

EARLY STAGES OF SILVER NANOPARTICLE FORMATION IN AQUEOUS SOLUTIONS BY PLASMA-CHEMICAL DISCHARGE*Skiba M. I.¹, Makarova A. K.¹, Vorobyova V. I.², Mahinya A. S.¹*¹Ukrainian State Chemical Technology University, Dnipro, Ukraine²National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine

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Metal nanoparticles (NPs) have attracted a great interest both in the area of scientific research and industrial applications. Silver (Ag) NPs have generated substantial interest not only in fundamental research and development, but also at the industrial scale due to their excellent properties. Hence, synthesis strategies that result in controlled AgNPs size, distribution, shape and stability are still an area of interest. Different methods have been employed in the production of nano-sized metallic silver particles with different morphologies and sizes.

One of the innovative and environmentally safe methods for preparation of nano-sized compounds is the use of plasma discharges of various configurations. Among plasma-chemical discharges, contact non-equilibrium low-temperature plasma (CNP) is a promising option from the point of view of practical application. Plasma discharge is generated between the electrode in the gaseous phase and surface of the liquid where the other electrode is located. Therefore, chemical transformations at the phase interface are conditioned by the combined effect of electrochemical oxidation-reduction; initiated photolysis reactions, UV radiation; flow of charged particles from the gaseous phase to the surface of the liquid medium.

In the present work, the theoretical and practical formation of Ag clusters in aqueous solution using of contact non-equilibrium low-temperature plasma have been investigated. We use the B3LYP level of approximation in the density functional theory (DFT) and the LANL2DZ basis set as implemented in the Gaussian 03 program. The practical research was carried out in the batch gas-liquid reactor.

The early stages of silver nanoparticle formation under the action of contact non-equilibrium low-temperature plasma technique have been investigated by first-principle theoretical calculations. The charge density of clusters turns out to be a molecular descriptor that is a key factor determining the selectivity among various growth pathways; an optimal charge density appears to control the selection between neutral and charged species in cluster growth. As a result, partially positively charged clusters are thermodynamically preferred that can serve as seeds for further growth.

In practice Ag^+ ions, in aqueous solution have been plasma-chemically reduced to produce Ag clusters. Our calculated results are consistent with experimental studies. UV-visible absorption spectral characteristics of Ag clusters obtained under different irradiation time, concentration of silver ions. On practice intermediates such as Ag_4^{+2} , Ag_8^{2+} was observed under the action of contact non-equilibrium low-temperature plasma with development of plasmon absorption band at about 360–325 nm. Processing during 1-5 minutes provides formation of silver nanoparticles. The formation of silver colloidal solutions in the presence of stabilizer is characterized by the presence of peak $\lambda_{\text{max}} = 400\text{--}440$ nm in the spectra. The average size of formed silver particles is up to 100 nm.