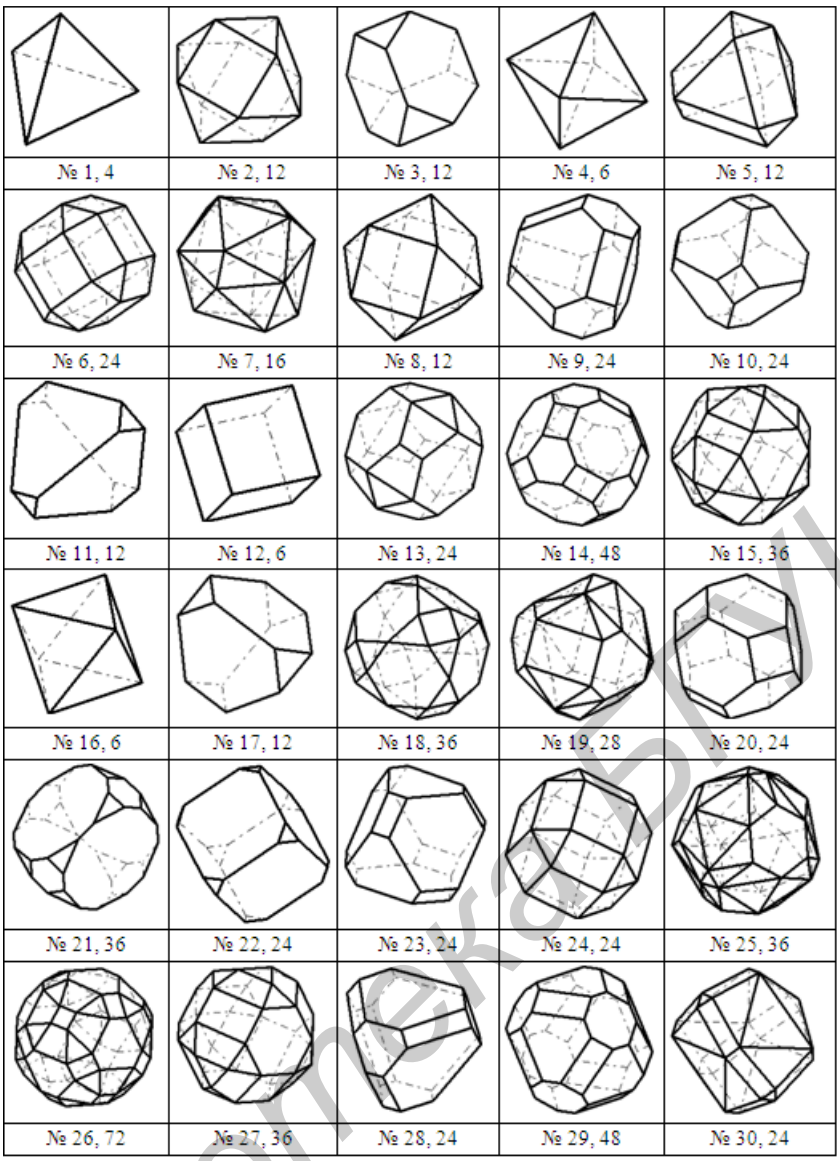

Figure 4 – Fd/3m. Diamond

This technique can be used for other crystallographic groups. In this case, it is necessary to use the method for crystals with a primitive Bravais cell.

Knowing the interconfiguration of atoms in a nanocrystal using the methods of statistical physics with the use of high-performance computations, it is possible to calculate the parameters of the physical properties of nanocrystals.

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