

Polarization and Optical Properties of n-Layer Doped with Au Nanoparticles

S. Mohammad Nejad¹

Nanoptronics Research Center, Iran University of
 Science and Technology
 Tehran, Iran
 shahramm@iust.ac.ir

S. G. Samani²

Nanoptronics Research Center, Iran University of
 Science and Technology
 Tehran, Iran
 s_ghatreh@yahoo.com

Abstract- In this paper, influence of gold nanoparticle size on polarization ratio and scattering element of n-layer doped with them are discussed. Simulation algorithms have been developed for calculation of extinction and absorption efficiency. It was found that polarization is strictly related to angle of incidence and nanoparticles size. We also studied design of antireflection thin film to adjust angle and select appropriate material.

Keywords- Nanoparticle(NP); Antireflection(AN); polarization; Scattering.

I. INTRODUCTION

Thin films are used to improve surface properties in various applications such as photodetectors, resistances, capacitors, sensor and etc. Its design tries to fulfill set targets as well as possible for surface properties. Designing for desired optical properties is rather more difficult and requires a deeper understanding of thin film structures. Antireflection coatings are the most common optical coating. They reduce the surface reflectivity and are usually designed for particular wavelength range and angle of incidence. In this paper, this subject is investigated.

Multilayer structures that are periodical in their optical properties in one direction, have been known for a long time and represents more than a century old subject of investigation [1]. Most common applications are various filter structures, which are standard parts of many optical systems [2]. It has been reported that the optical properties of thin film can be improved by doping with metal particles such as Ag, Au or Cu [3]. Nanoparticles of metals have recently become the focus of research because of their unique properties, which are different from those of bulk materials. These properties depend on the size, shape and differences in the environments of nanoparticles.

The size induced properties of nanoparticles make them suitable for many applications in various areas such as catalysis, optics, and life environments [4]. For thin film applications we are interested in controlling the peak resonance wavelength and relative contribution of absorption and scattering to extinction.

II. ANALYTICAL METHOD

For simulation of polarization and scattering element, Volkove equations are used [5]. These functions have the form:

$$a_n = \frac{\psi_N^n((\psi)_{N,N}^n - A_{N-1}^n(\kappa)_{N,N}^n) - m_N(\psi)_N^n(\psi_{N,N}^n - A_{N-1}^n\kappa_{N,N}^n)}{\xi_N^n((\psi)_{N,N}^n - A_{N-1}^n(\kappa)_{N,N}^n) - m_N(\xi)_N^n(\psi_{N,N}^n - A_{N-1}^n\kappa_{N,N}^n)} \quad (1)$$

$$b_n = \frac{m_N\psi_N^n((\psi)_{N,N}^n - A_{N-1}^n(\kappa)_{N,N}^n) - (\psi)_N^n(\psi_{N,N}^n - A_{N-1}^n\kappa_{N,N}^n)}{m_N\xi_N^n((\psi)_{N,N}^n - A_{N-1}^n(\kappa)_{N,N}^n) - (\xi)_N^n(\psi_{N,N}^n - A_{N-1}^n\kappa_{N,N}^n)} \quad (2)$$

Where $m = n + ik$ is the refractive index of the sphere relative to the ambient medium, $x=ka$ is the size parameter, a the radius of the nanoparticles, $k = 2\pi/\lambda$ is the wave number, and λ the wavelength and:

$$A_k^n = \frac{m_{k+1}\psi_{k+1,k}^n(\psi)_{k,k}^n - m_k(\psi)_{k+1,k}^n\psi_{k,k}^n + A_{k-1}^n a_k^n}{m_{k+1}\kappa_{k+1,k}^n(\psi)_{k,k}^n - m_k(\kappa)_{k+1,k}^n\psi_{k,k}^n + A_{k-1}^n \tilde{a}_k^n} \quad (3)$$

$$B_k^n = \frac{m_{k+1}\psi_{k,k}^n(\psi)_{k+1,k}^n - m_k(\psi)_{k,k}^n\psi_{k+1,k}^n + B_{k-1}^n b_k^n}{m_{k+1}(\kappa)_{k+1,k}^n(\psi)_{k,k}^n - m_k\kappa_{k+1,k}^n(\psi)_{k,k}^n + A_{k-1}^n \tilde{a}_k^n} \quad (4)$$

$$a_k^n = m_k\kappa_{k,k}^n(\psi)_{k+1,k}^n - m_{k+1}(\kappa)_{k,k}^n\psi_{k+1,k}^n \quad (5)$$

$$\tilde{a}_k^n = m_k\kappa_{k,k}^n(\kappa)_{k+1,k}^n - m_{k+1}(\kappa)_{k,k}^n\kappa_{k+1,k}^n \quad (6)$$

$$b_k^n = m_k(\kappa)_{k,k}^n\psi_{k+1,k}^n - m_{k+1}\kappa_{k+1,k}^n(\psi)_{k+1,k}^n \quad (7)$$

$$\tilde{b}_k^n = m_k(\kappa)_{k,k}^n(\kappa)_{k+1,k}^n - m_{k+1}\kappa_{k,k}^n(\kappa)_{k+1,k}^n \quad (8)$$

Where $\psi(p), \kappa(p)$ are Ricatti-Bessel functions and $\xi(p)$ is Hankel function [6].

An important consideration to be made is the number of terms a_n, b_n required in order for the scattering series to converge. The convergence criterion of Wiscombe is used,

even though it was derived for the homogeneous sphere problem [7].

$$n_c = \begin{cases} x + 4x^{1/3} + 1 & x \in [0.02, 8] \\ x + 4.05x^{1/3} + 2 & x \in [8, 4200] \\ x + 4x^{1/3} + 2 & x \in [4200, 20000] \end{cases} \quad (9)$$

The extinction, scattering and absorption cross section represent the optical area and are given in units μm^2 . Dimensionless optical efficiencies, Q_{ext} , Q_{sca} and Q_{abs} are defined as the optical cross section divided by the geometric cross section. Optical efficiencies enable comparison of optical interaction strength unbiased by particle size and they can be calculated by Bohren and Huffman equations [8].

Following equations for simulation of absorption, scattering and extinction has been used:

$$Q_{ext} = Q_{sca} + Q_{abs} \quad (10)$$

$$Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2) \quad (11)$$

$$Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n) \quad (12)$$

For obtaining detailed information on the shape of the angular scattering pattern, there is a need to calculate the scattering functions, denoted here by S_2, S_1 . These functions describe the scattered field.

$$S_1(\theta) = \sum_{n=1}^{n_c} \frac{2n+1}{n(n+1)} (a_n \pi_n + b_n \tau_n) \quad (13)$$

$$S_2(\theta) = \sum_{n=1}^{n_c} \frac{2n+1}{n(n+1)} (a_n \tau_n + b_n \pi_n) \quad (14)$$

Where π_n, τ_n are calculated by following functions:

$$\pi_n = \frac{2n+1}{n+1} \cos \theta \cdot \pi_{n-1} - \frac{n}{n+1} \pi_{n-2} \quad (15)$$

$$\tau_n = n \cos \theta \cdot \pi_n - (n+1) \pi_{n-1} \quad (16)$$

The scattered intensity denoted as $I_s(\theta)$ is directly related to the state of polarization of the incident light intensity I_0 to a particular scattering plane (i.e. in our case, the horizontal scattering plane). As a result it is often needed to obtain results for parallel, perpendicular polarization as well as unpolarised incidence.

In particular the ratio (S_{12}/S_{11}) which corresponds to the polarization ratio P . In as much using $P = \frac{S_{12}}{S_{11}}$, $|P| \leq 1$ the behavior of the scattered light can be determined. That is to say, if $P > 0$ the scattered light is partially polarized perpendicular to the scattering plane and if $P < 0$ the scattered light is partially polarized parallel to the scattering plane.

In as such, it can be shown that:

$$I_s(\theta) = \begin{cases} \frac{1}{x^2} (S_{11} + S_{12}) I_0 & \text{parallel polarisation} \\ \frac{1}{x^2} (S_{11} - S_{12}) I_0 & \text{perpendicular polarisation} \\ \frac{1}{x^2} (S_{11}) I_0 & \text{unpolarised} \end{cases} \quad (17)$$

III. SIMULATION

NP sizes vary considerably, from 5nm up to several nanometers. The variation of the polarization and the scattering are plotted against the wavelength for two layers, TiO2 and ZnO, doped with Au nanoparticle in a=50nm, 500nm and an incident laser power in 2mW. Fig. 1 shows the polarization ratio for Au doped into 2-layers for different size of Au nanoparticles. It is maximum and completely perpendicular at around the angle 90° .

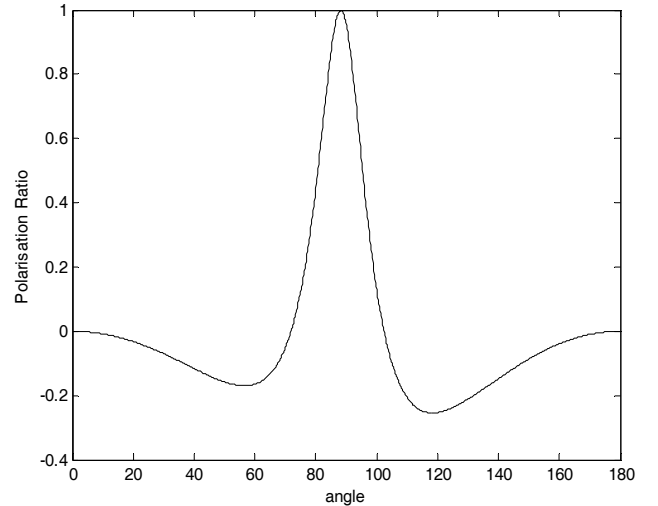


Figure 1. The scattered intensity's polarization ratio for 2-layer doped with Au NP with radius a=50nm

There are several important conclusions to be deduced from the results. First, the influence of the angle of incidence on scattering. Second, system acts as a filter for nanoparticle with radius about 50 nm. If the diameter of nanoparticles is about more than 50nm, the scattered intensity's polarization ratio will increase and both of parallel and perpendicular polarization will be existed so system is not proper filter.

To adjust angle we use antireflection coating that in the following we describe the most common types of AR coating. The first and most simple structure is a single layer with thickness $d = \frac{\lambda}{4n}$ and $n_0 < n < n_s$, where n_0 is the refractive index of propagation medium, n the coating

refractive index and n_s the substrate refractive index. A particular case for a single layer coating is when $n = \sqrt{n_0 n_s}$.

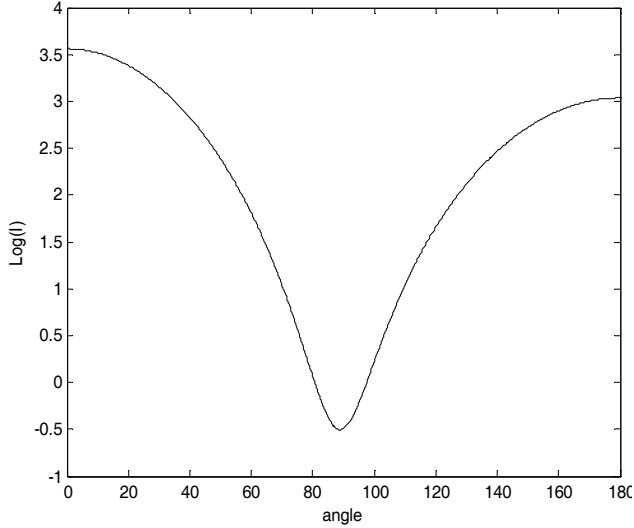


Figure 2. A 2-layer scattering model for polarized incidence for nanoparticles with $a=50\text{nm}$

The second category is two layer coating, also known as V-coating due to their reflectivity spectra in the AR-region, with $n_0 < n_1 < n_2 < n_s$. V-coating are very useful for the laser industry because of their simplicity and low reflectivity over a narrow bandwidth. A V-coating is easy to design since it can be analytically calculated as follows. The phase thickness for a thin film is:

$$\varphi_i = \frac{2\pi}{\lambda_t} n_i d_i \quad (18)$$

Where d_i is the thickness and n_i the layer refractive index of the i - layer. λ_t is the target wavelength. Table 1 lists the optical properties that were measured to analyze influence of nanoparticle on extinction and absorption.

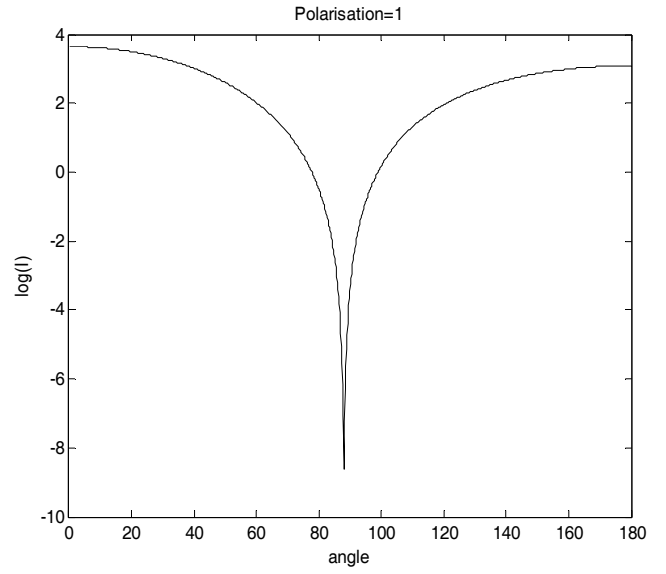


Figure 3. A 2-layer scattering model for unpolarized incidence for nanoparticles with $a=50\text{nm}$

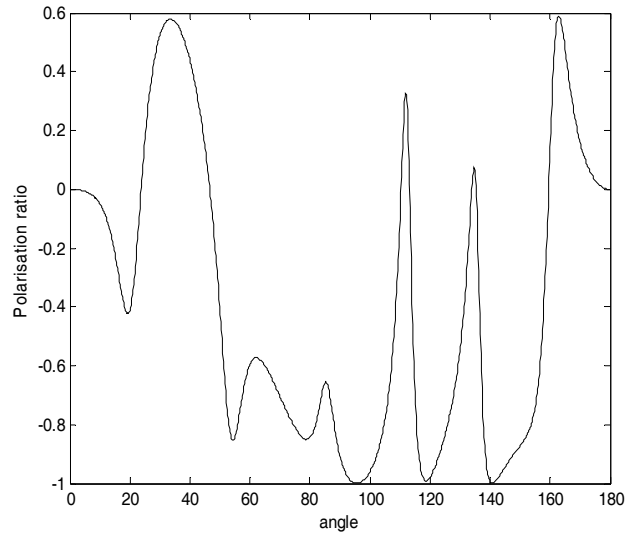


Figure 4. The scattered intensity's polarization ratio for 2-layer doped with Au NP with radius $a=500\text{nm}$

TABLE I. THE OPTICAL PROPERTIES FOR 2-LAYER DOPED WITH AU NANOPARTICLE AT $a=5\text{NM}$ AND $a=50\text{NM}$

$\lambda(\text{nm})$	Q_{sca}	Q_{ext}	Q_{abs}
300	11.63	14.5	2.92
350	6.25	8	1.8
400	7	7	0
500	9.5	10.9	1.4
550	6.5	9.2	2.7
600	7.2	10.7	3.5
650	7.7	17.8	10.12

700	17.65	50.9	33
750	14.2	15.8	1.6

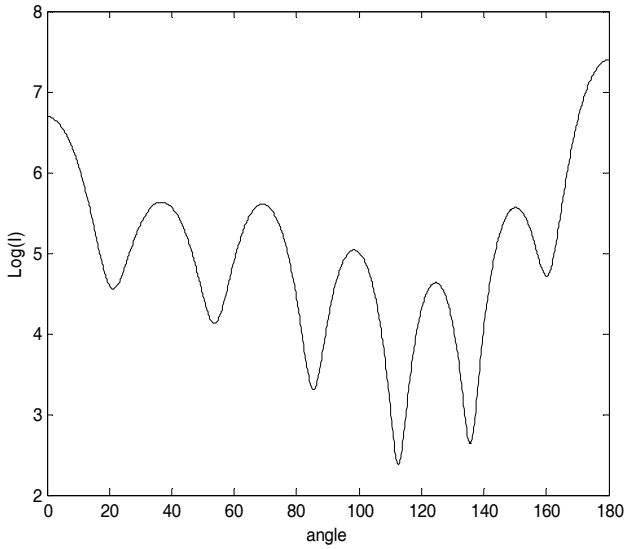


Figure 5. A 2-layer scattering model for polarized incidence for nanoparticles with $a=500\text{nm}$

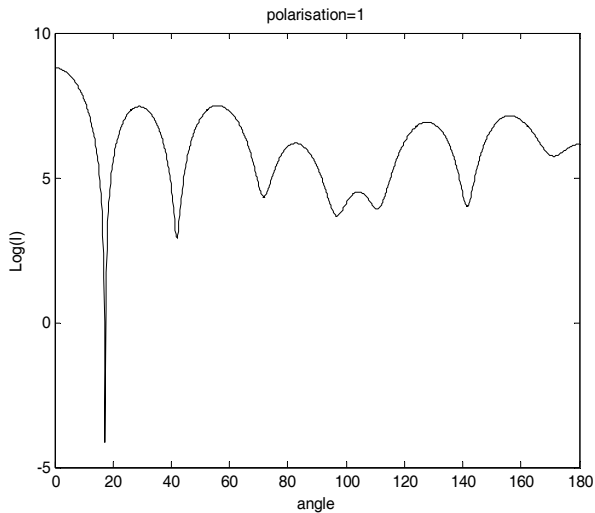


Figure 6. A 2-layer scattering model for unpolarized incidence for Au nanoparticles with $a=500\text{nm}$

IV. CONCLUSION

Polarization and optical properties of n-layer was found to be related to nanoparticle size and incident angle. It can be used antireflection coating for adjusting angle. If the diameter of nanoparticles is about more than 50nm, the scattered intensity's polarization ratio will increase and both of parallel and perpendicular polarization will be existed so system is not proper filter. Au nanoparticles have high absorption coefficient, so the charges depict very high

transition. That's why recombination electron - hole and noise decrease and absorption efficiency increases.

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