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Research Article

Computational Study of the Effect of the Size-Dependent Dielectric Functions of Gold Nanomaterials on Optical Properties

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The effect of size on the optical properties of gold nanomaterials has been studied using the theoretical Drude–Sommerfield model. The real and imaginary parts of the dielectric function of bulk as a function of wavelength due to free electron contribution and the real and imaginary parts of the dielectric function of nanogold materials as a function of wavelength due to free electron and bond electron contribution are calculated. The real and imaginary parts of the dielectric function of bulk as a function of wavelength due to the free electron contribution graph and The real and imaginary parts of the dielectric function of nanogold materials as a function of wavelength due to free electron and bond electron contributions are plotted. As we observed from the graphs, the real dielectric functions of both bulk and nanogold materials are inversely proportional to wavelength. The imaginary part of the dielectric function of bulk gold materials is independent of wavelength. At high wavelengths, the size of the gold nanomaterial is highly influenced by both real and imagined dielectric functions at high waves. As the wavelength increases, the effect of the size on the dielectric function also increases. The size-dependent dielectric function of nanomaterials is highly influenced by their optical properties and electrical structure.

1. Introduction

In recent decades, nanomaterials have gained widespread importance in academic and industrial research as well as in industrial, medical, and consumer applications. Their applications range from addition to cement and cloth to make them yet lighter and stronger, environmental remediation or cleanup to neutralize toxins and bind with, to electronics, and drug delivery. The surface area to volume ratio of nanomaterials is much higher than bulk, which means the large are on nanomaterials surface. This has very significant advantages for applications like catalysis. Nanomaterials, which can be synthesized utilizing the concepts of green chemistry and green engineering [1] or nanosized functionally advanced materials that have high-performance applications in energy generation and storage, carbon dioxide fixation, electronic devices, and are sustainable in terms of production and application with respect to the environment, have been labeled "green nanomaterials" [2–6]. Their function depends on the size of the materials [7]. A nanomaterial is a material with one of its dimensions ranging from 1 to 100 nm [8, 9]. If a material's size changes from bulk to nanoscale, its state also changes, which means that the material is nonmagnetic at bulk, but when it changes to nanoscale, it becomes magnetic [10].

In general, nanomaterials can be classified into five groups [10]: (1) based on origin, nanomaterials can be classified as artificial and natural nanomaterials; (2) based on size dimensions, nanomaterials can be classified as zero dimensions, one dimension, two dimension, and three-dimension nanomaterials; (3) based on structure configuration, nanomaterials can be classified as inorganic, organic, composite, and carbon-based nanomaterials; (4) based on potential toxicity, nanomaterials can be classified as persistent granular, fiber-like, and CMAR (carcinogenic, mutagenic, asthmagenic, reproductive toxin) nanomaterials; and (5) based on pore diameter dimensions, nanomaterials can also be classified as macroporous nanomaterials and mesoporous nanomaterials. Inorganic nanomaterials are nanoscale materials that do not have

carbon atoms. Metal-based nanomaterials are examples of inorganic nanomaterials, such as cadmium, aluminum, cobalt, gold, copper, iron, silver, zinc, and lead [11, 12]. These materials have extremely outstanding optical properties [13–15]. In addition to these integrations of gold and silver nanoparticles into hydrogels for commercial contact lenses [16]. Because of this, metal-based nanomaterials are becoming interesting research fields and nanotechnology application components. Specially gold nanomaterials are very sensitive for research [17] because they are used for many field of application such as magnetic resonance imaging [18], biooptical imaging [19], molecular imaging [20, 21], electrochemical imaging [22], radiotherapy and X-ray imaging [23], molecular TC/MR imaging of cancer [24–27], drug delivery [28–31], solar cell [32, 33], light-emitting diodes [34, 35], lithium-ion battery [36, 37], lithium air battery [38], lithium-oxygen battery [39], fluorescence microscopy [40, 41], communication [42, 43], spectroscopy [44, 45], cancer therapy [46, 47], biomedical sensors [48], diagnosis and therapy of disease [49, 50], nano electronics devices [51], bionano technology [52], green technology [53], agriculture [54, 55], photoluminescence [56], sensing detection [57], to develop new technologies [58], catalysis [59], water treatment [60], waste water treatment [61], water purification [62], soil fertility [63], soil productivity [63], antimicrobial activity [64], genetic engineering of plants [65], plant adaptation potential [66], plant disease diagnostics [67], plant disease management [68], animal health [69], animal breeding [70], metamaterials [71], plant breeding [72], and optical biosensors [73]. It should perhaps be noted here that microscopic investigations of gold particles and the determination of their dimensions are often regarded as the very beginning of colloid chemistry and, thus, also of nanotechnology [74, 75].

Nanomaterials have special functions, unlike bulk materials, as illustrated below. Nanomaterials have tunable optical properties that exhibit different optical properties and colors depending on their shape, composition, and size; they enhance nonlinear optics and optical emission [76]. Nanomaterials have higher nonlinear coefficients and photoluminescence compared to bulk materials [56]. Nanomaterials have the ability to be used in optical imaging [19] and sensing applications such as optical lenses [77] and probes such as fluorescence microscopy [40], photothermal therapy [46], and biosensors [51]. Nanomaterials have a great potential application in optical energy storage and conversion to improve the efficiency of solar cells [32], light-emitting diodes [34], and batteries [36–38].

In addition to this, because of their small size, nanomaterials have special magnetic, electrical, sensitivity, and physical features [10]. The dielectric function of a nanomaterial characterizes its optical properties, such as reflection, transmission, absorption, and dispersion, as a function of wavelength, frequency, and energy [10, 78]. The nanomaterial may have a high- or low-dielectric function [79]. This dielectric function (ε) consists of real and imaginary parts. The imaginary part of the dielectric function can also be expressed as complex numbers, which measure the ability of the dielectric losses and energy absorption of nanomaterials, but the real dielectric function is a measure of the ability of the nanomaterials to polarize [80]. The ability of nanomaterials to lose the tangent of dielectric materials can be expressed as the ratio of the imaginary dielectric constant to the real dielectric. This imaginary dielectric function is also related to the dissipation and absorption of electromagnetic radiation by an interactive material [81]. If a nanomaterial has a low imaginary dielectric function, it indicates that it has a low absorption coefficient. The main advantage of nanomaterials with high imaginary dielectric functions is that they enhance energy conversion; they have a high absorption coefficient; they are highly efficient at converting incident electromagnetic radiation into electricity and heat; and they are applicable to things such as solar cells and photodetectors [32, 33, 73].

High imaginary dielectric functions have the ability to improve contrast, which means that they create a high contrast between the reflected and transmitted. They are used for modulators and optical applications. They also have the ability to reduce scattering by improving the resolution and quality of the reflected or transmitted signal. Those nanomaterials are used for spectroscopy [44], imaging [19], magnetic recording media [82], and communication [42] applications. The main advantages of nanomaterials with high real dielectric function are increased capacitance, which has the ability to store more electric energy by field capacitance. The increased capacitances are used for energy storage, such as power supply. The nanomaterial has a high real dielectric function and has the ability to improve electric breakdown strength. It may withstand higher voltages, making it suitable without breaking down for the required amount. They improve antenna performance, which has a significant impact on transmission efficiency and radiation pattern. Lowering the real dielectric function of nanomaterials allows for reduced dielectric thickness; this reduction of the nanodielectric function thickness improves signal integrity by minimizing transmission line losses for very high-frequency circuits [80, 81, 83, 84].

The dielectric function of nanomaterials depends on the polarization of atoms in the nanomaterials, the density of the nanomaterial, the temperature, the frequency of the incident electromagnetic radiation, any surface defects, the size, shape, and free electrons of the nanomaterial. The dielectric function of nanomaterials is complex, which shows the ability of nanomaterials to respond to the applied electric magnetic field. It is also used for the calculation of the refractive indexes of nanomaterials. At optical frequency, there is no magnetic response; the electronics respond to incident electromagnetic radiation by dielectric function. The optical response of nano-size particles of dielectric function is in the visible-near infrared spectral range [85]. The main factors affecting the optical properties of gold nanomaterials are the shape, size, and dielectric function of the environment [86]. However, the extinction cross-sectional properties like peak position, amplitude of resonance, and full breadth at half the maximum value of gold nanomaterials and the optical density of gold nanomaterials depend on the dielectric function of gold nanomaterial [84, 86, 87].

The optical density of gold nanomaterials is the ability to measure whether the nanomaterials scatter or absorb

incident electromagnetic radiation (light). The extinction cross-section properties show the intensity of resonance peaks and their shape in the extinction spectrum. The collective oscillations of the electrons within the nanoparticles, known as surface plasmons, are represented by the resonance peaks [88]. The width of the resonance peak at half of its greatest value is known as the full breadth at half maximum or FBHM. The wavelength, or frequency, of the incident light that causes the greatest amount of extinction is known as the peak position. The greatest value of the extinction cross-section is known as the resonance amplitude.

Gold nanoparticle dielectric function modifies the resonance condition, damping factor, and radiative decay of surface plasmons, which in turn affects the optical density and extinction cross-sectional characteristics [89]. The ratio of the nanoparticles' dielectric function to that of the surrounding medium establishes the resonance condition, which in turn establishes the peak position. The FBHM is determined by the damping factor, which is influenced by radiation, interband transition losses, and electron scattering losses [90].

Many researchers have studied the optical properties and size-dependent dielectric function of Au nanoparticles in experimental and theoretical ways [90–93]. We are listing some of them below: In experimentally used spectroscopic ellipsometry, which measured the polarization of electromagnetic radiation, which is reflected from gold nanomaterials, and in differential interference contrast microscopy, they measured the real and imaginary parts of the dielectric function of gold nanomaterials. This method has the ability to provide high spectral sensitivity and spatial resolution over a broad range of wavelengths.

Gold nanoparticles have fascinating optical properties, while Au nanoparticles exhibit unique optical properties due to their surface-volume ratio, shape, and size [94–96]. They also have surface plasmon resonance properties, which occur when the incident light hits a gold surface. They have surface-enhanced Raman scattering properties when molecules are adsorbed onto the surface of gold nanoparticles [97]; the Raman scattering signals are significantly amplified; luminescence properties, which indicate Au nanoparticles emit "cold light" when excited [98, 99] and gold nanoparticles are biocompatible, minimizing adverse effects when used in biological systems [100, 101]. Due to these properties of Ag nanoparticles, they are used for improving bioimaging [102], optical biosensing, biosensors, imaging [10], therapeutic interventions [103], solar cells, photocatalysis [104], biomedicine [105], reduced air pollution [106], water purification [62], power cells [107], emission management, nanotechnology [106], their remarkable capacity to scatter and absorb light, absorb and convert optical energy into heat via nonradiative electron relaxation dynamics, and green nanotechnology. The theoretical Drude model, Drude–Sommerfield, and Mie theory methods have been used to study the optical properties of gold nanomaterials. Both in experimental and theoretical models, the dielectric function, such as plasma frequency, electron relation time, reaction wavelength, radii, plasma wavelength, damping constant for free electrons, damping constant for bond electrons, natural frequency, relaxation time, and dielectric function of Au nanomaterials at infinite radiuses, has been extracted. However, in this study, the Drude–Sommerfield theoretical model is also used to study the dielectric function of Au nanomaterials due to free electrons, bond electrons as a function of wavelength, and the dielectric function of Au bulk materials as a function of wavelength using the dielectric function parameters from experimental data. Anyone who studies the optical properties and the use of Au nanomaterials, and the users of Au nanoparticle materials must know these properties. Due to this reason, we have studied the impact of size on the optical properties of Gould nonparties based on the dielectric function article. Because of this study, we have the ability to fill the gap.

2. Mathematical Formulation of Bulk and Nanoscale Noble Metals' Using Drude–Sommerfeld Model

The Drude–Sommerfield model is used to study the optical properties of size-independent (bulk) and size-dependent (nanoscale) materials [108–112].

2.1. Mathematical Formulation of Bulk Noble Metals' Dielectric Function. The dielectric function of bulk materials is expressed as the permittivity of a medium as a function of angular frequency (ω), which is expressed in the real and imaginary parts as follows [113]:

$$\varepsilon_r = \varepsilon_1(\omega) + i\varepsilon_2(\omega). \tag{1}$$

Simplifying Equation (1), we get the following:

$$\varepsilon_r = 1 + \frac{\omega_p^2}{-\omega^2 - i\gamma\omega} = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}, \tag{2}$$

where ω is the angular frequency, γ is the damping constant of the oscillators w_p is plasma frequency occurs in the ultraviolet region of the spectrum, which is equal to $\frac{N^* e^2}{m\varepsilon_0}$, e is the charge of electron, m is mass of electron, ε_0 is permittivity of vacuum, N^* is the density of conduction electron.

The dielectric function of metals in their real parts is written independently as follows:

$$\varepsilon'(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + \gamma^2}. \tag{3}$$

The dielectric function of metals in their imaginary parts is written independently as follows:

$$\varepsilon''(\omega) = 1 - \frac{\omega_p^2 \gamma}{\omega(\omega^2 + \gamma^2)}. \tag{4}$$

For $\Gamma \ll \omega, \omega^2 + \gamma^2 \approx \omega^2$, Equation (3) is specified as follows and as a function of wavelength.

$$\varepsilon'(\omega) = 1 - \frac{\omega_p^2}{\omega^2}. \tag{5}$$

We know that the physical quantities, $\omega_p = \frac{2\pi c}{\lambda p}$, $\omega = \frac{2\pi c}{\lambda}$, $\tau = \frac{\lambda_\tau}{2\pi c}$, and $\Gamma = \frac{2\pi c}{\lambda_\tau}$.

Substituting these physical quantities in Equation (5), the dielectric function can be expressed as a function of wavelength as follows:

$$\varepsilon'(\lambda) = 1 - \frac{\lambda^2}{\lambda_p^2}. \tag{6}$$

The dielectric function of a metal's imaginary part is written independently as follows:

$$\varepsilon''(\lambda) = \frac{\omega_p^2 x\Gamma}{\omega^3}. \tag{7}$$

Substituting, $\omega_p = \frac{2\pi c}{\lambda p}$, $\omega = \frac{2\pi c}{\lambda}$, $\tau = \frac{\lambda_\tau}{2\pi c}$, and $\Gamma = \frac{2\pi c}{\lambda_\tau}$ into Equation (7), it is simplified as a function of wavelength.

$$\varepsilon''(\omega) = \frac{\lambda^3}{\lambda_\tau {\gamma_p}^2}. \tag{8}$$

The dielectric function of metal as a function of refractive index is as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = (n + ik)^2 = n^2 - k^2 + i2nk. \tag{9}$$

The real part of the dielectric function of Equation (9) is written as follows:

$$\varepsilon' = n^2 - k^2. \tag{10}$$

And also, the imaginary part of the dielectric function in Equation (9) is written as follows:

$$\varepsilon'' = 2nk, \tag{11}$$

where n is the real part of the refractive index and k is the imaginary part of the refractive index.

2.2. Mathematical Formulation of Size-Dependent Dielectric Function Nanoscale Using Drude–Sommerfeld Model. The total dielectric function of bulk metal is the sum of the dielectric function contribution of free electrons and the dielectric function contribution of band electrons [114–118].

$$\varepsilon(\omega) = \varepsilon_{\text{freeelectron}}(\omega) + \varepsilon_{\text{boundelectron}}(\omega). \tag{12}$$

The total dielectric function of bulk metal as a function of angular frequency is also expressed as follows:

$$\varepsilon(\omega) = \varepsilon(\infty) - \frac{\omega_p^2}{{\omega_0}^2 + \omega^2 + i\omega\gamma}. \tag{13}$$

$\varepsilon(\infty)$ is a high optical dielectric constant; its value for free electron gas is 1, for metal is from 1 to 10 [113], and Au is 1.53 [119, 120]. The total dielectric function of free electrons as a function of angular frequency is written as for free electron gas [92, 113], where γ_{free} is the damping constant of the oscillators of free electrons and $\omega_0 \approx 0$.

$$\varepsilon_{\text{freeelectron}}(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma_{\text{free}}}. \tag{14}$$

The real part of the dielectric function of a free electron contribution as a function of angular frequency in gas Equation (14) is given by the following:

$$\varepsilon'_{\text{freeelectron}}(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + {\gamma^2}_{\text{free}}}. \tag{15}$$

The optical dielectric constant of gold is equal to 1.35, and then the real part of the dielectric function of the free electron of gold metal as a function of angular frequency is given by the following:

$$\varepsilon'_{\text{freeelectron}}(\omega) = 1.53 - \frac{\omega_p^2}{\omega^2 + {\gamma^2}_{\text{free}}}. \tag{16}$$

The real part of the dielectric function of gold nanoparticles in Equation (14) as a function of wavelength can be expressed as follows:

$$\varepsilon'_{\text{freeelectron}}(\lambda) = 1.53 - \frac{4\pi c^2\lambda^2}{4\pi c^2\lambda^2 + {\gamma^2}_{\text{free}}\lambda^2{\lambda^2}_p}. \tag{17}$$

The imaginary part of the dielectric function of the free electron of gas as a function of the angular frequency of Equation (14) is given by the following:

$$\varepsilon''_{\text{freeelectron}}(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega^2 + {\gamma^2}_{\text{free}})}. \tag{18}$$

The imaginary part of the dielectric function of the free electron of Au as a function of the angular frequency of Equation (14) is given by the following:

$$\varepsilon''_{\text{freeelectron}}(\omega) = 1.53 - \frac{\omega_p^2}{\omega(\omega^2 + {\gamma^2}_{\text{free}})}. \tag{19}$$

The imaginary part of the dielectric function of gold nanomaterials in Equation (19) as a function of wavelength can be simplified and expressed as follows:

$$\varepsilon''_{\text{freeelectron}}(\lambda) = 1.53 - \frac{2\pi c\lambda^3}{4\pi^2\lambda_p c^2 + \lambda_p\lambda^2\gamma^2{}_{\text{free}}}. \tag{20}$$

The bound contribution of the total dielectric function of bulk materials is given [110, 117].

$$\varepsilon_{\text{boundelectron}}(\omega) = \varepsilon(\omega) - \varepsilon_{\text{freeelectron}}(\omega), \tag{21}$$

where $\varepsilon(\omega)$ is the experimental value of metals of Johnson and Christy [121], which is equal to 1.53 [119]. On the nanoscale of metal, the dielectric function of metals or particles is expressed as a function of radius [32].

$$\varepsilon(\omega, R) = \varepsilon_{\text{freeelectron}}(\omega) + \varepsilon_{\text{boundelectron}}(\omega). \tag{22}$$

The dumping constant of free electrons in a bulk metal is inversely proportional to the sum of the average time between electron–electron scattering, imperfections, and electron–phonon scattering.

$$\gamma_{\text{free}}{}^{\text{bulk}} = \frac{1}{\tau} = \frac{1}{\tau_{el-el}} + \frac{1}{\tau_{im}} + \frac{1}{\tau_{el-ph}}. \tag{23}$$

However, the dumping constant of free electrons in size-dependent materials or nanomaterials is the sum of the dumping constant of free electrons in the bulk metal and is inversely proportional to the average time between collisions of the free electrons with the boundary of particles. It can be expressed as follows:

$$\gamma^{\text{size}}{}_{\text{free}} = \gamma^{\text{bulk}}{}_{\text{free}} + \frac{CV_f}{r}, \tag{24}$$

where r is the radius of nanoparticles v_f is the velocity of free electrons at the fermi level, and C is the free electron scattering constant at the boundary.

The real part of the size-dependent dielectric function of gold nanomaterials as a function of the angular frequency of Equation (22) given by Graily-Moradi et al. [54].

$$\begin{aligned}\varepsilon'_{\text{freeelectron}}(\omega, R) &= 1.53 - \frac{\omega_p^2}{\omega^2 + (\gamma^{\text{size}}{}_{\text{free}})^2} \\ &= 1.53 - \frac{\omega_p^2}{\omega^2 + \left(\gamma^{\text{bulk}}{}_{\text{free}} + C\frac{V_f}{r}\right)^2}.\end{aligned} \tag{25}$$

The imaginary part of the size-dependent dielectric function of a gold nanomaterial as a function of angular frequency in Equation (22) is expressed as follows:

$$\begin{aligned}\varepsilon''_{\text{freeelectron}}(\omega, R) &= \frac{\omega_p^2\gamma^{\text{size}}{}_{\text{free}}}{\omega(\omega^2 + (\gamma^{\text{size}}{}_{\text{free}})^2)} \\ &= \frac{\omega_p^2\left(\gamma^{\text{bulk}}{}_{\text{free}} + C\frac{V_f}{r}\right)}{\omega\left(\omega^2 + \left(\gamma^{\text{bulk}}{}_{\text{free}} + C\frac{V_f}{r}\right)^2\right)}.\end{aligned} \tag{26}$$

The size-dependent total dielectric function of gold nanoparticles as a function of angular frequency and size of nanoparticles is the summation of the dielectric function due to free electrons and bound electrons, which is given as [110, 118].

$$\varepsilon(\omega, R) = \varepsilon_{\text{freeelectron}}(\omega, R) + \varepsilon_{\text{boundelectron}}(\omega). \tag{27}$$

The dielectric function of gold nanoparticles due to their bound electron contribution is also expressed as follows:

$$\varepsilon^L(\omega) = 1.53 + \frac{\omega_p'^2}{(\omega_0^2 - \omega^2) - i\gamma_{\text{bound}}}. \tag{28}$$

where γ_{bound} is the damping constant of the bond electron, ω_p' is analogy the plasma frequency under the applied electric field and ω_0 the resonance frequency of bound electron.

The real part of the bound electron dielectric function of gold as a function of angular frequency is given in [108].

$$\varepsilon'^L_{\text{bound}}(\omega) = 1.53 + \frac{\omega_p'^2(\omega_0^2 - \omega^2)}{\omega^2\gamma^2_{\text{bound}} + (\omega_0^2 - \omega^2)^2}. \tag{29}$$

The real part of the dielectric function of gold nanoparticles as a function of wavelength Equation (29) can be expressed in terms of wavelength.

$$\begin{aligned}&\varepsilon'^L{}_{\text{bound}}(\lambda) \\ &= 1.53 + \frac{2\pi c{\lambda_o}^2\lambda^3(\lambda - {\lambda_o}^2)}{\left(\lambda_p\lambda^4 + \lambda_p{\lambda^4}_0 - 2\lambda_p{\lambda_o}^2{\lambda_p}^2\right)\left(\lambda^2\gamma^2{}_{\text{bound}} + 4\pi^2c^2\right)}.\end{aligned} \tag{30}$$

The imaginary part of the bound electron dielectric function of gold particles as a function of angular frequency is given.

$$\varepsilon''^L{}_{\text{bound}}(\omega) = \frac{\omega_p'^2\omega\gamma_{\text{bound}}}{\omega^2\gamma^2_{\text{bound}} + (\omega_0^2 - \omega^2)^2}. \tag{31}$$

The imaginary part of the dielectric function of gold nanoparticles as a function of wavelength Equation (30) can be expressed in terms of wavelength as follows:

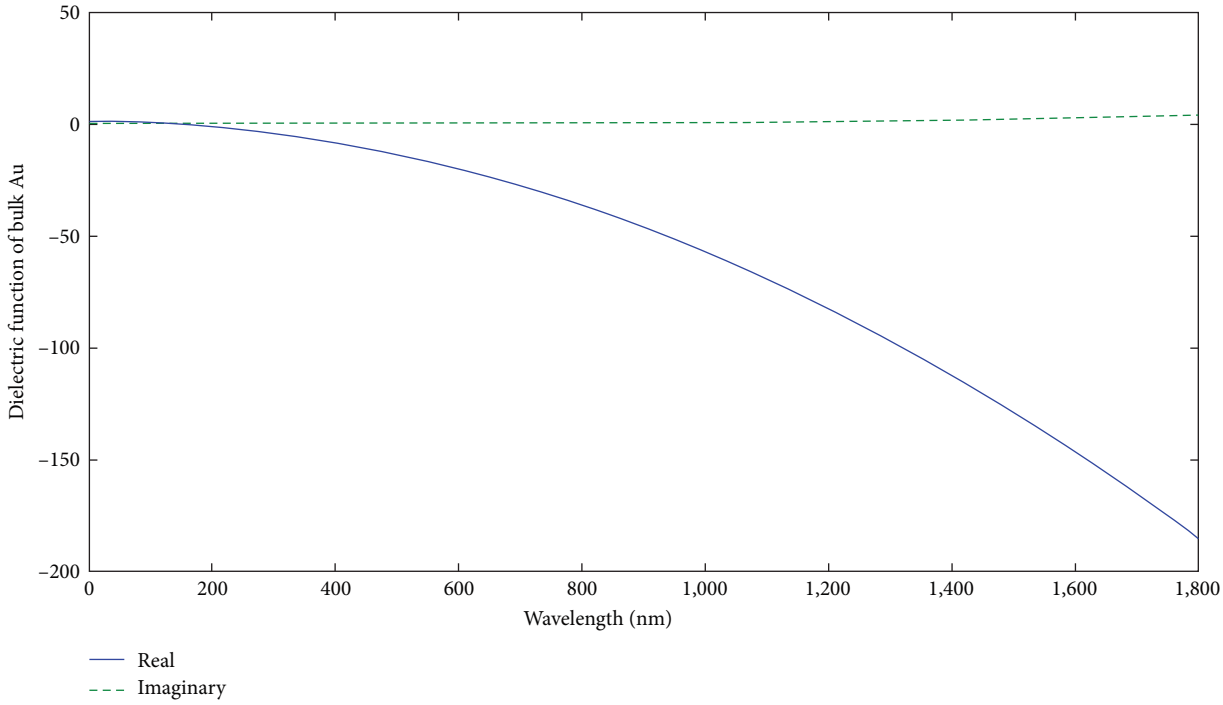

FIGURE 1: Dielectric function of bulk gold materials versus wavelength of free electron contribution.

$$\varepsilon''^{L}{}_{\text{bound}}(\lambda) = \frac{\lambda^3 \lambda^4{}_0 \gamma_{\text{bound}}}{\lambda_p \lambda^4{}_o \lambda^2 \gamma^2{}_{\text{bound}} + 4\pi^2 c^2 \lambda_p (\lambda^4 + \lambda_0{}^2 - 2\lambda_0 \lambda^2)}. \tag{32}$$

The dielectric function of gold nanoparticles as a function of wavelength and radius is the sum of the total dielectric function of free electron contribution and the dielectric function of bound electron contribution. It can be expressed as a function of wavelength mathematically as follows:

$$\varepsilon(\lambda, R) = \varepsilon'_{\text{freeelectron}}(\omega, R) + \varepsilon''_{\text{freeelectron}}(\omega, R) + \varepsilon'^{L}{}_{\text{bound}}(\lambda) + \varepsilon''^{L}{}_{\text{bound}}(\lambda). \tag{33}$$

Substituting Equations (25), (26), (30), and (32) into Equation (33) and simplifying, we get the following:

$$\varepsilon(\lambda, R) = 4.59 - \frac{2\pi c \lambda^3}{4\pi^2 \lambda_p c^2 + \lambda_p \lambda^2 \gamma^2{}_{\text{free}}} - \frac{2\pi c \lambda^3}{4\pi^2 \lambda_p c^2 + \lambda_p \lambda^2 \gamma^2{}_{\text{free}}} + \frac{2\pi c \lambda_o{}^2 \lambda^3 (\lambda - \lambda_o{}^2)}{\left(\lambda_p \lambda^4 + \lambda_p \lambda^4{}_0 - 2\lambda_p \lambda_o{}^2 \lambda_p{}^2\right)\left(\lambda^2 \gamma^2{}_{\text{bound}} + 4\pi^2 c^2\right)} + \frac{\lambda^3 \lambda^4{}_0 \gamma_{\text{bound}}}{\lambda_p \lambda^4{}_o \lambda^2 \gamma^2{}_{\text{bound}} + 4\pi^2 c^2 \lambda_p (\lambda^4 + \lambda_0{}^2 - 2\lambda_0 \lambda^2)}. \tag{34}$$

3. Result and Discussion

In the previous section, we calculated the real and imaginary parts of the dielectric function of bulk gold materials due to free electron contraption and the real and imaginary parts of the dielectric function of nanoscale gold materials due to free electron and bond electron contraption. In this section, we plot the real and bulk dielectric functions of bulk Au materials versus wavelength, the real and imaginary parts of the Au nanoscale and bulk dielectric functions of free electrons versus wavelength, the real part of the Au nanoscale and bulk dielectric function versus wavelength, and the imaginary part of the Au nanoscale and bulk dielectric function versus wavelength. The real and imaginary parts of the dielectric function of nanogold materials of bound electron contraption versus wavelength are plotted. Those graphs are plotted in MATLAB code using experimental values of dielectric function parameters, and these dielectric function gold parameters are listed below. $C = 0.8$, $v_f = 14.1 \times 10^{14}$ nm/s, $\omega_p = 13 \times 10^{15}$Hz, $\gamma_{\text{bulk}} = 1.1 \times 10^{14}$Hz, $K_{\text{bulk}} = 2.3 \times 10^{24}$, $\gamma_{\text{bound}} = 2.4 \times 10^{14}$Hz, $E_g = 2.1$ eV, $E_F = 2.5$ eV, $\omega_0 = 4.19 \times 10^{15}$Hz, $\omega' = 4.48 \times 10^{15}$Hz, $\varepsilon(\infty) = 1.53$, $\gamma_p = 17,000$ nm, $\lambda_p = 145$ nm, $\lambda_p = 8.4 \times 10^4$ nm [108, 114–116, 118–120].

The real and imaginary dielectric functions of bulk gold materials are plotted in Figure 1. As can be seen from this figure, the value of the imaginary dielectric function of bulk gold materials is near to independent of wavelength; its value is close to constant but not constant. This graph indicates that when the wavelength increases, the imaginary dielectric function increases very slowly. The imaginary part of the

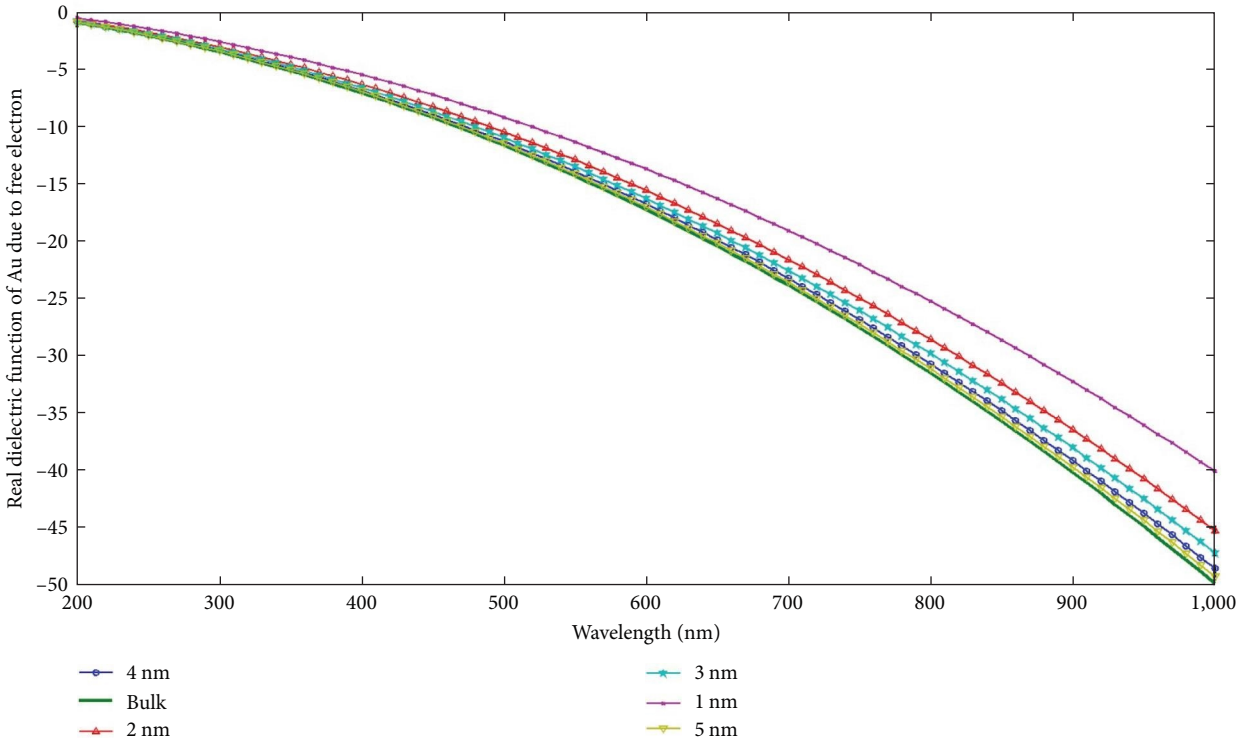

Figure 2: The real dielectric function of bulk and nanogold materials versus wavelength-free electron contribution.

dielectric function for bulk gold materials is indeed approximately constant across a wide range of wavelengths. This behavior is particularly prominent in the visible and near-infrared regions. Indeed, the imaginary part of the dielectric function for bulk gold (Au) is often assumed to be zero in many theoretical and practical contexts because gold behaves as a nonabsorbing material in visible light and near-infrared. This shows that in the visible light and near-infrared ranges, bulk gold particles do not significantly absorb light within this frequency range. Consequently, the imaginary part of the dielectric function is negligible. In addition to this, free electrons in gold metal collisions are relatively infrequent, especially in the optical range. In this case, the imaginary dielectric function of gold remains close to zero. However, at high frequencies in ultraviolet and beyond, gold does exhibit some absorption due to interband transitions. In these cases, the imaginary dielectric function becomes nonzero.

The curve of the imaginary part of the dielectric function versus wavelength of this study is exactly fitted to the theoretical and experimental studies [122, 123]. The value of the real dielectric function of bulk gold depends on wavelength; if the wavelength increases, the real dielectric function of bulk gold decreases rapidly, which means its value is exponentially inversely proportional to the wavelength of electromagnetic radiation. However, both the real and imaginary dielectric functions of bulk gold are independent of the size of gold materials.

This dielectric function of bulk gold materials versus the wavelength of the free electron contribution curve is fitted to the theoretical and experimental [88, 122, 123]. The real dielectric function of bulk and nanogold materials due to the free electron contribution graph is plotted in Figure 2. This figure shows that the real dielectric functions of bulk and nanoscale gold materials depend on the wavelength. As we observed in the graph, the real dielectric function of both bulk and nanogold materials is inversely proportional to wavelength. The real part of the dielectric function of bulk and nanogold is primarily responsible for surface plasmon resonance behavior. When light interacts with gold surfaces, it excites collective electron oscillations (plasmons). These plasmons resonate at specific wavelengths, leading to enhanced scattering. The frequency of the particle increases, and the scattering on the surface of materials also increases. It indicates that the real dielectric function of bulk and nanoparticles is directly proportional to frequency. When the wavelength of bulk and nanogold metals increases, the real dielectric function of bulk gold rapidly decreases. However, the real dielectric function of a gold nanomaterial also depends on its size. As the size of the gold nanomaterial decreases, the value of its dielectric function increases with a constant wavelength. For example, as shown in Figure 2, if the wavelength of electromagnetic radiation is 1,000 nm, the value of the real dielectric function of bulk gold material is −50, but the value of the real dielectric function of gold nonmaterial varies based on its size. At a wavelength of 1,000 nm, the real dielectric function of gold nanomaterials is −49.65 at a 5 nm radius, −48.76 at a 4 nm radius, −46.3 at a 3 nm radius, −45.59 at a 2 nm radius, and −40.04 at a 1 nm radius. But at the 200 nm wavelength, at all radii, including bulk, they have an approximately equal value near −2.03.

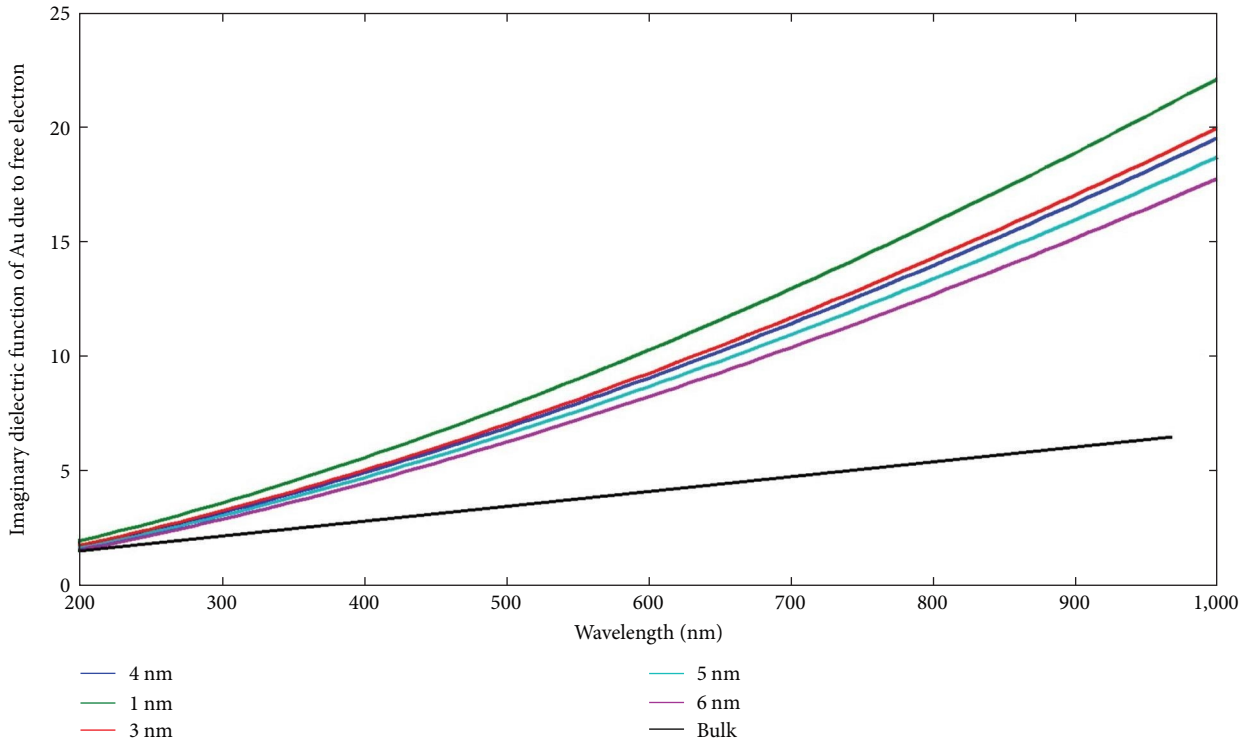

Figure 3: Imaginary dielectric function of bulk and nanogold materials versus wavelength-free electron contribution.

The curve of the real dielectric function of bulk and nanogold materials versus wavelength-free electron contribution is fitted to the theoretical and experimental studies [108, 122, 123].

The imaginary dielectric functions of bulk and nanogold materials due to the free electron contribution graph are plotted in Figure 3.

Figure 2 shows that the imaginer dielectric functions of nanoscale gold materials depend on the wavelength of electromagnetic radiation. As we observed in the graph, the imaginary dielectric function of nanogold materials is exponentially proportional to wavelength. The imaginary dielectric function of a gold nanomaterial depends on its size. As the size of the nanomaterial gold increases, the value of its dielectric function decreases. As Figure 3 shows, at a wavelength of 1,000 nm, the imaginary dielectric function of gold nanomaterials is 17.67 at a 5 nm radius, 18.34 at a 4 nm radius, 19.06 at a 3 nm radius, 19.97 at a 2 nm radius, and 22.36 at a 1 nm radius. But at the 200 nm wavelength, at all radii, the value of the imaginary dielectric function is approximately equal to or near 2.57. However, the value of the imaginary dielectric function of bulk gold is independent of size and wavelength; its value is approximated at 2.57. The imaginary part of the dielectric function of nano and bulk gold particles in this study graph is fit to the theoretical and experimental studies graphs [108, 122, 123].

The dielectric functions of gold nanomaterials depend on their size and wavelength. The surface-to-volume ratio of nanogold particles is greater than that of bulk gold particles; when the size of nanoparticles decreases, the surface-to-volume ratio increases. The surface-to-volume ratio significantly influences the dielectric function of nanomaterials due to enhanced surface effects, quantum size effects, surface plasmons, size-dependent resonance peaks, interband transitions, wavelength dependence, and local field enhancement of nanogold particles. Therefore, the real and imaginary parts of the dielectric function of gold nanoparticles depend on their size and the incident wavelength. These properties are shown in Figures 2–5. We have explained in detail about the dielectric functions of gold nanomaterials depend on their size and wavelength as below. The light interaction on the nanoparticles is greater than that on the bulk materials when the skin depth is greater than the size of the nanoparticles. It suggests an increase in surface scattering. Effects of quantum size: The dielectric function of the nanoparticles greatly affects the size and form of the particle when the wavelength of light is larger than the particle's size. When gold nanoparticles are smaller than the Bohr radius, the energy level becomes distinct, and all electrons are contained. This is how the quantum confinement effect manifests itself.

Because of their confinement within nanoparticles, electrons exhibit quantized behavior at the nanoscale. The quantity of electrons accessible for collective oscillations (like plasmons) varies as the size of the gold nanoparticle reduces. The real and imaginary components of the dielectric function are also strongly impacted by these quantum-scale effects. Surface plasmons: Surface plasmons are a collective oscillation of free electrons that are seen in gold nanoparticles. The size, shape, and surroundings of the nanoparticle all affect surface plasmon sensitivity. Surface plasmon phase velocity is influenced by the refractive index, which is directly connected to the real part of the dielectric function. The

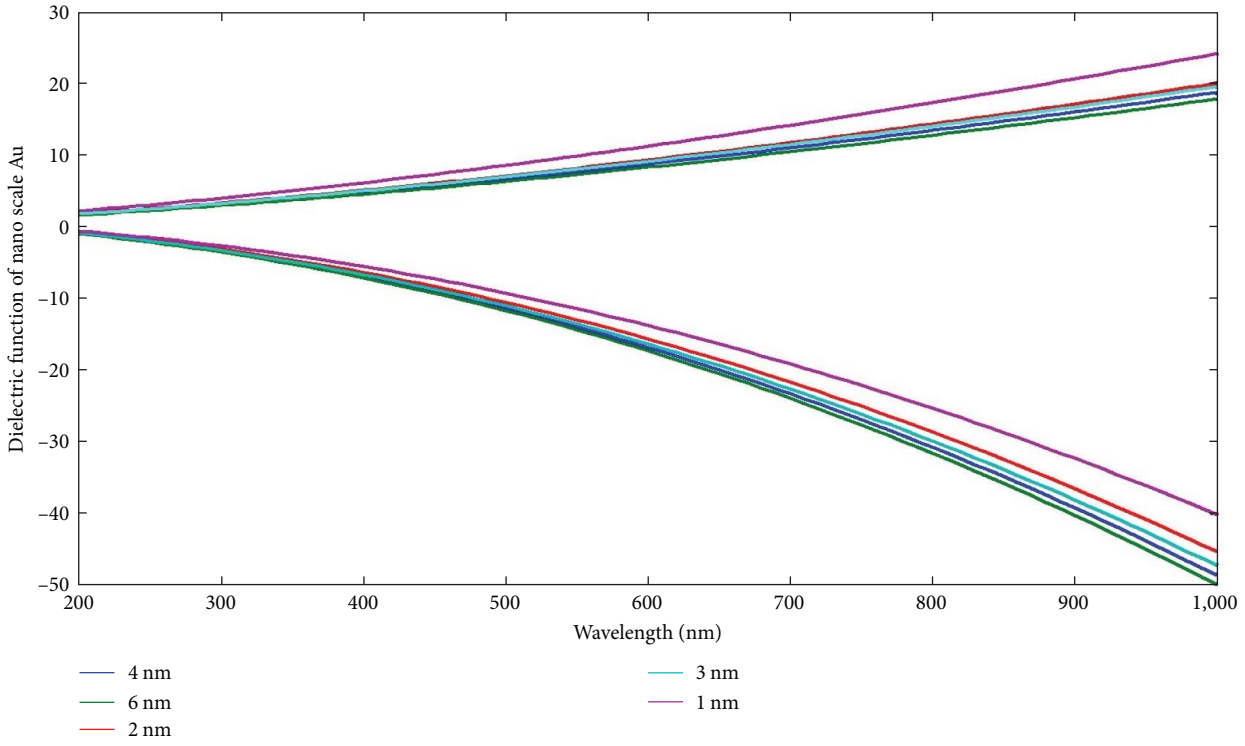

Figure 4: Imaginary and real dielectric functions of nanogold materials versus wavelength-free electron contribution.

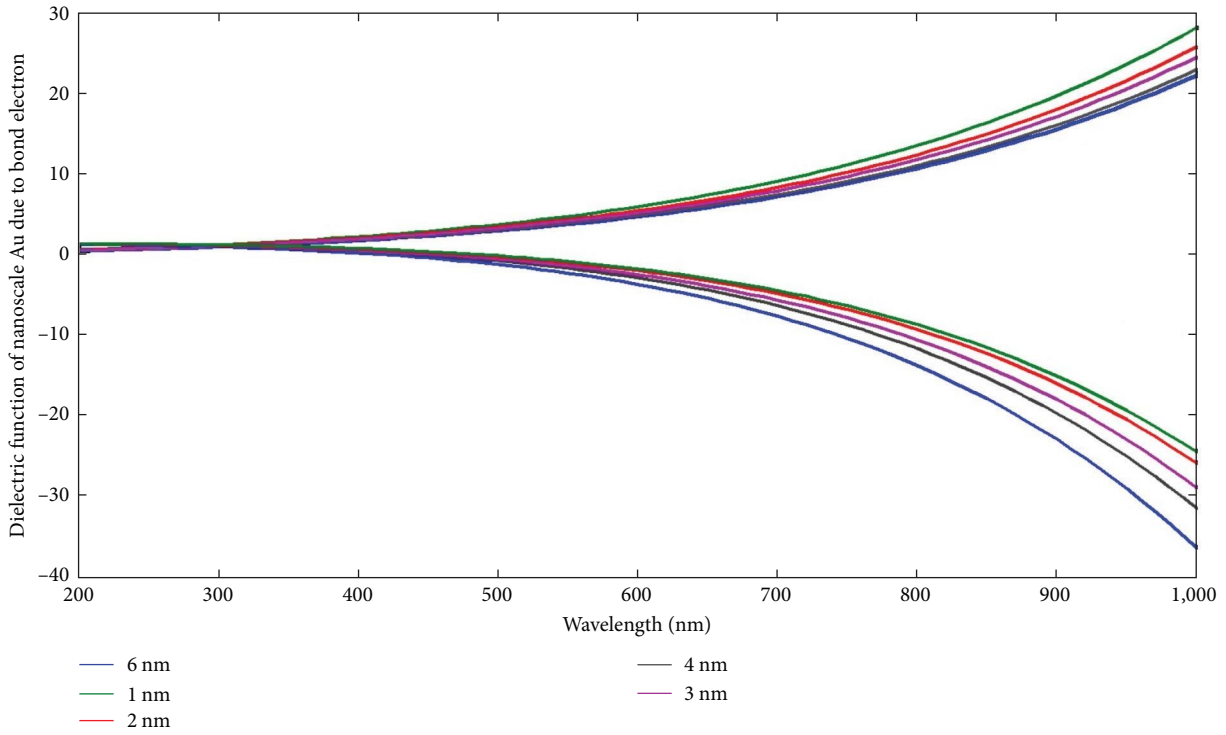

Figure 5: Imaginary and real dielectric functions of nanogold materials versus wavelength bond electron contribution.

imaginary part is equivalent to the energy absorbed during plasmon resonance. Dependence on wavelength: The dielectric function changes depending on the incident light's wavelength. Strong absorption happens when the wavelength coincides with the surface plasmon resonance condition. The imaginary part of the dielectric function reflects this absorption. Size-dependent optical features result from the diverse ways that different wavelengths interact with the nanoparticle. Size-dependent resonance peaks: The resonance peaks in the absorption spectra shift in response to variations in nanoparticle size. The real and imaginary components of the dielectric function are intimately correlated with these shifts. Interband shifts: Interband transitions, or electron transitions between energy bands, happen in bulk gold at particular energies. Quantum confinement causes these transitions to alter at the nanoscale. These electronic changes have an impact on the dielectric function's real part. Local field enhancement: When a gold nanoparticle is present, the surrounding local electric field is strengthened. The dielectric response of molecules or other nanoparticles in the vicinity is impacted by this field augmentation. In this augmented field region, the dielectric function's real and imaginary components change.

The imaginary and real dielectric functions of nanogold materials' free electron contribution graphs are plotted in Figure 4.

As we observed from Figures 2–4, both the imaginary and real dielectric functions of gold nanomaterial depend on its size and wavelength. As Figure 4 illustrates, as the wavelength increases from 200 to 1,000 nm, the real part of the dielectric function of the gold nanomaterial exponentially decreases, but simultaneously, the imaginary part of the dielectric function exponentially increases. If the size of the nanomaterial decreases, the real and imaginary dielectric functions of the gold nonmaterial increase due to the free electrons contribution. This curve of imaginary and real dielectric functions of nanogold materials versus wavelength-free electron contribution is fitted in [108, 116, 122, 123] studies.

The imaginary and real dielectric functions of nanogold materials due to the bound electron contribution graph are plotted in Figure 5. Figure 5 indicates that the real and imaginary parts of the dielectric functions of gold nanomaterials depend on both size and wavelength. The real dielectric function of gold nanomaterials from 200 up to 386 nm decreases slowly, nearing constant, but the wavelength from 386 to 1,000 nm is exponentially decreasing. The imaginary dielectric function of gold nanomaterials from 200 up to 386 nm increases slowly, near to constant, but the wavelength from 386 to 1,000 nm is exponentially increasing. The size of the gold nanomaterial is highly influenced by both real and imaginary dielectric functions at high wavelengths. The effect of size on dielectric function decreases as the wavelength increases. The graph of imaginary and real dielectric functions of nanogold materials versus wavelength-bound electron contribution is exactly fitted in the study [108].

4. Conclusion

The real and imaginary parts of the dielectric function of gold nanomaterials depend on the size of the materials, temperature, frequency, and wavelength. The nonmaterial size is highly influenced by dielectric functions such as the nonlocal response effect, the surface scattering effect, and the quantum confinement effect. When the size of nanomaterials is less than the Bohr radius, their energy levels change to discrete. This process is highly influenced by the optical properties of nanomaterials, such as emission and absorption spectra. When the skin depth is greater than the size of the nanomaterials in gold, the interaction of electromagnetic waves with the surface of the nanomaterials is greater than the bulk of the materials. The size effect on dielectric function is increased at a wavelength greater than 386 nm due to bond electron contribution, but in free electron contribution, its effect appears at a wavelength of 200 nm. Gold nanomaterials are used in many fields of application, such as medicine, electronics, green technology, nanotechnology, and agriculture.

Data Availability

The data underlying the results presented in the study are available in the manuscript.

Conflicts of Interest

Regarding the publishing of this paper, the authors state that they have no conflicts of interest.

Authors' Contributions

Bawoke Mekuye has written the manuscript, and Rainer Höfer and Gedefaw Mebratie have edited the manuscript.

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