NUCLEATION AND NANOSYSTEMS

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Formation of condensed phases is started by an appearance of nonoscale nucleuses. It is known many other nanoparticles such as inclusions, giant clusters [1], macrocycles [2], giant icosahedral keplerates [3] and so on. However, crystal nucleus is growing up to macrocrystal but a size of mentioned other particles is stabilized in nanoscale region. The aim of this investigation is thermodynamical analysis of size stability and shaping of nanoparticles. The nanoparticles are classified under two types: nanoparticle with filled volume and nanoparticle with cavity inside.

Gibbs capillarity theory can be used for an explanation of size stabilization of nanoscale "giant" atomic or molecular clusters. In these cases a surface tension of nanoparticle depend on its size. It can be a reason of an increase of chemical potential of building units (atoms, molecules, clusters and so on) in particles under further aggregation in fluid or solid solution. Another case of size stabilization can be connected with a blocking the surface by anyone chemical component even by precursor. According to the capillarity theory a particle shape must be described by Laplace and Wulf equations, and it can be presented by spherical and facet forms. The latter is often close to icosahedra.

The nanoparticles such as molecular macrocycles, for example cucurbit(n)uril, and keplerates such as polyoxometalate clusters with nanoscale cavities inside can not considered in view of the capillarity theory because of the position uncertainty of dividing surface what is a base for determining surface tension. In these occasions it is fruitful to consider nanoparticle like a shell. This shell is elastic deformed by an anisotropy of chemical composition in normal direction to the surface. A sing of the chemical potential derivatives of building unit in such nanoparticles is defined by the magnitudes of stress and strain as well as their size derivatives under unit aggregation. Positive derivative of chemical potential and, hence, a size stability might be appeared as a result of Derjagin dejoined pressure and nanoparticle deformation when the shell is locked by the latest building units.

Full thermodynamical analysis nanoparticle formation includes:
1. Identification of nanoparticle: with filled volume or with cavity.
2. Recognition of building units and their precursors.
3. Change analysis of chemical potential of building units under their aggregation, using:
-capillarity theory for volume fulled nanoparticles,
- theory of elastic deformed shell for macrocycles, keplerates and so on.
4. Substantiation necessity of realization of either open or closed chemical system. Open system is preferred for formation of size-stabilized nanopartickes.
5. A choice of building unit concentration in solution for formation of a required aggregation degree.

References.

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