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Analysis of the scattering properties of a core-shell nanoparticle deposited on a plane surface via rigorous computer model

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The discrete sources method has been extended to analyze the scattering behavior of a core-shell nanoparticle (nanoshell) deposited near a plane surface in an evanescent wave field. The rigorous computer model based on DSM, which allows one to take into account all features of the scattering problem, has been realized. The dependence of the scattering spectra of core-shell particles on size, shell thickness and core-shell asphericity is discussed.

Keywords: core-shell nanoparticle; rigorous model; light scattering; discrete sources method

1. Introduction

Interest in scattering by core-shell nanoparticles has increased rapidly within the last few years. Nanoshells are a new type of nanoparticle composed of a dielectric core coated with an ultra-thin noble metallic shell. Such particles are of great interest in different scientific, medical and technological applications due to their scattering behavior and their ability to demonstrate a tunable plasmon resonance response in the visible range of the spectra. They are considered to be an improvement on solid noble particles with similar characteristics (*1, 2*), which have been used before. It has been detected that the resonance frequency of a nanoshell depends on its properties (size, shape, shell thickness, etc.) (*3–6*). Varying those parameters enables one to shift the plasmon resonance peak to the required frequency domain. Due to these abilities nanoshells became of interest for a wide variety of applications: environmental, Raman, chemical and biological sensing, surface-enhanced and near field scanning optical microscopy.

Nanoshells produced for biomedical applications are composed of a dielectric core with a gold shell (*7*), as gold stays neutral within biological tissue. The working principle of a nanoshell, which is used for viruses' detection, is based on the evanescent waves scattering. An experimental setup includes the incident unpolarized light, which is coupled

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into a glass prism and hits the glass–water interface with an angle slightly exceeding the critical angle of total internal reflection. This generates an exponentially decaying evanescent field near the interface in the lower refractive index medium (water). The nanoshell particle is deposited in the medium to transform an evanescent field in the vicinity of the surface. The scattered light is detected by an objective lens. Even a small change of the refractive index of the ambient media, caused by the presence of viruses, leads to a shift of the plasmon resonance. So, from detection of the position of a plasmon resonance peak one can get information about the refractive index of an ambient media and detect its deviation from the known refractive index of the water. A similar principle is used, for example, for immunoglobulin detection (*7*).

Modern detecting devices used for plasmon resonance studies are able to detect a resonance shift of about 1 nm. This means that synthesis of core-shell nanoparticles requires clear understanding of their functional abilities in a frequency domain (*8, 9*). Even slight deviation in core-shell particle properties can complicate measurement interpretation. Additionally, for biomedical applications nanoshells must provide a high and narrow spectrum peak in the wavelength range of 700–1100 nm, which is known as the 'biological window' region of transparency in biological tissue. That is why a detailed theoretical analysis of the scattering properties of core-shell nanoparticles seems to be very important.

One of the advanced methods for the scattering analysis for different kinds of particles located near a plane interface is the discrete sources method (DSM) (*10*). The DSM allows one to take into account the whole environment of the scattering problem including the complete interaction of the particle and the interface, actual objective aperture, core-shell asphericity, etc. Recently the DSM has been applied to the investigation of the scattering by solid noble nanoparticles on a plane surface (*11*). In this paper the DSM is extended to simulate light scattering by core-shell nanoparticles. The main goal of our research is a detailed investigation of the scattering behavior of the spectral resonance of core-shell particles and 'optimal' choice of their parameters, which enables one to provide a shift of the resonance peak beyond 700 nm. For this purpose computer simulation analysis based on the DSM model has been performed.

The paper consists of three parts: in the first one the brief outlines of the DSM theory are given, the second part is devoted to the numerical scheme and in the final part of the paper we present simulation results and discussion.

2. Discrete sources method

In this section we would like to provide a short sketch of the DSM theory (*10, 11*).

Consider an axial symmetric penetrable particle with an interior domain D_i covered with a layer D_l and smooth boundaries $\partial D_{i,l}$ deposited on the plane prism surface Σ. We denote the prism domain by D_1 and the ambient space exterior to the particle by D_0. Let us introduce a Cartesian coordinate system Oxyz by choosing its origin O at the interface surface and the Oz axis coincides with the axis of symmetry of the particle and is directed into domain D_0 so, that the plane $z = 0$ corresponds to the Σ plane. We assume that the exciting field $\{\mathbf{E}^0, \mathbf{H}^0\}$ is a plane wave propagating from D_1 at the angle θ_1 with respect to the z axis (Figure 1).

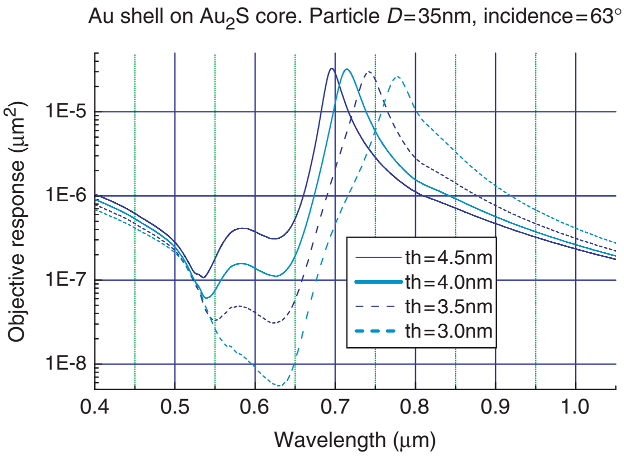

Figure 3. Objective scattering response versus wavelength for core-shell particle $D = 35$ nm with different shell thicknesses. (The colour version of this figure is included in the online version of the journal.)

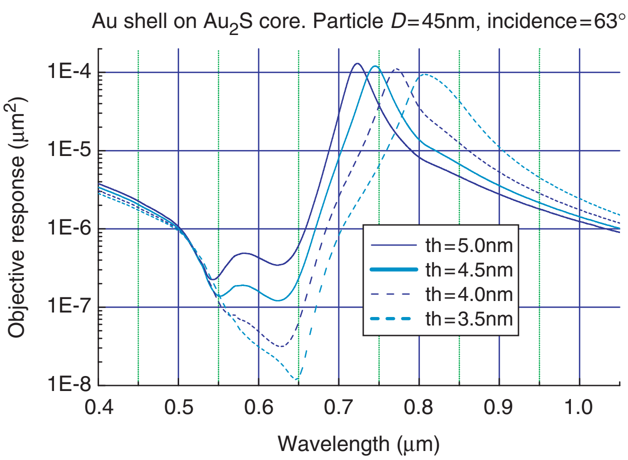

Figure 4. Objective scattering response versus wavelength for core-shell particle $D = 45$ nm with different shell thicknesses. (The colour version of this figure is included in the online version of the journal.)

The optimal diameter which provides relatively high intensity together with still not so wide peak corresponds to $D = 45$ nm. Now let us fix both particle diameter and shell thickness and get back to the choice of our incident angle that up to now we have kept fixed.

Figure 6 presents the objective response for the core-shell particle of $D = 45$ nm and a shell thickness of 4.5 nm for different incident angles. From the results one can see that the pattern stays the same, but intensity decreases with increasing incident angle.

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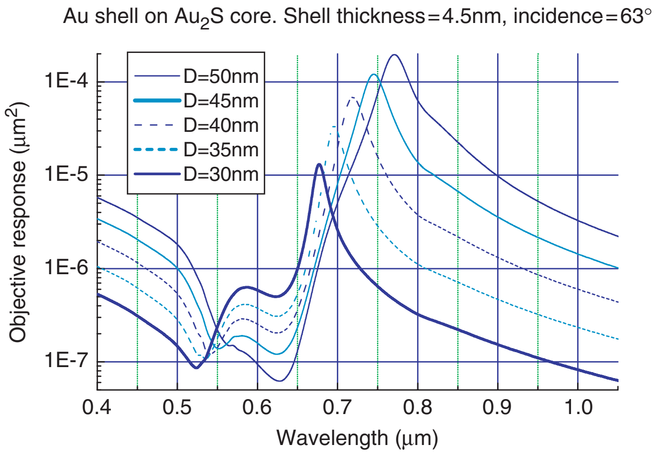

Figure 5. Objective scattering response versus wavelength for core-shell particle of different diameters with fixed shell thicknesses. (The colour version of this figure is included in the online version of the journal.)

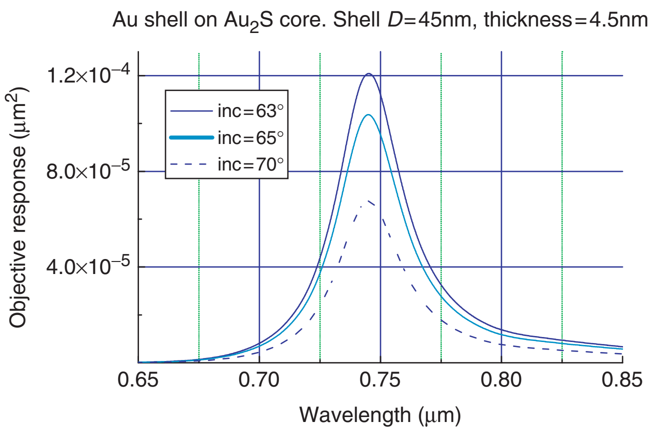

Figure 6. Objective scattering response versus wavelength for core-shell particle of $D = 40$ nm with shell thickness of 4.5 nm for different incident angles. (The colour version of this figure is included in the online version of the journal.)

Figure 7 shows the objective response for particles of $D = 45$ nm with different shell thickness at a fixed wavelength of 750 nm (the wavelength corresponding to the maximum of the scattering response) versus incident angle. The response curves first are very close to a straight line with a local maximum in the area of the critical angle (about 62°) and then a rather fast decrease with an increase of the incident angle above the critical one. These results allow one to explain the results presented in Figure 6: the closer the incident angle to the critical one, the higher the objective response. From the last result it is clear why the

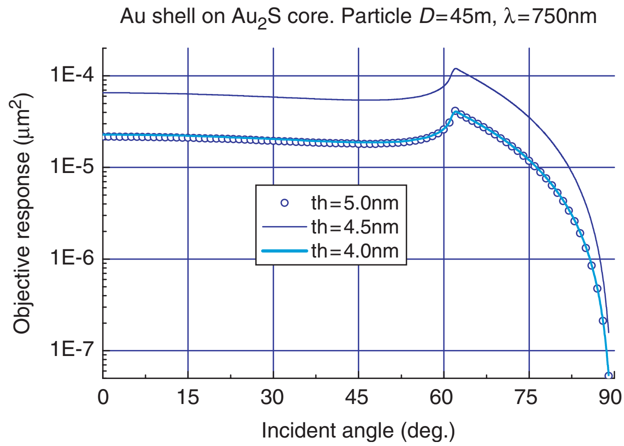

Figure 7. Objective scattering response versus scattering angle for core-shell particle of $D = 45$ nm under wavelength of 750 nm for different shell thicknesses. (The colour version of this figure is included in the online version of the journal.)

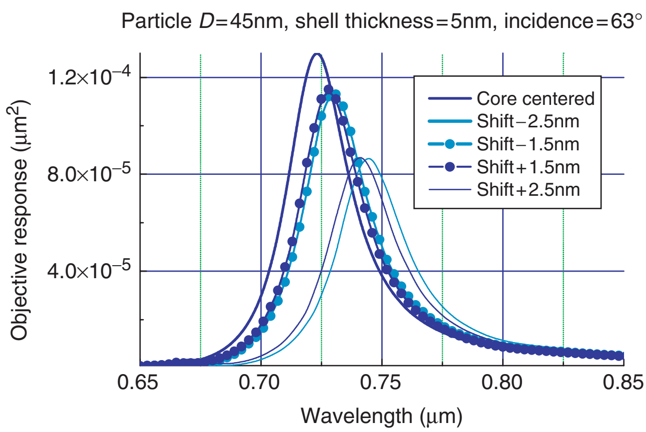

Figure 8. Objective scattering response versus wavelength for core-shell particle of $D = 45$ nm with shell thickness of 5 nm for different asymmetry models. (The colour version of this figure is included in the online version of the journal.)

response for the core-shell particle with shell thickness of 4.5 nm is much higher than for particles with a shell thickness of 4 and 5 nm, since the variety of thickness is just about 1% of the total particle diameter. This gives our choice of 'optimal' shell thickness.

Now, as we have already learned how sensitive the objective response is to the core-shell properties, we would like to analyze another important aspect – the core-shell asymmetry. Core-shell asymmetry, which is seldom taken into account in theoretical investigations, takes place in reality rather often (*16*). Figures 8 and 9 present the scattering

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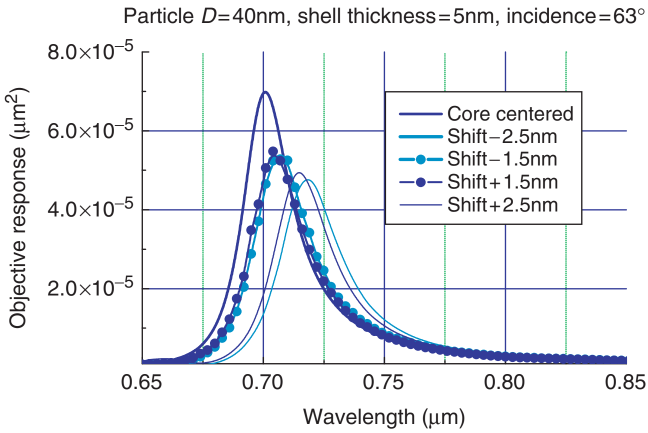

Figure 9. Objective scattering response versus wavelength for core-shell particle of $D = 40$ nm with shell thickness of 5 nm for different asymmetry models. (The colour version of this figure is included in the online version of the journal.)

response from core-shell particles of $D = 45$ nm (Figure 8) and $D = 40$ nm (Figure 9) with a shell thickness of 5 nm under the incidence of 63° for different core depositions inside the particles. A shift in this case means that the centre of the core is shifted up (+) or down (−) inside the particle. From the simulations one can see that even such a small core shift of 2.5 nm shifts the maximum of the response about 30 nm and essentially decreases its intensity. So, a possible asymmetry of the core-shell particles should be taken into account in the design, as in sensitive systems the shift of the resonance peak by 30 nm could lead to the wrong interpretation of the experimental results.

5. Conclusion

In this paper DSM has been applied to the scattering analysis of a core-shell nanoparticle deposited on a prism surface. The main goal of the investigation was to clarify the scattering behavior of core-shell particles with their parameters: diameter, shell thickness and core-shell asymmetry. The results obtained by simulations allow one to choose the optimal parameters for nanoshell synthesis, which provides maximum enhancement and a shift of the resonance into the window of biological transparency. It has also been shown that the scattering behavior of nanoshells strongly depends on the core-shell asymmetry, which may lead to the wrong interpretation of experimental results.

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