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Numerical Study of Plasmon Resonance Silver Nanoparticles Coated Polyvinyl Alcohol (PVA) using Bohren-Huffman-Mie Approximation

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Abstract In this study, we have investigated the LSPR spectra of the silver nanoparticles (Ag-NPs) coatedby polyvinyl alcohol (PVA) by means of a numerical study using Bohren-Huffman-Mie (BHMie) approximation. The LSPR of Ag-NPs shifted to red-shift as the diameter size of Ag-NPs and the thickness of PVA increased. The peak of the LSPR spectra exponentially increased as the thickness increased. Interestingly, there have three characteristic of the LSPR spectra, small, intermediate, and large diameter. In small diameter, the dipole resonant mode contributed to the LSPR spectra while in large diameter, the LSPR spectra originated from the quadrupole resonant mode. In contrast to intermediate diameter, the LSPR spectra originated from the competition between the dipole and the quadrupole mode. For this reason, at small and large diameter the LSPR peak has one peak and increased then until a certain thickness showed constant. Different at intermediate diameter, the LSPR peak appeared more one peak with major peak increased then until a certain thickness trend to decrease and minor peak followed at small diameter behavior.

Keywords: Silver nanoparticle, BHMie approximation, PVA coating, dipole and quadrupole expansion

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1. Introduction

In decades, the noble nanoparticlesresearch has been a great attention because of its potential application such as electronics, environments, computers, biotechnology, sensors, pharmacy, etc based on the localized surface plasmon resonance (LSPR) effect [1].The silver nanoparticles (Ag-NPs) is a part of the noble nanoparticles has also attracted many researchers since their application in biosensor, biomedical, and, antimicrobial [2]. To maintain the stability of the Ag-NPs for practical purpose, usually Ag-NPs combined with some polymeric composites such as polyvinyl alcohol (PVA), polypyrrole (PPy), carbonxymethyl cellulose (CMC) [3,4], biocompatible molecu-lessuch as bovine serum albumin (BSA) [5,6] and semiconductor such assilica [7]. Numerous studies have been also reported in numerical approximation to investigate the LSPR spectra, such as determining the interaction between Ag-NPs and PVA using density functional theory (DFT) to calculate the binding energy [8], finite different time domain (FDTD)method to produce the LSPR spectra Ag-NPs nanocubes [9], and

the calculation the scattering intensity in the nanoshell model [10,11]. However, there have been little studies in the LSPR spectra to Ag-NPs coated PVA with respect to the thickness of PVA variation.

In this study, we have systematicallyinvestigatedthe LSPR spectra corresponds to the diameter of Ag-NPs and the thickness of PVA variation based on Bohren-Huffman-Mie approximation (BHMie). From this approximation, we can produce the LSPR spectra that consists of the absorption, scattering, and extinction cross section as a function of the wavelength. According to this study, we can analyze the effect of the diameter size of Ag-NPs and the thickness of PVA to the LSPR spectra Ag-NPs.

2. Numerical Method

We have performed the LSPR spectra of Ag-NPs coated PVA by means of BHMie approximation [12,13] which was written in Matlablanguage. According to BHMie, we calculated theabsorptionC_{abs}, scatteringC_{sca}, and extinction C_{ext}cross section as a function of the wavelength function, were written as:

$$\begin{aligned} C_{sca} &= \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)(|a_n|^2+|b_n|^2), \\ C_{ext} &= \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)\Re(a_n+b_n), \\ C_{abs} &= C_{ext} - C_{sca} \end{aligned} \tag{1}$$

with

$$\begin{aligned} a_n &= \frac{\psi_n(y)[\psi'(m_2y) - A_n\chi_n'(m_2y)] - m_2\psi_n'(y)[\psi_n(m_2y) - A_n\chi_n(m_2y)]}{\xi_n(y)[\psi_n'(m_2y) - A_n\chi_n'(m_2y)] - m_2\xi_n'(y)[\psi_n(m_2y) - A_n\chi_n(m_2y)]} \\ b_n &= \frac{m_2\psi_n(y)[\psi_n'(m_2y) - B_n\chi_n'(m_2y)] - \psi_n'(y)[\psi_n(m_2y) - B_n\chi_n(m_2y)]}{m_2\xi_n(y)[\psi_n'(m_2y) - B_n\chi_n'(m_2y)] - \xi_n'(y)[\psi_n(m_2y) - B_n\chi_n(m_2y)]} \\ A_n &= \frac{m_2\psi_n(m_2x)\psi_n'(m_1x) - m_1\psi_n'(m_2x)\psi_n(m_1x)}{m_2\chi_n(m_2x)\psi_n'(m_1x) - m_1\chi_n'(m_2x)\psi_n(m_1x)} \\ B_n &= \frac{m_2\psi_n(m_1x)\psi_n'(m_2x) - m_1\psi_n(m_2x)\psi_n'(m_1x)}{m_2\psi_n(m_1x)\chi_n'(m_2x) - m_1\chi_n(m_2x)\psi_n'(m_1x)} \end{aligned} \tag{2}$$

where $k^2 = \omega^2\mu, x = kD, y = k(t+D)$, m_1 and $m_2$denoted the refractive index Ag-NPs and coating PVA respectively, and the functions ψ_n, $-\xi_n$, and $\chi_n$were Ricatti-Bessel function. In this study, we used a single sphere model of Ag-NPs and coated by PVA. The diameter D of Ag-NPs was varied from 20 nm to 100 nm and the thickness t of PVA was from 10 nm to 200 nm. The property of dielectric constant Ag-NPs used from Palik's experiment [14], the refractive index of PVA was n_{PVA} = 1.531 [15], and the refractive index of the medium was n_a = 1.3334 [16]. The illustration model of Ag-NPs coated by PVA is shown as Fig. 1.

3. Results and Discussion

Fig. 2 showed the LSPR spectra of Ag-NPs, the absorption, scattering, and extinction as a function of the wavelength from D = 20 nm to 100 nm with respect to the thickness of

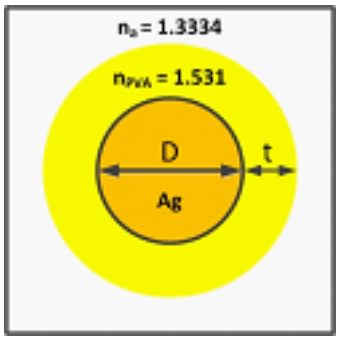

Figure 1: The illustration model of the Ag-NPs coated by PVA, D is diameter ofAg-NPs, t is the thickness of PVA, n_{PVA} is the refractive index of PVA and n_a is the refractive index of medium.

PVA. The LSPR spectra exhibited shifting to larger wavelength or red-shift as the size of Ag-NPs and the thickness of PVA increased. Similar observations were also reported by Ananth [6] and Mbhele [17]. The red-shift phenomenon of the LSPR Ag-NPs was simply can examined by scattering [18]. Increasing the particle size will increase the scattering process and the external driving field becomes non uniform across each particle. For this reason, the peak LSPR spectra will shift to larger of wavelength or red-shift.

Next, we have also determined the peak of LSPR spectra based on Fig. 2 and were plotted as the thickness of PVA which was given in Fig. 3. The peak of LSPR was obtained from the absorption cross section with reason it was simply determined than scattering or extinction cross section. As look details, we have observed that the LSPR spectra can be divided by three regions. First region located in small diameter (D = 20-50 nm) with the LSPR spectra showed one peak. Second region in intermediate diameter (D = 60-80 nm) with the peak of LSPR showed one more peak, first peak appeared at low wavelength and second peak at high wavelength. Third region in large diameter (D > 80 nm) and the peak of LSPR became one peak again. Furthermore, it was found that the peak of LSPR spectra exponentially increased as the thickness of PVA increased. Similar pattern was also reported by Chumanov [19]. In the case of small and larger diameter, the peak of LSPR spectra increased then until a certain thickness exhibited constant. In contrast to intermediate diameter, the peak of LSPR spectra increased then until a certain thickness of PVA trend to decrease. The peak of LSPR showed higher than small and large diameter for the second peak and relatively same for the first peak. Further analyzed, we have found the dipole and quadrupole resonant mode contributed to the LSPR spectra of Ag-NPs coated PVA. For small diameter, the plasmonic resonant mode was dominantly first-order quasi-static dipole. The electromagnetic energy caused the electron cloud displacement forming the dipole field in the particle. At this condition, the external driving field relatively showed uniform and the absorption process was more dominant. So, it was clear the peak of LSPR appeared only one peak. Then, increasing the particle size, the interaction between the incident energy with the particles produced the external driving field was not uniform. Therefore, the dynamic depolarization happened in the particle and the second-order LSPR such as quadrupole resonant mode will contribute to the LSPR spectra. Thus, the dipole and the quadrupole resonant mode attributed the LSPR spectra at intermediate

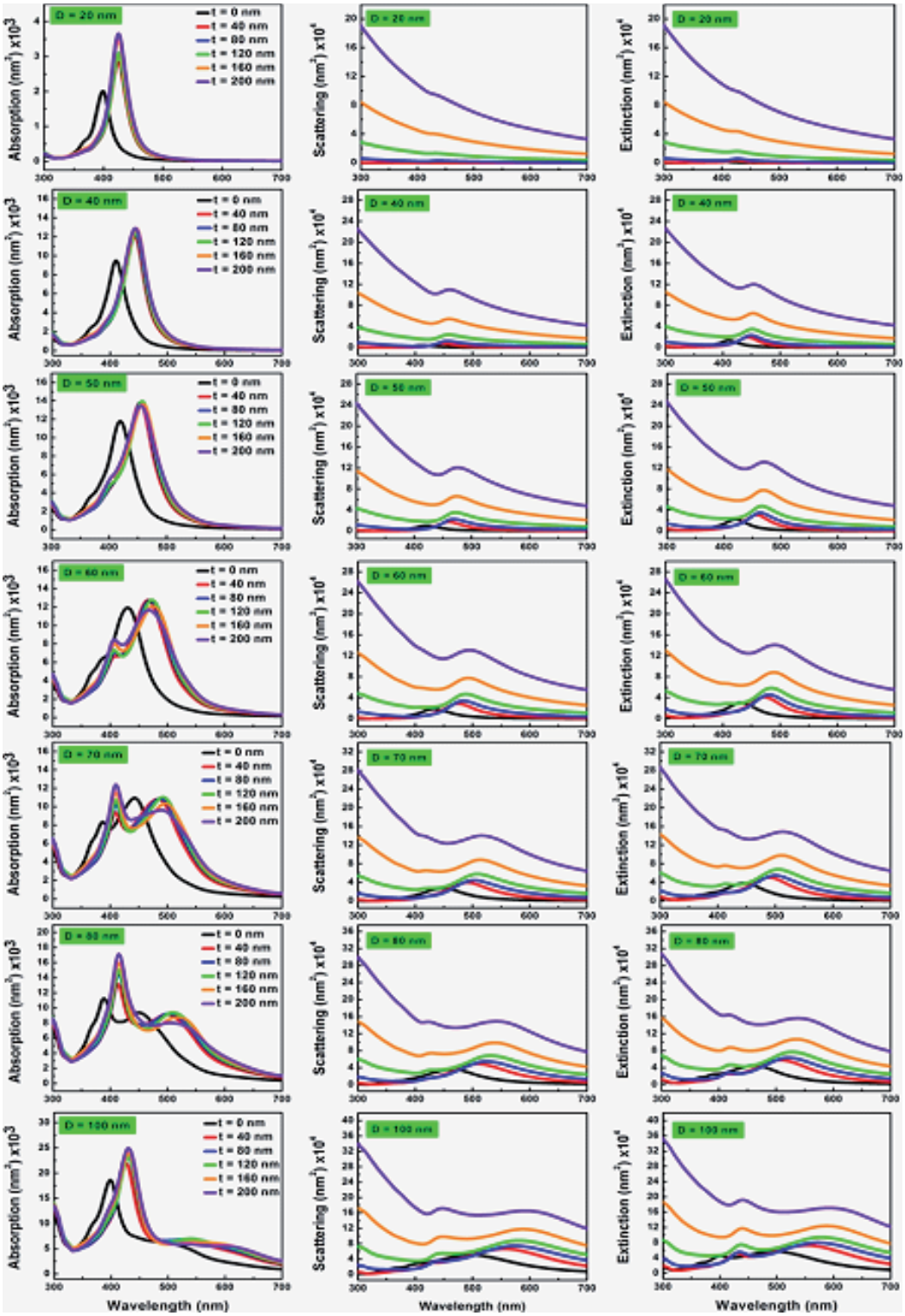

Figure 2: The LSPR spetra of Ag-NPs coated PVA from diameter D = 20 nm to D = 100 nm with respect to PVA thickness variation from t = 10 nm to t = 200 nm.

diameter. Consequently, one more peaks was found in the LSPR spectra. Then, the quadrupole resonant mode became dominant in the LSPR spectra in large diameter [20].

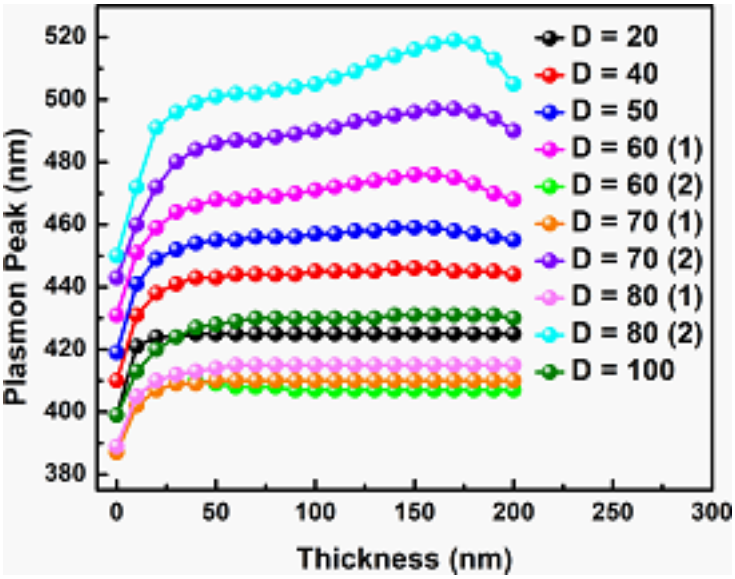

Figure 3: The peak of the LSPR spectra of Ag-NPs coated PVA with respect to diameter of Ag-NPs (D = 20-100 nm) and thickness of PVA variation (t = 0-200 nm).

4. Conclusions

In conclusions, we have systematically investigated the LSPR spectra of Ag-NPs coated PVA by means of numerical study based on BHMie approximation. The LSPR spectra shifted to red-shift as the diameter and the thickness increased. It was found the LSPR spectra showed three characteristic for small, intermediate, and large diameter. At small diameter, the dipole resonant mode contributed to the LSPR. At intermediate diameter, the dipole and the quadrupole resonant mode competed to the LSPR spectra. At large diameter, the quadrupole resonant mode was dominant to the LSPR spectra. Consequently, the LSPR spectra showed one peak at small and large diameter and more one peak at intermediate diameter.

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