ATOMIC STRUCTURE OF MONOELEMENT NANOCRYSTALS

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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.

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

Figure 1 – Fm3m. Face centered cubic
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.

REFERENCES