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Tuning plasmon frequency by the external electric field and its applications

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ABSTRACT

In this paper, plasmon frequency manipulation using an external electric field was investigated. Using an external electric field with the right intensity can change the density of charge carriers in materials such as metals and semiconductors. This phenomenon can be used to design a tunable multi-range radiation detector. The density distribution formula of electric charge carriers is proposed as a function of the external electric field, dimension, initial density, and temperature. The validity of this formula was tested by comparing it with the Maxwell distribution function. The use of the formula on the formation of a hot point on the gp120-CD4 connection of HIV-1 and host cells was considered as a practical example. Finally, the effects of Johnson thermal noise and shot Coulomb noise are calculated to accurately determine the external electric field required.

1. Introduction

Coherent mass oscillation of electron density in materials is known as plasmon [1-3]. Drude and Lorentz proposed the classical model for such oscillations in metals [4], which proves that conductive materials absorb incident electromagnetic radiation at the plasmon frequency, while frequencies lower than the plasmon frequency can penetrate materials. On the other hand, light with a frequency higher than the plasmon frequency cannot be transmitted and the material is blurred for radiant radiation in this case. Even for metal nanostructures, this model can be used without considering quantum mechanical methods, because high-density free electrons have energy levels comparable to K_BT thermal excitation energy at room temperature [5]. The optical response strongly depends on the considered plasmon frequency of the material [6, 7]. In micro and nanoscale systems, the phenomenon of "surface plasmon resonance" (SPR) is predominant. SPR refers to the collective oscillations of electrons in the metal and at the interface between metal and dielectric. These collective surface waves propagate due to the confinement of light in small structures and have tremendous potential in many applications [8, 9].

Controlling the absorption frequency by the size, shape, and composition of nanoparticles is one of the interesting fields that has been studied by scientists in recent years. As a result of these studies, IR and NIR frequency detectors have been manufactured [10-13]. This technique can be applied to many devices. Some important applications include plasmonic waveguides, solar cells, photovoltaic devices, nanoantennas, switching devices between electronics and photons, increasing the efficiency of solar cells, and photothermal therapy [14-19]. In photothermal therapy, nanoparticles absorb the incident light, which raises the local temperature of the cells, resulting in cancer cells, viruses, and DNA, or any other target will be damaged without affecting the surrounding healthy cells [20-24]. All of these applications are based on the effective absorption of plasmon light. Plasmon particles as nanoparticles play an important role in detecting electromagnetic waves [25, 26]. These nanoantennas can be used as detectors and biosensors by detecting Near field rot [19, 27]. moreover, the control of the spectral range that can be absorbed by such a device provides terahertz detectors. [28, 29]. These methods are related to the size, shape, and type of nanoparticles considered.

This paper presents a method for controlling the absorption frequency of plasmon by applying an external electric field to a specific material. The magnitude of the applied electric field is then used to manipulate the density distribution of conducting electrons and their plasmon absorption frequency in the sample. The results of this model are used to paralyze the HIV-1 virus and are confirmed by other scientific results. [30].

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2. Model and calculations

To introduce a tunable detector, a rod with uniform electron density distribution is considered (Fig. 1a). After applying an external electric field, a gradient of electron density distribution is created in the rod. The low-density electron side produces a low plasmon frequency in the IR range, and the other side produces a high plasmon frequency that absorbs UV radiation. By connecting the two sides of the rod and using an ammeter, the absorbed radiation can be detected on each side (Fig. 1b).

To calculate localized surface plasmon frequency, the following distribution function is suggested:

$$\frac{n-n_0}{n_0} = \alpha E e^{-\beta E x^2} \tag{1}$$

Parameters n, n_0, E, α, and β are the final electron density, initial electron density, magnitude of the external electric field, and two constants that should be determined later, respectively. In Eq.1, the linear part is due to Coulomb's law applied to the electron density, while the exponential part is held for electron mutual repulsion. When the external electric field is activated, the electrons move toward the positive electrode and partially accumulate at the end of the rod, the length of the side where the electrons are accumulated is suggested to be equal to δ. This accumulation creates an induced electric field in the opposite direction of the applied electric field leading to an electron density saturation, so an exponential function of the electric field is considered. To determine α and β, an analytical dimension is employed. Since the $(n\text{-}n_0)/n_0$ is non-dimensional, hence αE should be non-dimensional

$$[\alpha] = \frac{1}{[E]} \tag{2}$$

Knowing that the electric field in the rod is related to the electric current density (J) and the conductance of the rod σ according to the relation $E = \frac{J}{\sigma}$. On the other hand, $J = \frac{I}{S}$ where S is the cross section of the rod and the electric current $I = nevS = \frac{e}{SL} vS$, with L length of the rod, e the elementary charge, and v the velocity. As a result, one can obtain the following formula

$$E = \frac{ev}{\sigma SL} \tag{3}$$

By substituting $\sigma = \frac{n_0 e^2 \tau}{m}$ in Eq. 3, the equation becomes

$$E = \frac{mv}{n_0 e \tau SL} \tag{4}$$

Due to this relationship, the Coulomb repulsion force among electrons becomes significant with increasing temperature because the microscopic velocity is directly related to temperature. As a result, more external electric fields must be applied. It is known that at the microscopic level, the average kinetic energy is related to temperature as follows, assuming that the motion of the electrons is one-dimensional:

$$\frac{1}{2} m v^2 = \frac{1}{2} k_B T \tag{5}$$

Where k_B represents the Boltzmann constant, by substituting in Eq.4 the relation becomes

$$E = \frac{k_B T}{n_0 e S L^2} \tag{6}$$

consequently, according to Eq. 2, the expression of α should be as following

$$\alpha = \frac{n_0 e S L^2}{k_B T} \tag{7}$$

and that of β is

$$\beta = \frac{\alpha}{L^2} = \frac{n_0 e S}{k_B T} \tag{8}$$

By substituting α and β in Eq. 1, and by taking into consideration that electric field $E = \frac{V}{L}$, the expression of the electron density becomes

$$n = n_0 \left(1 + \frac{n_0 e S}{k_B T} L V e^{-\frac{n_0 e S}{k_B T} \frac{V}{L} x^2}\right) \tag{9}$$

From this equation, it can be seen that with increasing temperature, a significant resistance against the accumulation of electrons is created, so to overcome this resistance, the applied voltage must be increased. For this purpose, the relationship between the accumulation length and the external electric field must be calculated.

By calculating the full width at half maximum (FWHM) and substituting the accumulation length (δ), the following equation is obtained

$$\delta = \frac{\Delta x}{2} = \left(\frac{k_B}{n_0 e S \mathrm{v}}\right)^{1/2} \tag{10}$$

the accumulation volume is given by $\mathrm{V} = \delta S$

$$V = \frac{k_B T}{n_0 e \mathrm{v}} \frac{L}{\delta} \tag{11}$$

For N particle:

$$V = \frac{N k_B T}{n_0 e \mathrm{v}} \frac{L}{\delta} = \frac{k_B T}{e} \frac{L}{\delta} \frac{n_e}{n_0} \tag{12}$$

where n_e represents the density of electrons in the accumulation section of the rod. Finally, the required electric field is given by

$$E = \frac{k_B T}{e \delta} \frac{n_e}{n_0} \tag{13}$$

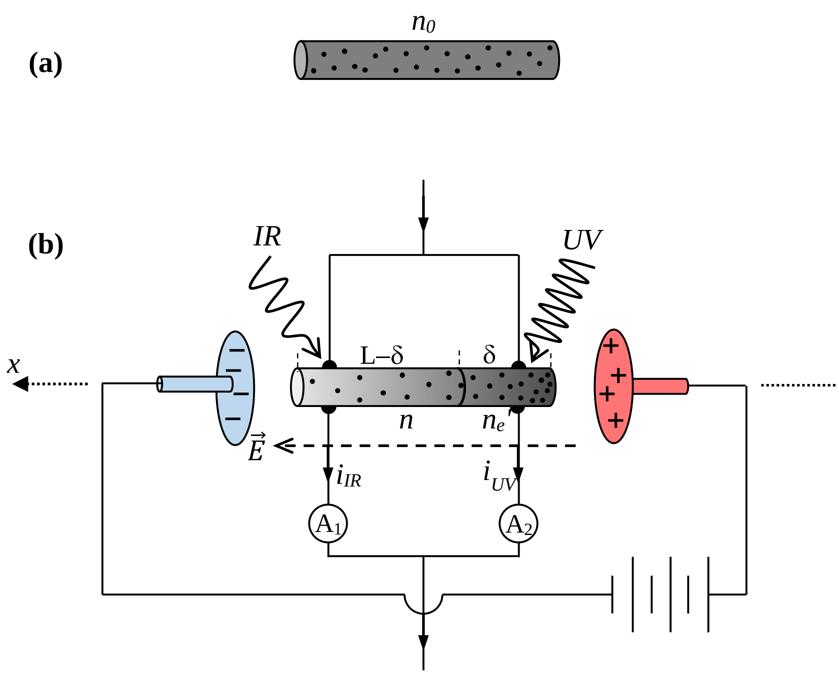

Fig.1. The effect of the electric field on the plasmon frequency. (a) Without an external electric field, the distribution of electron density is uniform in the rod. (b) Changing of electron density distribution under the effect of electric field. The color gradient and the dots in the rod show the electron density distribution.

3. Tuned plasmon application

Eq. 13 can be used for many applications, one of which is HIV-1 paralysis. Due to the number of free electrons under the applied voltage V, the distribution of free electrons was the same before the voltage was applied. After applying the potential difference with the mean of the negative and positive electrodes, kinetic energy is induced in the free electrons. As a result, these electrons accumulate in a small area near the positive electrode. The following equation can describe this phenomenon [31]:

$$eV = K_B T \, \frac{n_e}{n_0} \tag{14}$$

Furthermore, by considering the relation $E = -\nabla V$, the following statement is obtained

$$E = -\frac{K_B T}{n_0 e} \nabla n_e \tag{15}$$

and by integrating over the length where the electrons are accumulated, the density of electrons in the accumulation section can be calculated:

$$n_e = -\int_L^{L-\delta} \frac{n_0 E e}{K_B T} dl = n_0 e \delta \tag{16}$$

By substituting the obtained density function that it is tuned by controlling the external electric field in the equation of charge conservation, the free electron density of diluted area can be obtained:

$$N' + N = N_0 \quad \rightarrow \quad \frac{n'\delta + n(L-\delta)}{L} = n_0 \tag{17}$$

Where N_0, N, and N' are the number of free electrons on the entire surface, diluted section, and accumulation section, respectively respectively. Related plasmon frequencies are derived as below

$$\omega_p = \left(\frac{ne^2}{\varepsilon_0 m}\right)^{\frac{1}{2}} = \left[\frac{n_0 e^2}{\varepsilon_0 m}\left(1 + \frac{n_0 eSLV}{K_B T} e^{-\frac{n_0 eSV}{K_B TL}x^2}\right)\right]^{\frac{1}{2}} \tag{18}$$

$$\omega'_p = \left(\frac{n'e^2}{\varepsilon_0 m}\right)^{\frac{1}{2}} = \left[\frac{n_0 e^2}{\varepsilon_0 m}\left(1 - \frac{\delta}{L-\delta}\frac{n_0 eSLV}{K_B T} e^{-\frac{n_0 eSV}{K_B TL}x^2}\right)\right]^{\frac{1}{2}} \tag{19}$$

where n and n' are the electron density of the accumulation section of length δ and the electron density of the diluted section of length L-δ, respectively.

The effect of the external electric field, the size, and the cross-section shape of the rod can be analyzed in this equation for special objects including in vivo targets and viruses.

4. Human immune deficiency virus

HIV-1 is a group of RNA viruses that insert a copy of their genome into a host cell to replicate themselves. This type of virus is called a retrovirus [30, 31]. The virus contains glycoproteins (gpl20) that allow HIV to attack receptor cells (CD4) [32]. At the end of 2015, 36.7 million people worldwide were living with HIV [33, 34].

The fusion mechanism involves the binding of CD4 protein to gpl20. When gpl20 is bound to CD4, RNA is injected into the host cell, which causes a structural change. This change exposes the binding domains of gp41 chemokines and allows them to interact with the target chemokine receptor. As a result, a more stable two-pronged attachment can be achieved, which allows the N-terminal gp41 fusion peptide to penetrate the cell membrane, as shown in Fig. 2 [35, 36].

In any structure, there are free electrons that can oscillate coherently at their resonant plasmon frequency. This phenomenon applies to a protein whose corresponding plasmon frequency has been calculated in this paper. The plasmon frequency equation can be used for HIV-1 containing gp120 as mentioned earlier. The Gp120 can be considered rod-shaped due to its curved shape. Plasmon frequency can be adjusted by carrier density. When a protein absorbs a photon at a frequency equal to its plasmon frequency, it melts and its function is lost.

If this mechanism is applied on gp120, it will be disconnected from the receptor (CCR5), as a result, the progress of the disease will be blocked before being spread.

By referring to Eq. 18 and Eq. 19 For hot points, the regulated plasmon frequencies as a function of the external electric field are plotted in Fig. 3. Obviously, with increasing external electric field, the frequency of the diluted part decreases, and the frequency of the accumulation part increases, where the extremum The accumulation point is located around 2×107 (N/C), which is the optimal range to control the paralysis process.

The free electron density energy has the same K_BT thermal excitation scale at room temperature, therefore, the Drude interpretation of the classical model is chosen to control this mechanism. An important step in using the classical equation for plasmon frequency is to calculate the electron density for the connection point (Eq. 14). By exposing this point to an external one by applying a laser beam with a frequency equal to the plasmon resonant frequency, the connection point at gp120 is disrupted as previously described.

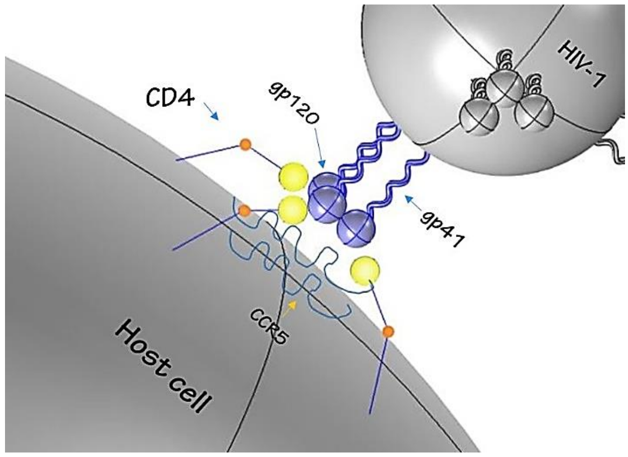

Fig. 2. HIV-1 connected to the CD4 from gp120 terminals and injecting RNA to the host cell

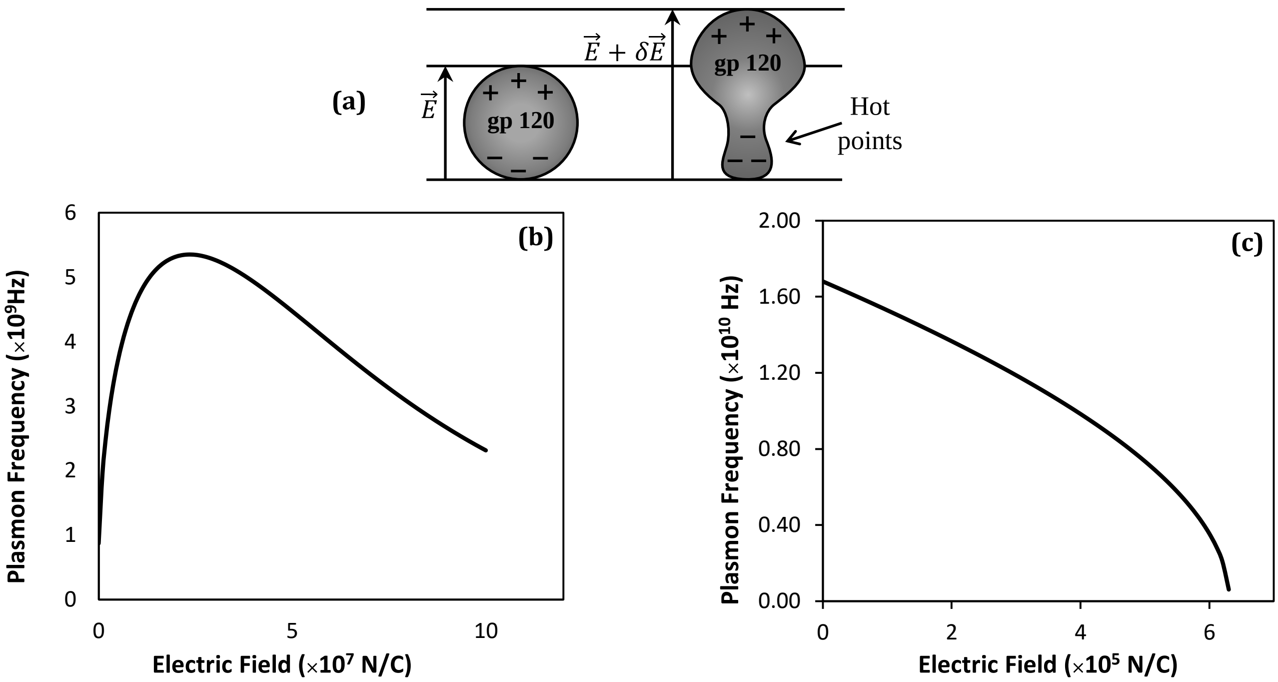

Fig. 3. (a) Creation of hot point on gp120 due to the external electric field, (b) plasmon frequency of the accumulation section, (c) diluted section

5. Johnson thermal noise

By applying an electric field, the electrons move rapidly. As a result, the temperature of the rod accumulation section increases due to the kinetic energy of the electrons, hence, the thermal noise of Eq. 19 can appear [37, 38]. Johnson noise appears due to the thermal stirring of charge carriers, which are usually electrons inside an electrical conductor. This thermal noise occurs regardless of the external electric field because the charge carriers vibrate as a result of the temperature. Therefore, this vibration depends on the temperature, so if the temperature rises, it reaches a higher level of thermal noise. The amount of thermal noise can be obtained with the following formula

$$V_{j,Th} = (4k_BTBR)^{\frac{1}{2}} \tag{20}$$

where R is the total resistance of the system and B is the frequency bandwidth. Total resistance could be rewritten as below

$$R = \rho \frac{L}{S} = \frac{L}{\sigma S} = \frac{m v}{n_0 e^2 S} \quad (21)$$

By substituting Eq. 21 in Eq. 20, the following equation can be obtained

$$V_{j,Th} = (\frac{4 K_B T m v}{n_0 S e^2} B)^{\frac{1}{2}} \quad (22)$$

by replacing mv by $(mkBT)^{\frac{1}{2}}$, the expression of $V_{j,Th}$ becomes

$$V_{j,Th} = C\, T^{\frac{3}{4}} \quad (23)$$

where C is given by the expression

$$C = (\frac{4 K_B^{\frac{3}{2}} m^{\frac{1}{2}}}{n_0 S e^2} B)^{\frac{1}{2}} \quad (24)$$

In the case of HIV-1 virus, for band width between 0 to 10^{16} Hz, the results achieved are shown in Fig. 4.

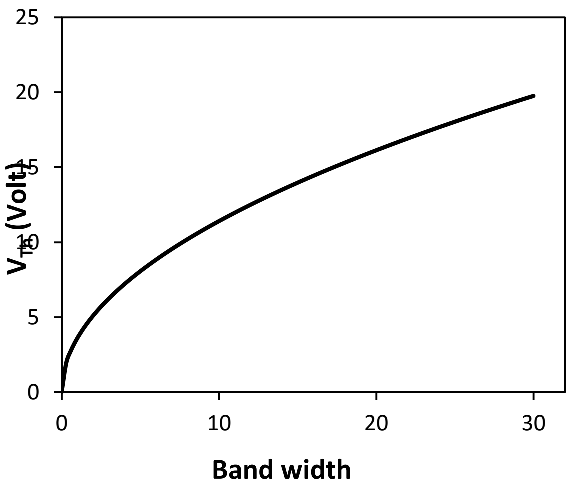

Fig. 4. Johnson noise voltage plotted for a range of band width

As shown in Fig.4, thermal voltage is increased due to the high bandwidth ranges.

6. Long-range coulomb's interaction

When an electron moves in an electric field, the electrostatic wall stops aggregating the electrons. This phenomenon is known as "long-distance Colombian interaction" in "shot noise" in vacuum tube devices that are smaller than microscale [39-42]. In this phenomenon, charge carriers move in the medium, this movement with self-adaptive potential creates an area that affects the velocity of the carriers themselves. This velocity changes the range of the electric potential to give the desired frequency in an area defined as gp120. The velocity equation is related to the square root temperature.

$$v_{c,Th} = (\frac{2\, K_B T}{\pi\, m})^{\frac{1}{2}} \quad (25)$$

regarding the following equations

$$I_{c,Th} = n e v_{c,th} A \quad (26)$$

and

$$V_{c,Th} = I_{c,Th} R = n e v_{c,th} A \left(\rho \frac{L}{A}\right) = n e \rho L v_{c,th} \quad (27)$$

By substituting $v_{c,th}$ with its expression from Eq. 25, the expression of the voltage becomes

$$V_{c,th} = n e \rho L (\frac{2 K_B T}{\pi m})^{\frac{1}{2}} \quad (28)$$

Accordingly, by considering thermal noise, and long-range Coulomb's effect, the total applied voltage could be as follow

$$V_{Total} = V + V_{j,th} + V_{c,th} = AT + CT^{1/4} + DT^{1/2} \quad (29)$$

with

$$D = n e \rho L (\frac{2 K_B}{\pi m})^{\frac{1}{2}} \quad (30)$$

Eq. 30 shows that in addition to the linear relationship with the temperature of Eq. 14, Johnson and Columbus's noises affect the desired external potential. This appropriate potential can control the hot point plasmon frequency at the connection point of CD4-gp120.

7. Conclusion

Applying an external electric field can change the electron density distribution, this feature can be used for many plasmon frequency applications. In this paper, the distribution of free electrons was studied and the effects of electron density on plasmon frequency were presented. Plasmon frequency regulation can also be used as a tunable detector in the UV to NIR range and HIV-1 paralyzation. For this purpose, the optimum potential voltage was shown as a function of the thermal effect by considering the shot noise and the Johnson effect. The use of an external electric field with a frequency of resonance of HIV-1 paralysis at the CD4 connection point raises the temperature and thus can damage gp120 glycoprotein, which plays an important role in HIV-host cell connection.

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