Theoretical and experimental studies of the morphology and optical properties of photochemically / thermally synthesized nanoparticles with characteristic surface plasmon resonance spectra

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Results

Scientific interest in noble metals nanoparticles (NPs) and nanostructured metal surfaces formed by their deposition is caused by their unique physical properties, including surface enhancement of linear and nonlinear optical phenomena in the media in contact with such nanostructures. Morphological characteristics of NPs determine their catalytic, sensor, optical properties. Thus, it is of great importance to identify factors that affect the morphology of nanoparticles formed in multicomponent solution with regard to kinetic phenomena in solution and on the NPs surface. This is ecomplished in present work with help of numerical simulation methods developed by the authors.

Numerical study of 3D model of nanoparticles diffusion growth, whose internal structure corresponds to the different types of crystalline lattice is carried out. Self-consistent nanocrystals / environment system is considered. Dynamics of cluster's surface particles, which may change their position at the transition to nearest neighbor vacancies or detach from the surface with various degree of probability, is considered. The obtained results demonstrate the basic principles of shape control of nanoparticles growing from the initial nucleus of small size. It is shown that for the same crystal lattice nanoparticles of different shapes can be obtained; even regular polyhedrons are formed in nonequilibrium growth mode; the cluster form evolution can be controlled by changing the temperature and free atoms concentration in the environment surrounding the growing cluster. It is found that well-defined surface features are obtained for relatively narrow ranges of parameter values, for those quantities which are related to the on-surface diffusion rate and to temperature.

The research results demonstrate the possibility of controlled synthesis, modification and management of optical characteristics of nanostructured systems. The obtained theoretical findings are used to develop methods for controllable photochemical / thermal synthesis of Ag and Au NPs in colloids and transparent silica films with known nanoclusters morphology

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