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Spectral Analysis of Gold Nanorods as Active Plasmonic Media in Dielectric Environments (Air and Water) across Visible and Different NIR Wavelengths

Hanaa Jassim Mohamed[1,*], Maher Abdulfadhil Gatea[1,2]

[1]*Department of Physics, College of Science, University of Kufa.*
** Education Ministry, Najaf, Iraq. hanaaj.alabasi@student.uokufa.edu.iq*

[*]Corresponding Author E-mail: mahera.alibraheemi@uokufa.edu.iq

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ABSTRACT

Gold nanorods (GNRs) have emerged as pivotal nanostructures in optical and electronic applications due to their unique localized surface plasmon resonance (LSPR) properties, which are highly sensitive to particle geometry and the surrounding medium. This study investigates the effects of spatial variations, radius of the cylindrical structure, surrounding media, and insulating layers on the scattering behavior of GNRs under illumination at selective wavelengths (610, 710, 810, 910) nm. Three key simulation models were developed: The first simulation model was on the impact of varying interparticle distances in different media (air and water), revealing significant shifts in scattering intensity and plasmonic spectra due to enhanced interactions at closer proximities. The second simulation model explored the role of insulating layers, demonstrating that coatings such as silica altered electric field distributions and attenuated environmental influences, resulting in modified scattering spectra. The third simulation model focused on the impact of varying the radius of GNRs in different media (air and water), again showing notable shifts in scattering intensity and plasmonic behavior. The results clearly highlight the critical role of gold nanoparticles as active nanostructures in controlling the optical response, particularly through the LSPR mechanism. This emphasizes their potential in nanophotonic applications, such as high-sensitivity optical sensors, nanoscale imaging systems, and optoelectronic devices. The findings also show that the maximum benefit of nanostructures in medical fields can be obtained by carefully designing these structures.

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التحليل الطيفي لقضبان الذهب النانوية كأوساط بلازمونية فعالة في بيئات عازلة مختلفة (الهواء والماء) عبر أطوال موجية في النطاق المرئي وتحت الأحمر القريب

هناءجاسم محمد [1,*] , ماهر عبد الفاضل كاطع[1,2]

قسم الفيزياء , كلية العلوم , جامعة الكوفة [1]

وزارة التربية, النجف , العراق*

الـــخُـــلاصـــة

برزت قضبان الذهب كهياكل نانوية محورية في التطبيقات البصرية والإلكترونية نظرًا لخصائصها الفريدة للرنين البلازموني السطحي الموضعي(LSPR) ، والتي تتميز بحساسية عالية لهندسة الجسيمات والوسط المحيط. تبحث هذه الدراسة في آثار الاختلافات المكانية ونصف قطر الهيكل الأسطواني والوسائط المحيطة والطبقات العازلة على سلوك التشتت لقضبان الذهب النانوية تحت الإضاءة عند أطوال موجية انتقائية (610،710،810،910) نانومتر. قادت ثلاثة نماذج محاكاة رئيسية: نموذج المحاكاة الأول تأثير المسافات المتغيرة بين الجسيمات في وسائط مختلفة (الهواء والماء)، مما يكشف عن تحولات كبيرة في شدة التشتت والأطياف البلازمية بسبب التفاعلات المحسنة عند التقارب. استكشف نموذج المحاكاة الثاني دور الطبقات العازلة، موضحًا أن الطلاءات مثل السيليكا غيرت توزيعات المجال الكهربائي وخففت التأثيرات البيئية، مما أدى إلى تعديل أطياف التشتت. نموذج المحاكاة الثالث يرصد تأثير تغيير نصف قطر جسيمات النانو النانوية في بيئات مختلفة (الهواء والماء)، كاشفًا عن تحولات كبيرة في شدة التشتت والأطياف البلازمية نتيجةً لزيادة التفاعلات عند مسافات أقرب. تُقدم هذه النتائج رؤىً قيّمة في مجال التحكم في خصائص البلازمون، مما يُسهم في تطوير أجهزة استشعار بصرية عالية الحساسية، وأنظمة تصوير نانوية، وأجهزة إلكترونية بصرية. تُظهر النتائج أنه يمكن تحقيق أقصى استفادة من البنى النانوية في المجالات الطبية من خلال التحكم في تصميم هذه البنى.

الكلمات المفتاحية:

الاعواد النانوية
التشتت البلازموني
الازدواج البيني
البيئة العازلة
علم الفوتونيات النانوي
المقطع العرضي للتشتت
القلب والقشرة

1. INTRODUCTION

The study of nanoparticles has become a keystone of modern science and technology, because the nanoparticles display unique properties that are different from those of their bulk complements. Among the diverse types of nanoparticles, gold nanorods GNRs have involved particular attention due to their distinctive optical, electronic, and plasmonic characters, which enable a broad range of applications in fields such as photo thermal therapy[1], bio sensing[2], optical imaging[3], and nanophotonics [4]. Localized surface plasmon resonance (LSPR) occurs when conduction electrons on the surface of gold nanorods oscillate in response to incident light. This resonance is responsible for their unique optical behavior. Gold nanorods support two distinct plasmon modes: longitudinal and transverse. In contrast, spherical nanoparticles exhibit only symmetric resonance patterns[5].

When two GNRs were placed close together and illuminated with light of different wavelengths range 610,710,810,910) nm, gold (e.g. nanorods has a distinctive scattering pattern due to their strong plasmonic response. This response is an important finding of publication [6]. In nanoscale imaging, the ability of GNRs to scatter light efficiently enhanced the contrast and resolution of the images by using GNRs with SiO_2 promising new contrast agents that can be controlled to have specific scattering and absorption properties in the near-infrared region(NIR), and are widely utilized in biomedical imaging applications due to their highly tunable scattering and absorption characteristics ,making them excellent candidates for light-responsive contrast enhancement[7]. The scattering intensity and spectral profile of GNRs are influenced by a combination of intrinsic and extrinsic factors, including interparticle distance, insulating layer coatings, surrounding media and nanorod material and diameter. Each of these parameters plays a crucial role in determining the strength and nature of plasmonic coupling, and the overall optical response of the nanorods [8].

One of the most significant factors that are affecting the scattering properties of GNRs is the distance between adjacent nanorods. The spacing between adjacent gold nanorods plays a central role in determining their scattering behavior. The distance between adjacent gold nanorods has a profound effect on their light-scattering characteristics. When two nanostructures are brought sufficiently close, their localized electric fields begin to interact, leading to a phenomenon known as plasmonic coupling. This coupling results from the merging of intense near-field zones on each particle's surface, causing noticeable shifts in plasmonic resonance energies[9]. Understanding this phenomenon is particularly important for applications that require controlled interaction between light and metal at the nanoscale. Examples include photonic circuits, high-resolution bioimaging, and plasmonic waveguides, where accurate tuning of optical responses directly impacts performance[10, 11].

The optical behavior of nanoparticles can be effectively tuned by coating them with dielectric layers. These layers help stabilize and regulate the local surface plasmon resonance (LSPR) peak, making the nanoparticle’s response more predictable and less susceptible to environmental fluctuations[12, 13].

The scattering cross-section was found to increase with the diameter of gold nanorods (GNRs), as a result of light interacting with a larger volume of material. Moreover, a larger diameter enhances near-field effects and strengthens plasmonic coupling between particles. These phenomena play a critical role in applications such as surface-enhanced spectroscopy and nanoscale plasmonic sensing, where increased interaction leads to improved signal detection and sensitivity[14].

This study aims to establish a systematic framework for enhancing the optical scattering behavior of gold nanorods (GNRs). The investigation focuses on three key variables: varying the nanorod diameters (10–60 nm), adjusting the inter-rod spacing, and introducing insulating dielectric layers around the particles. By analyzing the influence of these parameters, the study seeks to optimize light–matter interactions at the nanoscale [15].

The main objectives of this research are: a- Investigate how varying the diameter of gold nanorods (from 10 nm to 60 nm) affects the scattering cross-section and plasmonic behavior. b- Evaluate the impact of interparticle distance on plasmonic coupling and resonance shift. c- Assess the influence of dielectric insulating layers (e.g., silica) on the optical stability and tunability of LSPR. These objectives aim to enhance the design of plasmonic nanostructures for optimized light–matter interaction, with implications for advanced imaging and sensing technologies.

2 . Numerical Modeling of Gold Nanorod

In this study, the length of the two gold nanorods was kept constant across all simulations. The analysis was conducted in three stages: First, the interparticle distance was varied to examine its effect on the scattering cross-section. Second, the diameters of the nanorods were systematically adjusted to evaluate the influence of size. Finally, dielectric shells with thicknesses of 5 nm and 10 nm were added around each gold-rod to assess the role of insulation in modulating the optical response. Then, in the second part, we kept the length the same but with different radii to understand how the rod size influences the scattering behavior.

COMSOL Multiphysics 6.1 was used to model the scattering behavior of gold nanorods with varying radii. The finite element method (FEM) applied with carefully defined boundary conditions to ensure accurate results. The extinction cross-section simply tells us how much light is lost due to both absorption and scattering by the nanoparticle as show in eq. (1)

$$\sigma_{ext} = \sigma_{abs} + \sigma_{sca} \qquad (1)$$

σ_{abs} : Absorption cross section

σ_{sca} : Scattering cross section

An electromagnetic wave frequency domain model was employed to numerically compute the scattering cross section of two adjacent GNRs in different surrounding media, as described in equation (2), and the geometrical mesh structure of two GNRs showed in figure (1).

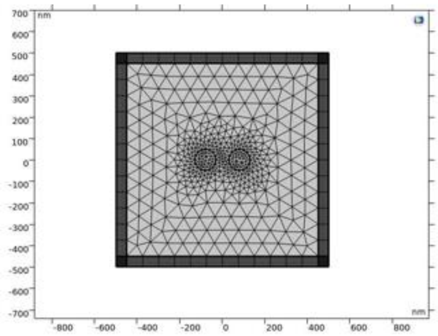


Fig. 1 Geometrical mesh structure of two GNRs

$$\boldsymbol{\sigma_{sca}} = \frac{\boldsymbol{k^4}}{\boldsymbol{6\pi}} |\boldsymbol{\alpha}|^2 \qquad \textbf{(2)}$$

Where K, The wave vector of incident light, α, is the polarizability.

3 . Computational Data

The simulation of light scattering by gold nanorods (GNRs) was performed using COMSOL Multiphysics software, based on the finite element method (FEM). The geometry was modeled using cylindrical nanorods with diameters ranging from 10 to 60 nm, placed in different dielectric media (air and water) with variable interparticle spacing. The incident wavelengths were selected as 610 nm, 710 nm, 810 nm, and 910 nm. Perfectly matched layers (PML) were used as boundary conditions to absorb scattered waves and minimize reflection. The mesh size was optimized to ensure accuracy, especially near the nanorod surfaces. Optical constants of gold were defined using experimental data for the real and imaginary parts of the refractive index. The simulations included cases with and without dielectric coatings (such as silica) to analyze their effect on the electric field distribution and scattering intensity. Table 1 : Physical Quantities, Symbols, and Units Used in This Study

Physical Quantity	Symbol	Unit
Wavelength	λ	nm
Scattering cross-section	. σ_{sca}	m^2
Absorption cross -section	σ_{abs}	m^2
Wave vector of incident light	K	m^{-1}
Polarizability.	α	m^3

4 . Results and discussion

The investigation into interparticle distance offers valuable insights for designing plasmonic systems with tunable coupling effects, which are essential for applications such as near-field communication devices. Meanwhile, the analysis of insulating layers provides critical data for developing stable and robust GNR-based sensors in complex environments [16, 17]. The scattering behavior of (GNRs) under changing inter particle distances investigated in two different media: air and water. Part of the analysis focuses on how the medium and inter particle spacing influence the localized surface plasmon resonance (LSPR) characteristics, particularly the scattering intensity and peak position [18]

Fig.(2). Illustrates the scattering cross section as a function of the lateral (x-axis) separation between two gold nanorods, varying from 20 to 100 nm. The nanorods have a fixed length and radius, and the simulations conducted in two different surrounding media air and water. In the case of GNRs dispersed in air were they are equal in size, we also noticed that scattering was less for the shorter wave length of the laser used [19].

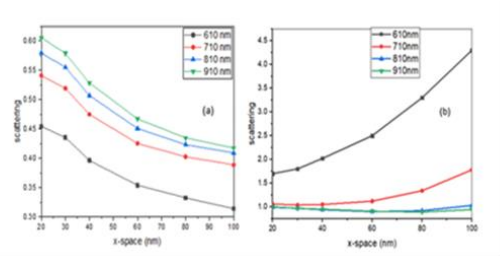
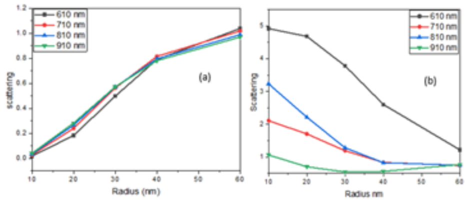


Fig.2 Scattering vs. inter-nanorod distance in air and water

When increase the distance between two (GNRs), and then illuminated them with a laser light of a different wavelengths about (i.e. 610, 710, 810, 910) nm, it was noticed that the scattering cross section decreases with increasing distance between two GNRs, due to reducing the phenomenon of coupling effect, and the refractive decreasing which led to decreasing in scattering, it was also noticed that scattering less for the shorter wave length of the laser used [19].

In water, the scattering cross-section increased gradually with the increase in the distance between the two rods, due to the large refractive index of water, which reduces the plasmonic coupling between the two rods, which in turn increases the scattering cross-section.[20]. The influence of varying the radius of gold nanorods (GNRs) on the scattering behavior analyzed in two different media: air and water can be seen in Fig (3).

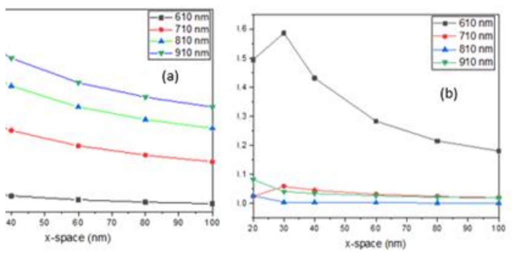


The radii considered in this study were (10 nm, 20 nm, 30 nm, 40 nm, and 60 nm). The objective of behind this comparison is to understand how changes in nanorod size affect the scattering cross section in different dielectric environments [21].

In air, it was noticed that the increase in scattering cross section with an increase in the radius of GNRs can be attributed to the larger surface area of the GNRs. While in water the scattering cross section decreases as the increase of the GNRs radius. A laser with a shorter wavelength has greater scattering cross section. . The explanation for that can be that, in air, the speed of light is greater than its speed in water because the refractive index of water is greater than the refractive index of air .As the radius of GNRs increases, the size of the surface that interacts with the incident light increases, which increases the scattering cross section. As in water where the speed of light is lower, the amount of light interacting with the nanorod decreases ,and thus the scattering cross section decreases [22].

The scattering estimation in point between two GNRs at (a) 5nm SiO_2 shell (b) 10 nm SiO_2 shell can be demonstrated in Fig.4. The scattering behavior of gold nanorods (GNRs) coated with silica shells of varying thicknesses was systematically studied to evaluate the influence of the insulating layer on their localized surface plasmon resonance (LSPR) characteristics. Specifically, two scenarios were considered: GNRs with a 5 nm silica shell and GNRs with a 10 nm silica shell. The results highlight the critical role of shell thickness in modulating the scattering intensity and spectral profile of GNRs under laser excitation[23].

Fig.4, shows the scattering cross section between two GNRs, coated with two different thicknesses of SiO2, in each thickness we noticed there is decreases of scattering cross section with increases of the space between two gold nanorod after irradiated them by laser light due to decreases of the coupling effect between them and then decreases the scattering[24].



In general, a thinner SiO2 layer enhances coupling and reduces scattering, while increasing the layer thickness leads to reduced coupling and increased scattering[25].

5 - Conclusion

The results showed that increasing the distance between the nanorods in air increased the scattering cross-section, while in water the opposite occurred. Furthermore, increasing the diameter of the nanorods reduced the scattering cross-section in air and increased it in water. The results also showed that coating the rod with a thin layer of SiO2 improved optical scattering. All of these results are fully consistent with previous research and studies in this field.

6 – Reference

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