The Influence of the Electroneutrality of the Metal Layer on the Plasmon Spectrum in "Dielectric-Metal-Dielectric" Structures

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Abstract— **In this paper proposed a model that takes into account the discretization of the Fermi wave vector and energy levels (bound states), as well as the condition of electroneutrality when investigating the influence of metal thickness on the spectrum of SPPs waves in heterogeneous (dielectric-metal-dielectric) structures. The results of mathematical modeling show that for atomically thin metal films the influence is significant and has some specific properties.**

Keywords—plasmon spectrum, metal layer thickness, Fermi wave vector, electronuetrality

I. Introduction

The experimental results published in [1,2] allow us to state that the spectrum of plasmonic excitations considerably depends on the thickness of the metal layer in cases when we deal with atomically thin films that consist of few monolayers. In our previous work [3], we considered the dependence of dielectric permittivity function on the thickness of a metal. And it was shown that taking into account of geometric properties of a metal qualitatively changes the behaviour of the plasmon spectrum for atomically thin films. In addition, the description of quantum-sized effects on nanoscales and their influence on characteristics of metal films [4,5,6] pushed us to an assumption that these effects also should be taken into consideration. Because in the abovementioned works shown that with the change of a metal thickness wave vector and configuration of bound states change too. On both these parameters depends the model proposed in [6], so, naturally, arose the question about how taking into account of a change of these parameters will affect a plasmonic spectrum.

In subsequent chapters, the model proposed in [3] is supplemented by a description of the width of the asymmetric rectangular potential well in which the width depends on the thickness of the metal film and the environment that surrounds this film (insulators).

II. Ease of Use

As in our previous work, the geometrical structure of the considered model consisted of atomically thin metal film sandwiched between two dielectric environments (Fig. 1). Dielectric permittivity of insulators $\varepsilon_1(\omega)$ and $\varepsilon_3(\omega)$ are taken in the high-frequency approximation, thus, they are functions of the time variable / frequency. On the contrary, the dielectric permittivity of a metal depends on both time variable and spatial coordinates $\varepsilon\left(\vec{r},\vec{r}',t-t'\right)$.

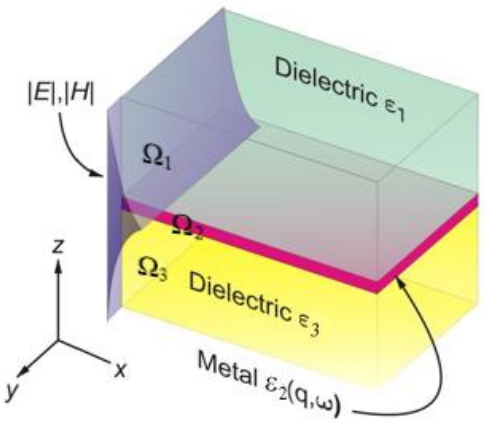

Figure 1. Schematic representation of model geometry

$$\varepsilon_2 = \varepsilon\left(\vec{r},\vec{r}',t-t'\right). \tag{1}$$

Given the assumption of the absence of external charges ρ, the Maxwell system of equations are such

$$\begin{aligned} &div\vec{D}=0,\ div\vec{B}=0,\\ &rot\vec{H}=\frac{\partial\vec{D}}{\partial t},\ rot\vec{E}=\frac{\partial\vec{B}}{\partial t}. \end{aligned} \tag{2}$$

Here $\vec{H}$ and $\vec{E}$ are vectors of magnetic and electric strength and $\vec{D}$ and $\vec{B}$ are vectors of electric and magnetic flux density. Interconnection between $\vec{D}$ and $\vec{E}$ vectors is non-local because the process is non-stationary

$$\vec{D}(\vec{r},t)=\int\limits_{\Omega} d\vec{r}'\int\limits_{t} dt'\varepsilon(\vec{r},\vec{r}',t-t')\vec{E}(\vec{r}',t'). \quad (3)$$

Considered transverse magnetic (TM) polarization of vectors of strength $\vec{H}$ and $\vec{E}$

$$\begin{aligned}&\vec{H}=\left(0,H_y,0\right),\ \vec{E}=\left(E_x,0,E_z\right),\\&\vec{H}=H(z)\mathrm{e}^{ik_x x}\mathrm{e}^{-i\omega t}\end{aligned} \quad (4)$$

together with the system (2) of Maxwell's equations yield the following system of wave equations

$$\begin{aligned}&\frac{\partial^2 H_y}{\partial z^2}+\left(k_0^2\varepsilon_1(\omega)-k_x\right)H_y=0,\quad z<-L/2,\\&\frac{\partial^2 H_y}{\partial z^2}+\left(k_0^2\varepsilon_2(\omega,z)-k_x\right)H_y=0,\quad -L/2<z<L/2,\\&\frac{\partial^2 H_y}{\partial z^2}+\left(k_0^2\varepsilon_3(\omega)-k_x\right)H_y=0,\quad z>L/2;\end{aligned} \quad (5)$$

Solutions of which describe the behavior of the electromagnetic wave near the dielectric-metal surface.

III. Description of the dielectric permitivitty of a metal layer

Based on the results obtained in [3] for a metal layer, we considered a model of an electron gas in an asymmetric rectangular potential well of finite depth. The dielectric function based on the diagonal component of the dielectric permittivity tensor [7] has the following form for this model:

$$\varepsilon_2(\omega,z)=1-\frac{\omega_p^2}{2\pi n_e\omega^2}\sum_{i=1}^{n_{\max}}\left(k_F^2-\alpha_i^2\right)\left|\varphi_i(z)\right|^2. \quad (6)$$

Here n_e - electron concentration in a metal, $\omega_p=\sqrt{4\pi n_e e^2/m_e}$, k_F - Fermi wave vector [8], α - quantum numbers of the bound states.

The presence of surfaces is described by potential

$$U(z)=\begin{cases}U_1\ if\ z<0,\\0\ \ if\ 0<z<L,\\U_2\ if\ z>L,\end{cases} \quad (7)$$

where L - thickness of the metal layer Function

$$\psi_n(z)=\sqrt{2/S}e^{i(\vec{q}\cdot\vec{r})}\varphi_n(z) \quad (8)$$

is a wave function of an electron in metal, $\vec{q}=\left(k_x,k_y\right)$, $\vec{r}=\left(r_{\|},z\right)$, $\varphi_n(z)$ - the solution of the Schrödinger equation

$$\begin{aligned}&-\frac{\hbar^2}{2m}\frac{d^2\varphi_n(z)}{dz^2}+U(z)\varphi_n(z)=W\varphi_n(z),\\&\lim_{z\to\pm\infty}\varphi_n(z)=0.\end{aligned} \quad (9)$$

Equation (9) together with potential (7) give the following expression for the wave function $\varphi_n(z)$ [6]:

$$\begin{aligned}&\varphi_n(z)=C\begin{cases}\frac{\alpha}{s_1}e^{\sqrt{s_1^2-\alpha^2}z}\ if\ z\le 0,\\\sin\left(az+\arcsin\frac{\alpha}{s_1}\right)\ \ if\ 0<z<L,\\\sin\left(Lz+\arcsin\frac{\alpha}{s_1}\right)e^{-\sqrt{s_2^2-\alpha^2}(z-L)}if\ z\ge L,\end{cases}\\&s_i=\sqrt{2m/\hbar^2 U_i},\ i=1,2,\end{aligned} \quad (10)$$

$C=C(\alpha)$ - normalizing constant [6]

$$C(\alpha)=\frac{\sqrt{2}}{\sqrt{L+\frac{(\alpha/s_1)^2}{\sqrt{s_1^2-\alpha^2}}+\frac{(\alpha/s_2)^2}{\sqrt{s_2^2-\alpha^2}}-\frac{1}{\alpha}\sin(\alpha L)\cos(\alpha L+2\arcsin\alpha/s_1)}}. \quad (11)$$

Equations for finding quantum numbers of bound states and the maximum number of energy levels, in turn, have the following form

$$\alpha L=\pi n-\arcsin\frac{\alpha}{s_1}+\arcsin\frac{\alpha}{s_2}, \quad (12)$$

$$n_{\max}=\left[\frac{1}{\pi}\left(L\min(s_1,s_2)+\arcsin\frac{\min(s_1,s_2)}{s_1}+\arcsin\frac{\min(s_1,s_2)}{s_2}\right)\right]. \quad (13)$$

Two approaches to describing the width of a potential well are considered and compared. In the first case, the width of the pit is equal to the width of the metal layer, and in the second it is stated that the width depends on the thickness of the metal layer and the dielectric parameters of the surrounding environment [6], which is depicted in Fig. 2

$$L_{well} = L + d_1 + d_2.$$
$$d_i = \frac{3\pi}{8k_F} + \frac{\pi^2}{8k_F^2 L_{well}} - \frac{3}{4k_F} \times \quad (14)$$
$$\times \left(\sqrt{\frac{s_i^2}{k_F^2} - 1} + \left(2 - \frac{s_i^2}{k_F^2}\right) \arcsin \frac{k_F}{s_i} \right), i = 1, 2.$$

The Fermi wave vector can be found from the condition of electroneutrality [6]

$$\frac{2}{3r_s^2} = \frac{1}{L} \sum_{n=1}^{n_{\max}} \left(k_F - \alpha_n^2\right). \quad (15)$$

r_s - Wigner-Seitz radius [8].

IV. Dispersion relatoin and results of modeling

In work [3] it is shown that the dielectric permittivity function and (6) the wave function (10) significantly depends on coordinates only at the interfaces dielectric-metal and metal-dielectric.

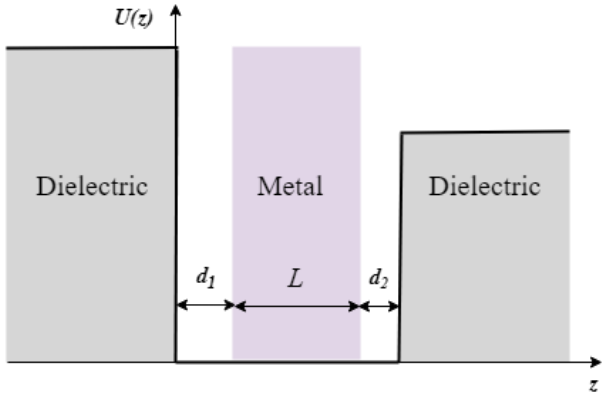

Figure 2. Schema of rectangular potential well with thickness different from the thickness of a metal subtrate.

Consequently, we can make the following assumption about the dielectric function (6)

$$\varepsilon_2(z, z', \omega) = \left(\varepsilon_2(L, \omega) + \alpha \Delta\varepsilon_2(z, \omega)\right) \delta(z - z'), \quad (16)$$

$$\varepsilon_2(\mathrm{L}, \omega) = \frac{1}{L} \int_0^L \varepsilon_2(z, \omega) dz =$$
$$= 1 - \frac{\omega_p^2}{2\pi n_e \omega^2} \sum_{n=1}^{n_{\max}} \left(k_F^2 - \alpha_n^2\right) \left|\overline{\varphi}_n(z)\right|^2, \quad (17)$$
$$\left|\overline{\varphi}_n(z)\right|^2 = \frac{1}{L} \int_0^L \left|\varphi_n(z)\right| dz.$$

Value $\Delta\varepsilon_2(z, \omega)$ describes the behaviour of the function (6) on the borders of the potential well.

After expansion of the function of the magnetic field strength $H_y(z, \omega)$ into series in powers of λ

$$H_y(z, \omega) = \sum_{m=0}^{\infty} \lambda^m H_{ym}(z, \omega) \quad (18)$$

and substitutions in (5) we obtain a system of recurrent differential equations for finding $H_y(z, \omega)$.

In this case, we limited ourselves to considering the first equation of the system

$$\frac{\partial^2 H_{y0}(z)}{\partial z^2} + \left(k_0^2 \varepsilon_2(\omega, z) - k_x\right) H_{y0}(z) = 0. \quad (19)$$

For such an equation, the dispersion relation is known and has the following form [9]

$$e^{-4k_1 L/2} = \frac{k_1/\varepsilon_1 - k_2/\varepsilon_2}{k_1/\varepsilon_1 + k_2/\varepsilon_2} \frac{k_3/\varepsilon_3 - k_2/\varepsilon_2}{k_3/\varepsilon_3 + k_2/\varepsilon_2}, \quad (20)$$
$$k_i = \sqrt{k_x^2 - k_0^2 \varepsilon_i}, \quad k_0 = \omega/c.$$

Study of the obtained model were conducted for such structures "Vacuum/Ag/SiO_2" and "Vacuum/Ag/Al_2O_3", characteristics of the metal are taken from [8] and of the dielectrics from [4]. The results of simulation are shown in Fig 3-4.

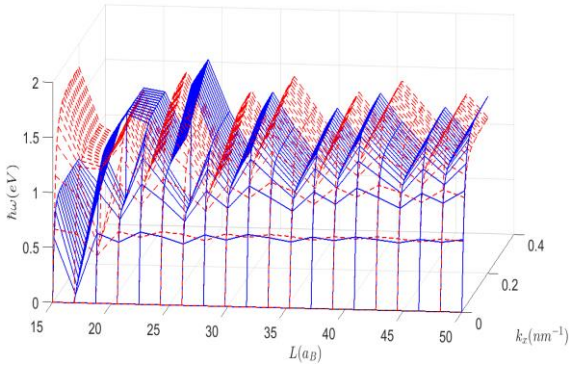

Figure 3. Dependence of plasmon spectrum on metal thickness for "Vacuum/Ag/Al_3O_2" structure. L_{well}=L - red lines and L_{well}=L+ d_1+d_2 - blue lines

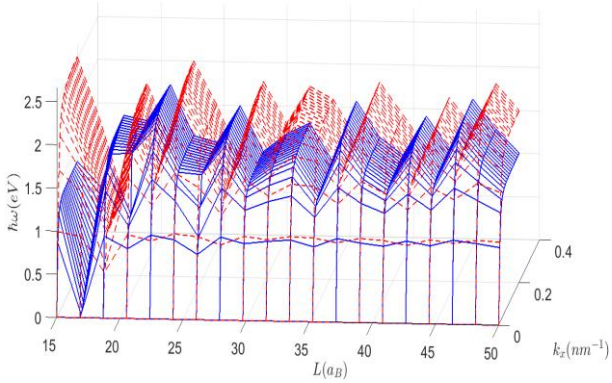

Figure 4. Dependence of plasmon spectrum on metal thickness for "Vacuum/Ag/SiO_2" structure. L_{well}=L - red lines and L_{well}=L+ d_1+d_2 - blue lines

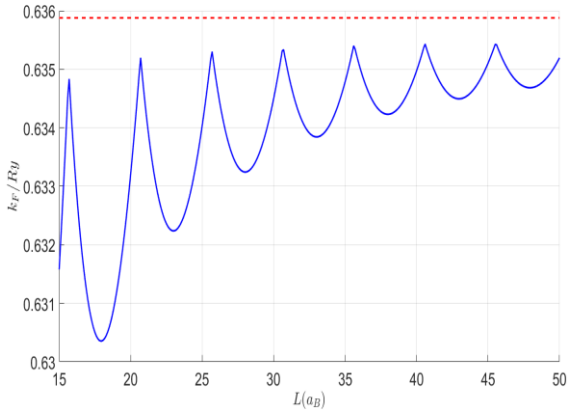

Figure 5. Dependence of Fermi wave vector on metal thickness for "Vacuum/Ag/SiO_2" structure. L_{well}=L - red lines and L_{well}=L+ d_1+d_2 - blue lines

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