همایش نانوفوتونیک ایران ۱۳۹۹- ۱ و ۲ آبان

Iranian Nano-Photonic Conference 2020
October 23 and 24

Optical Properties of Gold Nanoparticles: Shape and Size Effects

Parisa Khajegi[1,*], Majid Rashidi Huyeh[1]

Dept. of Physics, Faculty of Sciences, Sistan and Baluchestan University, Zahedan, Iran.

Abstract- Nobel metal nanoparticles (NPs) are widely used in various applications including optical and biological sensors, biomedicine, photocatalysts, electronics, and photovoltaic cells. Optical properties of gold NPs are surveyed in this paper under the Surface Plasmon Resonance (SPR) effect, which increases the light absorption and scattering at the SPR wavelength. This SPR frequency depends on the various factors, including the shape and size of the particles. Here, the optical response of gold NPs with different shapes and sizes is investigated using the finite element method (FEM) with COMSOL Multiphysics. The results show that the bandwidth, amplitude, and SPR wavelength depend on the shape and dimensions of the NPs as well as the polarization of the incident light. The SPR wavelength changes from 515 nm to 760 nm for different shapes of the NPs. To study the size effects, the spherical NPs absorptions are determined for different NPs size. As the particle size increases, absorption per unit volume decreases, and the bandwidth increases.

Keywords: Gold Nanoparticles; Surface Plasmon Resonance; Absorption Cross Section; Scattering Cross Section, Shape Effect.

[1*]parisakhajegi@gmail.com

1. Introduction

As the dimensions of the material decrease to the nanometer scale, their magnetic, electronic, and optical properties change. The optical properties of the noble metal NPs are dominated by the surface plasmon resonance (SPR) phenomenon. This phenomenon is related to the collective oscillation of the metal NPs free electrons under the electromagnetic waves (EMWs) excitation, and result in an absorption pick in a wavelength, known as SPR wavelength. So, these NPs are proposed in a wide range of medical and photonic devices applications [1-3]. The optical properties of metal NPs depend on the structure, composition, and shape of the NPs. Such effects have been studied, experimentally as well as theoretically, by different groups [4-7]. In these works, absorption and/or extinction coefficient were reported for different shapes of NPs. In this paper, are studied the shape and size effects of the gold NPs on their optical properties. For this, are calculated the absorption and scattering cross-sections (CSs) of the NPs by different shapes and sizes, using COMSOL Multiphysics®.

2. Model

The FEM method is used to model the NPs in the dielectric medium, using the COMSOL Multiphysics® software package. A scattering calculation is used, instead of the full field calculation, wherein a background field with a specific polarization is applied as the source to excite the particle. The model calculates the Helmholtz equations for EMW and the emerged results are obtained using a perfectly matched layer (PML) as an absorber layer in the outer domain of the modeling environment. The thickness of the PML must be at least equal to half of the local wavelength of the EMW in the dielectric media ($\lambda_0 / 2n$, in a media with a refractive index of n) and the same distance must be considered between the PML and the active region of the modeling domain (i.e. NP in the present work). The scattering boundary condition is used at the outer boundaries of the PML to ensure that the light cannot be reflected in the modeling domain. The absorption and the scattering CSs are obtained from equations 1:

$$CS_{abs/scat} = \frac{W_{abs/scat}}{\frac{1}{2}\sqrt{\frac{\varepsilon}{\mu}}\left|E_{e0}\right|^2} \tag{1}$$

where, $W_{abs} = \frac{1}{2}\int_{\Omega} \mathbf{J}\cdot\mathbf{E}dv$, $W_{scat} = \int_{S_c} \mathbf{n}\cdot\langle\mathbf{S}_{scat}\rangle dS = \frac{1}{2}\int_{S_c} \mathbf{n}\cdot\mathrm{Re}\left\{\mathbf{E}_s \times \mathbf{H}_s^*\right\}dS$ are absorbed power in the NP and scattered power around it, respectively. **J**, **E**, **H**, **S**, and **n** represent current density, electric field, magnetic field, Poynting vector, and the normal vector of particle surface respectively [8]. The model is first validated by comparing the results for a spherical nanoparticle with those obtained using Mie theory [9].

3. Shape effect

To investigate the effect of NPs shape on the optical properties, the absorption and scattering CSs per particle volume are compared for different shapes of spherical, ellipsoid, cubic, and triangular NPs. For asymmetric particles, in which the intensity of absorption depends on the polarization of the incident light, effective polarization (polarization with the highest absorption intensity) is considered. The results are shown in Figure 1. The arrows, indicated on each particle, represent the effective polarization of the NP. The SPR wavelength for spherical, cubic, elliptical, and triangular particles is located at 515, 580, 640, and 760 nm, respectively (Figure 1a). The SPR bandwidth depends also on the particle shape (see inset in Figure1a). The absorption bandwidth for cubic and elliptical NPs are wither than those the spherical and triangular NPs. This phenomenon can be related to edge mode and multipolar effects [2, 10]. The absorption and scattering amplitude increase for the NPs with more edges and vertices (triangular and cubic shapes). For such shapes of NPs, several SPR peaks may be observed and the SPR wavelength is located in longer wavelength. These behaviors have also been reported by many authors [2].

4. Size effect

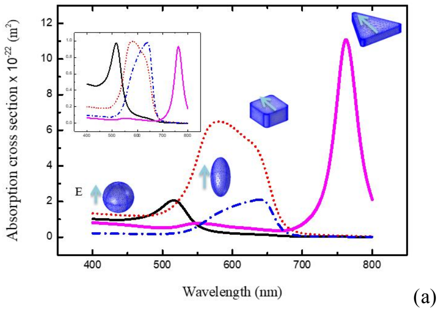

Figure 1. Absorption (a) and scattering (b) cross-section per particle volume fo elliptical (15×7×7 nm), triangular prism (8×50×55 nm) and rectangular cube (direction of light polarization. The insets show the normalized absorption values

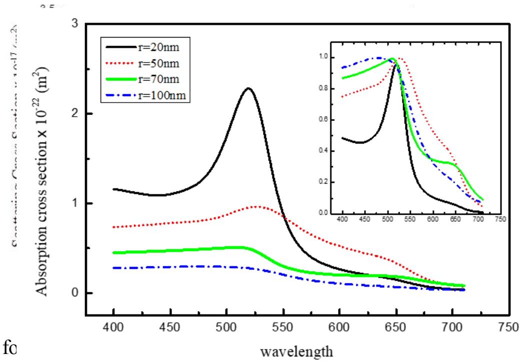

Figure 2. Absorption cross-section per NP volume for gold spherical NPs by different radii of 20, 50, 70, and 100 nm. The inset shows the normalized absorption CS per NP volume.

To study the NPs size effect on the optical properties, the absorption CS per particle volume is calculated for spherical NPs with different sizes, varying from 20 to 100 nm of the radius. The results are presented in Fig. 2. It can be seen that as the particle size increases, the absorption per unit volume decreases, and the SPR bandwidth increases, but the SPR wavelength doesn't change significantly in this range of NPs size (see the inset in the Fig. 2). It can be also seen that another SPR peak, located at a longer wavelength, appears for large particles. This effect can be contributed to the electric multipolar effects. In fact, for the particle with a dimension very smaller than the incident electromagnetic wavelength, just electric dipole may be excited, but for the particle with a size comparable by the incident EMW, the electric multipolar can be excited [11,12].

5- Conclusion

In this communication, were studied the shape and size effects of NPs on their optical properties. The results showed that the shape of the NP affects the SPR wavelength and amplitude. The SPR wavelength of NPs with sharp edges and vertices (triangular and cubic shapes) shows a redshift comparing with other NPs shape and their absorption and scattering CSs amplitude are more significant. Moreover, the SPR bandwidth and amplitude depend on the particle size.

References

1. H. Kang *et. al.* **Chem. Rev 119**(1) 664-99, (2018).

2. M. Sharifi *et. al.* **Controlled Release 311** 170-189, (2019).

3. S. Castelletto *et. al.* **Nano-sci & Nano-tech. Let 5**(1) 36-40, (2013).

4. R .D . Averitt *et. al.* **JOSA. B 16(10)** 1824-1832, (1999).

5. R. Rodríguez-Oliveros *et. al.* **Optics express 20**(1) 621-626, (2012).

6. X. Huang *et. al*. **advanced research 1**(1) 13-28, (2010).

7. G. S. He *et. al.* **Physical Chemistry C 114**(7) 2853-2860, (2010).

8. A. Doicu, *Light scattering by systems of particles. null-field method with discrete sources: theory and programs,* New York: Springer-Verlag, Ch.1, (2006).

9. G. Mie. **Ann. Phys**. 25, 377, (1908).

10. L. J. Sherry *et. al*. **Nano letters 6**(9) 2060-2065, (2006).

11. J. Y. Yan, **Phys. Rev. B 77**(16) 165301, (2008).

12. J. Z. Zhang, *Optical properties and spectroscopy of nanomaterials*, World Scientific, Ch.7 , (2009)