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Dependences of optical properties of spherical two-layered nanoparticles on parameters of gold core and material shell

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ABSTRACT

Modeling of nonlinear dependences of optical properties of spherical two-layered gold core and some material shell nanoparticles (NPs) placed in water on parameters of core and shell was carried out on the basis of the extended Mie theory. Efficiency cross-sections of absorption, scattering and extinction of radiation with wavelength 532 nm by core–shell NPs in the ranges of core radii $r_{00}=5$–40 nm and of relative NP radii $r_1/r_{00}=1$–8 were calculated (r_1—radius of two-layered nanoparticle). Shell materials were used with optical indexes in the ranges of refraction $n_1=0.2$–1.5 and absorption $k_1=0$–3.5 for the presentation of optical properties of wide classes of shell materials (including dielectrics, metals, polymers, vapor shell around gold core). Results show nonlinear dependences of optical properties of two-layered NPs on optical indexes of shell material, core r_{00} and relative NP r_1/r_{00} radii. Regions with sharp decrease and increase of absorption, scattering and extinction efficiency cross-sections with changing of core and shell parameters were investigated. These dependences should be taken into account for applications of two-layered NPs in laser nanomedicine and optical diagnostics of tissues. The results can be used for experimental investigation of shell formation on NP core and optical determination of geometrical parameters of core and shell of two-layered NPs.

1. Introduction

During the past years many research efforts have been focused on preparation and investigation of spherical hybrid core–shell nanoparticles (NPs) because of their unique size-dependent physical and chemical properties [1–26]. First of all, core–shell silica–gold [1–3] and silver–gold and vice-versa gold–silver [4,5] NPs were prepared and experimentally investigated and applied in nanomedicine, imaging, labeling and laser medicine. After that many hybrid two-layered NPs with different materials for core and shell were synthesized and investigated in Refs. [6–10]. The design of core–shell NPs with chosen and adjusted properties is possible by the selection of core and shell materials and material composition. Plasmonic properties of nanoscale two-layered NPs depend on their dimensions, shapes, optical properties of the materials of core, shell and surrounding medium [2,4,11–19]. By varying core size and shell thickness plasmon resonance of core–shell hybrid NPs can be adjusted across a broad range of the optical spectrum [2,4,11–15]. This tunability of plasmon resonance is an interesting property of core–shell NPs and makes them ideal nanostructures for incorporation into different systems.

Core–shell NPs are used in many different fields of research and technology including nanomedicine, optical diagnostics and imaging, catalysis, nanophotonics [1,3,15, 20–26]. Two-layered NPs were used for the purposes of

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photothermal and photoacoustical applications in nanomedicine [1–3,23,25], molecular imaging of tumors [24,25], for optical diagnostics of materials and nanocomposites [21], for use of core–shell NPs in different sensors [26], for methanol oxidation [22], and in other applications.

Many two-layered NPs were synthesized on the basis of gold-core and some material-shell composition during the last years [4–15,20–26]. For shell materials different metals (silver, cuprum, platinum, etc.) [4,5,8,10,13–15,20–22,25,26], silica [1–3,9–11,24], some polymers [6,7,10], and others were used [10,14]. Vapor nanoshells (bubbles) were created under laser action on gold NPs placed in water (blood) contained tissues [27–30]. It means origination of two-layered gold core–water vapor shell NPs. Applications of amplified scattering effects from gold core–water vapor shells NPs was proposed in Refs. [27–30] for increasing the detection sensitivity.

Shell formation on gold core can be used for the preservation of NP in some chemically active media, for achievement of different physical and chemical properties of core–shell NPs in comparison with homogeneous gold NP and other purposes. For example, silica shell on gold core was also used for increasing the stability of NP in chemically active liquids (salt liquids, blood), for the possible increase of absorbance of NP or shift of resonance wavelength in different regions of optical spectrum [1–3,9–11,24].

Wide applications of gold core–some material shell NPs are based on investigations of their optical properties which make them very attractive hybrid NPs. Optical characteristics of gold core–material shell NPs were experimentally investigated in Refs. [2,4,11–15] by the methods of optical spectroscopy, light microscopy and optical transmission diagnostics. Geometrical (core size and shell thickness) and internal characteristics of NPs were investigated by transmission electron microscopy [11–15]. Theoretical investigations of optical properties of core–shell NPs were carried out in Refs. [2,12,16–19]. We have to note that these experimental and theoretical results have limited the investigations of the dependences of extinction (scattering) optical properties on radiation wavelengths λ under fixed values of core radius r_0 and shell thicknesses [2,12,17] or the dependences of properties on core radius r_0 under fixed values of shell thickness and wavelength λ [18,19].

We are going to investigate nonlinear dependences of optical properties (effective cross-sections of absorption, scattering and extinction) on geometrical (core radii r_{00} and relative NP radii r_1/r_{00}) and optical parameters of gold core–material shell NPs. It is very interesting to find and determine the regions with sharp decrease and increase of absorption, scattering and extinction of radiation by NPs. Achievement of maximal values of efficiency cross-sections of absorption of radiation σ_{abs} that will lead to minimizing the values of laser intensity for thermooptical and thermoacoustical applications in laser nanomedicine and nanotechnology will be discussed. Determination of maximal or minimal values of efficiency cross-sections of scattering σ_{sca} and extinction σ_{ext} of radiation is important for the purposes of optical scattering diagnostics and imaging. It is important to develop the optical method for the determination of geometrical (core radius and shell thickness) characteristics on the basis of investigated optical properties of NPs.

Principal novelty and difference of our investigations compared with previous publications [2,12,16–19] is the investigations of optical properties of core–shell NPs in the wide ranges of the core radii r_{00}=5–40 nm and of relative NP radii r_1/r_{00}=1–8 for wide range of optical indexes of shell materials (including metals, dielectrics, gas, vapor).

2. Results of computer modeling of optical properties of spherical gold core–material shell NPs

It is assumed that spherical two-layered NP consists of a spherical homogeneous core of radius r_{00} with the complex refractive index $m_0=n_{00}-i\kappa_0$ of gold, enveloped by spherically symmetric homogeneous shell of radius r_1 with the complex refractive index $m_1=n_1-i\kappa_1$ of shell material. The particle is located in the homogeneous non-absorbing medium with a refractive index n_2. The set of geometrical and optical parameters of core—r_{00}, m_0, shell—r_1, m_1, medium—n_2 determines optical properties of two-layered NP placed in some medium. Optical characteristics of two-layered sphere (absorption, scattering and extinction effective cross-sections) are expressed in terms of amplitude coefficients given by the theory of diffraction of radiation on two-layered spherical particle [16,18]. Calculations of such characteristics for two-layered particles are much more cumbersome than for homogeneous spherical particles [16].

Consider two-layered spherical NPs with gold (Au) core and shell material. We used gold for core material because gold has appropriate properties for many applications and is widely used in experiments [1–15]. Optical indexes of Au were used from Ref. [37]. Optical indexes for shell material were used in the ranges n_1=0.2–1.5 for refraction and k_1=0–3.5 for absorption. These values of n_1 and k_1 present the optical properties of wide classes of shell materials (dielectrics, metals, glasses, gases, etc.). For example, for air, water vapor n_1=1.001–1.01, k_1=0, for silica n_1=1.5–1.45, k_1=0, for some metals n_1=0.2–1.5, k_1=0–3.5. Two-layered NPs with gold core and some material shell are created as a result of different chemical or physical procedures [8–10]. Two layered system (NP) of gold core and water vapor shell is created under laser pulse action on NPs placed in water contained tissues [27–30]. We should take into account that lines in Figs. 1–7 are presented for NPs with the values of core r_{00} and relative radii r_1/r_{00} (r_1—radii of NP, thickness of shell $\Delta r_1=r_1-r_{00}$). The point r_1/r_{00}=1 in Figs. 1–7 means the presentation of optical properties of homogeneous gold NP with value of r_{00}. Increase of r_1/r_{00} means the increase of shell thickness under constant value of core radius r_{00}=const. It is correlated with the growth of shell on core as a result of chemical reaction or expanding of vapor shell after its origination.

Gold NPs have strong plasmon resonance in the spectral interval 520–540 nm. Laser wavelength 532 nm belongs to this plasmon resonance interval and is widely used in experiments. We use wavelength 532 nm in our investigations because of significant influence of gold core on optical