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CALCULATION OF THE LINEAR ATTENUATION RATE FOR 1-DIMENSIONAL NANO-SIZED WAVEGUIDES

Abstract – Within semi-classical RPA-type approach it was calculated the linear attenuation of the electric field intensity of plasmon waves that travel along a nano-sized waveguide. The waveguide is considered as long 1D-array made of metal spherical nanoparticles, on one of which there is a source of excitation of plasmon oscillations. The results of calculations for Au/Ag/Cu-nanochains “immersed” in vacuum or silicon dioxide are presented (the nanosphere radius $a=25$ nm; the center-to-center distance $d=75$ nm). The obtained results were compared with similar data of other authors.

Keywords: surface dipole oscillations, metal nanoparticles, nanoscale waveguides, linear attenuation rate.

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РАСЧЕТ ПОГОННОГО ЗАТУХАНИЯ ДЛЯ ОДНОМЕРНЫХ НАНОМАСШТАБНЫХ ВОЛНОВОДОВ

В рамках метода RPA вычислено погонное затухание поверхностных дипольных колебаний, распространяющихся вдоль линейной цепочки, составленной из сферических наночастиц благородных металлов. Подобные волноводы рассматриваются как одномерные массивы конечной длины, в начальной точке которых находится внешний источник периодических возмущений. Вычисления проводились для наноразмерных Ag/Au/Cu-волноводов, погруженных в различные диэлектрические среды. Полученные расчетные данные находятся в хорошем согласии с результатами численных экспериментов других авторов.

Ключевые слова: поверхностные дипольные колебания, металлические наночастицы, наноразмерный волновод, погонное затухание.

Introduction

Experimental and theoretical studies of plasma oscillations in metallic nanoparticles, besides of purely scientific interest, are also of great practical importance. It is found that one-dimensional periodic structures of metallic nanoparticles can serve as a plasmon waveguide [1-3]. In this case, as it shown by experiments [3-7], the frequency both of the plasmonic and the light waves may coincide, but the length of the plasma wave will be significantly less than the length of the light wave. Therefore considered chains of nanoparticles can be successfully used in modern optoelectronic devices [8, 9]. When studying plasma oscillations in nanoparticles as small as 5 nm or less, the method of quantum-mechanical density functional theory or the “local-density approximation” method (LDA) as well the “time-dependent LDA” method (TDLDA) are generally used [9-12]. When studying plasma oscillations in metallic nanoparticles of several tens of nanometers the “random phase approximation” method (RPA) can be successfully used [13-16].

The results of computer simulation of “long” (the array of 1000 nanoparticles, radius $a=10$ nm) 1-dimensional waveguides were presented in [17], and in [18] it was presented results of modeling of optical frequencies’ excitation transport along a “short” nanoscale waveguide (the array of 80 nanoparticles, radius $a=10$ nm). But in these studies the linear attenuation rates of the propagation of surface plasmons were not shown.

It is known that the RPA method gives us the principal opportunity to find the *exact* solution of the basic equations that model this phenomenon [19, 20]. Providing calculus within the RPA method permits to avoid some unclear and disputable properties of group velocities of collective surface plasmons for both longitudinal and transversal polarization with respect to the nanochain orientation, as well their attenuation rates.

The aim of this work was to find within the framework of the RPA method the damping coefficients of the collective surface plasmon excitations travelling along 1D nanoscale waveguides (“nanochains”) which are composed of Au/Ag/Cu-nanospheres and immersed into different dielectric medium.

1. Propagation of surface plasma oscillations along the linear array composed of Metal spherical nanoparticles

Let us consider rather a long “chain” composed of metal (e.g. Au, Ag, Cu) nanoparticles of spherical shape of radius a and immersed into a dielectric medium with the permittivity of ϵ_h . We suppose that the nanospheres are arranged along an axis Z at the equal distance of $d > 2a$ from each other (i.e., their centers are spaced at equal distances from each other). Let the origin of coordinates be in the center of one of the particles, for example, in the nanosphere with the index of $l = 0$ (Fig. 1).

Further, one assumes that there is an external source of the electric field, which is located on one of the particles of the nanochain, for example, on the same particle with index $l = 0$. This electric field creates a point

dipole moment in the center of the particle with $l = 0$, and that point dipole, in turn, also produces the certain electric field.

Let the value of $\vec{E}_0(0, z, t)$ be the electric field intensity of the radiated electric field at any point of the axis Z at any given time t . Thus, the projections of the considered electric field intensity onto the coordinate axes X and Z at each l -th node of the chain, where the metal nanoparticles are located, will be determined by the following relations: $\vec{E}_{0\alpha}(0; ld; t) = \lim_{z \rightarrow ld} E_{0\alpha}(0; z; t)$, – here and elsewhere in this paper: $\alpha = x, z$. It means that at the center of each metal nanoparticles (see [15], p. 124322, Eq. (27)) it will arise additional dipole moments, committing with time compelled transverse and longitudinal vibrations.

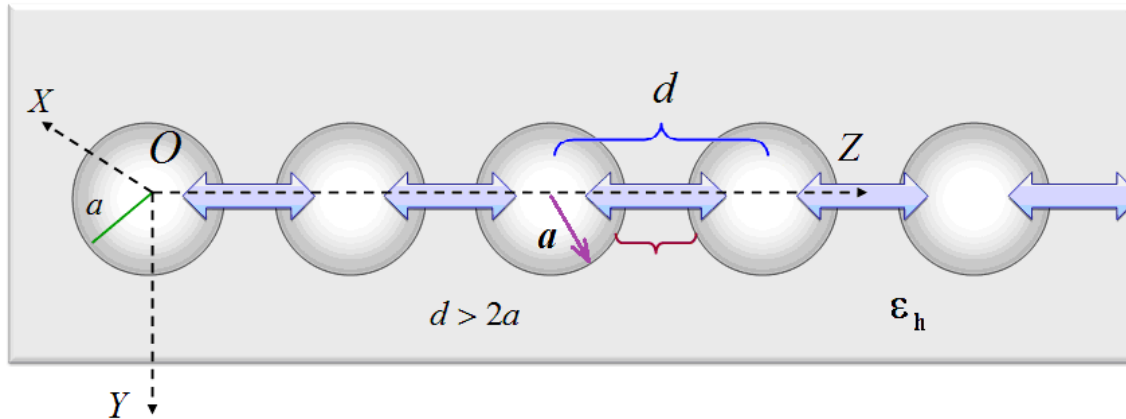


Figure 1. A schematic representation of the linear array of metallic spheres of radius a , which are spaced by the distance of d (immersed in dielectric medium)

In [16] it was shown that the dipole moment $\vec{D}(\vec{R}, t)$ of any nanoparticle satisfies the following DE :

$$\frac{\partial^2}{\partial t^2} \vec{D}(\vec{R}, t) + \frac{2}{\tau_0} \frac{\partial}{\partial t} \vec{D}(\vec{R}, t) + \omega_{p,h}^2 \vec{D}(\vec{R}, t) = \varepsilon_h a^3 \omega_{p,h}^2 \vec{E}(\vec{R}, t). \quad (1)$$

Here:

- $\omega_{p,h} = \omega_p / \sqrt{3\varepsilon_h}$, where ω_p is the bulk plasma frequency of the metal nanoparticles;
- τ_0 is the decay time of plasma oscillations: $\frac{1}{\tau_0} = \frac{v_F}{2} \left(\frac{1}{\lambda_b} + \frac{1}{a} \right)$, where v_F is the Fermi velocity, λ_b

is the mean free path of an electron in a bulk metal [13-15].

If there are N electric field sources located at points with coordinates \vec{R}_i ($i = 1, 2, \dots, N$), and the center of the particular metallic nanosphere is located at the point \vec{R}_0 , then Eq. (1) takes the form:

$$\frac{\partial^2}{\partial t^2} \vec{D}(\vec{R}_0, t) + \frac{2}{\tau_0} \frac{\partial}{\partial t} \vec{D}(\vec{R}_0, t) + \omega_{p,h}^2 \vec{D}(\vec{R}_0, t) = \varepsilon_h a^3 \omega_{p,h}^2 \sum_{i=1}^N \vec{E}(\vec{R}_{i0}, \vec{R}_i, t) \quad (2)$$

where $\vec{R}_{i0} = \vec{R}_i - \vec{R}_0$.

Further, accordingly to the general theory [21, 13], the dipole moment $\vec{D}(\vec{R}, t)$ of any nanoparticle that is located at the point \vec{R} can produce the electric field with its intensity of $\vec{E} = \vec{E}(\vec{R}, t)$ at the point $(\vec{R} + \vec{R}_0)$ which one can describe as follows:

$$\begin{aligned} \vec{E}(\vec{R}; \vec{R}_0; t) = & \frac{1}{\varepsilon_h} \left(-\frac{1}{R_0^3} - \frac{1}{R_0^2} \frac{1}{v_h} \frac{\partial}{\partial t} - \frac{1}{R_0} \frac{1}{v_h^2} \frac{\partial^2}{\partial t^2} \right) \vec{D}(\vec{R}; t - R_0/v_h) + \\ & + \frac{1}{\varepsilon_h} \left(\frac{3}{R_0^3} + \frac{3}{R_0^2} \frac{1}{v_h} \frac{\partial}{\partial t} + \frac{1}{R_0} \frac{1}{v_h^2} \frac{\partial^2}{\partial t^2} \right) \vec{n}_0 \cdot (\vec{n}_0 \cdot \vec{D}(\vec{R}; t - R_0/v_h)), \end{aligned}$$

where $\vec{n}_0 = \vec{R}_0/R_0$, $v_h = c/\sqrt{\varepsilon_h}$.

In that case, if at the particles of the array with index m , which are adjacent to the particle with index l ($m \neq l$), plasma oscillations occur, i.e. electric dipole moments $\vec{D}(md, t)$ arise, they establish the electric field whose intensity vector at the point where the particle is located, accordingly to the equation above, equals to

$$E_z(R_m, R_{ml}, t) = \frac{2}{\varepsilon_h d^3} \left(\frac{1}{|m-l|^3} + \frac{d}{v_h |m-l|^2} \frac{\partial}{\partial t} \right) D_z \left(md; t - \frac{|m-l|}{v_h} d \right), \quad (3a)$$

$$E_x(R_m, R_{ml}, t) = -\frac{1}{\varepsilon_h d^3} \left(\frac{1}{|m-l|^3} + \frac{d}{v_h |m-l|^2} \frac{\partial}{\partial t} + \frac{d^2}{v_h^2 |m-l|} \frac{\partial^2}{\partial t^2} \right) D_x \left(md; t - \frac{|m-l|}{v_h} d \right). \quad (3b)$$

Then, accordingly to Eq. (2), one can get the equations that describe the dipole moment $\vec{D}(ld, t)$ of the l -th nanoparticle:

$$\frac{\partial^2}{\partial t^2} D_\alpha(ld, t) + \frac{2}{\tau_0} \frac{\partial}{\partial t} D_\alpha(ld, t) + \omega_1^2 D_\alpha(ld, t) = \varepsilon_h a^3 \omega_1^2 \left(\sum_{\substack{m=-\infty \\ (m \neq l)}}^{+\infty} E_\alpha(R_m, R_{ml}, t) + E_{L\alpha}(ld, 0, t) + E_{0\alpha}(0, ld, t) \right),$$

where $\alpha = (x, z)$. Note: here it was included the existence of the Lorentz frictional force (or *Lorentz friction* [21]), the electric field intensity of which \vec{E}_L one can find accordingly to the following equation [14-16]:

$$\vec{E}_L(ld, 0, t) = \frac{2e\sqrt{\varepsilon_h}}{3c^3} \frac{\partial^3}{\partial t^3} \vec{D}(ld, t) = \frac{2}{3d^3 \varepsilon_h} \left(\frac{d}{v_h} \right)^3 \frac{\partial^3}{\partial t^3} \vec{D}(ld, t).$$

As it known, the Lorentz friction for dipole surface plasmons in metallic nanospheres is of great significance as it determines both the resonance frequency and the damping of plasmons [13-16, 22].

After certain transformations of the equation above one will get the following solution of it (see [23]):

$$D_{0\alpha}(ld, t) = \text{Re} e^{-t/\tau_0} \cdot \int_0^{2\pi} A_\alpha(k) \cdot \exp(-i \cdot (\Omega \cdot t - k \cdot ld)) \cdot dk,$$

where

- k is the wave number;
- Ω is the frequency of eigenwaves in a 1D-array composed of the same particles [24];
- A_α is an arbitrary periodic function of k .

As one can see, the obtained function describes a wave packet traveling along the nanochain in the positive direction (*longitudinal waves*). There are the EM signal propagation effective lengths L_z for different nanochains in [24]. And as one can see, for interesting in the context of technology Au-waveguides with the proper geometrical parameters (i.e. the nanoparticle radius $a = 25$ nm and the center-to-center distance $d = 3a$) it was estimated that the value of L_z is about 965 nm. The mentioned wave packet can run the distance within the time of τ_0 (it is the decay time of plasma oscillations due to their interaction with phonons of bulk metal and surface of the nanoparticles [24], in the current case it is about 2×10^{-14} s).

We shall further consider only surface plasma oscillations that arise under the influence of an external uniform electric field. One assumes that the external electric field source creates the field with periodically varying field strength at the point z : $\vec{E}_{0\alpha}(z, t) = \vec{E}_{0\alpha}(z) \cdot \cos(F, t)$, here F is the frequency of the field strength oscillation of the external alternating electric field.

Let the intensity of this radiated electric field at any point of the Z axis at time t be equal to $\vec{E}_0(z, t)$. Then the projections of the mentioned electric field intensity on the coordinate axes X and Z at each l -th node of the chain will be determined by the following relations: at $z \rightarrow ld$ it leads to following: $\vec{E}_{0\alpha}(z, t) = \vec{E}_{0\alpha}(ld, t)$ (note: here and elsewhere $\alpha = x, z$). Accordingly to Eq. (1) this fact means that additional dipole moments will occur in the center of each metallic nanoparticle of the array, and it will cause forced transverse and longitudinal oscillations over time.

Thus, the differential equation below determines the time dependence of the longitudinal and transverse electric dipole moments $D_\alpha(z, t)$ of a point dipole located at the z -point of the chain made of metal nanoparticles:

$$\left(\frac{\partial^2}{\partial t^2} + \frac{2}{\tau_0} \frac{\partial}{\partial t} + \omega_\alpha^2(kd) \right) D_\alpha(z, t) = \varepsilon_h a^2 \omega_{p,h}^2 E_{0\alpha}(z, t).$$

Substituting $z = l \cdot d$ one can determine the dipole moment of the particle located at the l -th node of the infinite chain considered by us [23]:

$$\frac{\partial^2}{\partial t^2} D_\alpha(ld, t) + \frac{2}{\tau_0} \frac{\partial}{\partial t} D_\alpha(ld, t) + \omega_{p,h}^2 D_\alpha(ld, t) = \varepsilon_h a^3 \omega_{p,h}^2 \left(\sum_{\substack{m=-\infty \\ (m \neq l)}}^{+\infty} E_\alpha(R_m, R_{ml}, t) + E_{L\alpha}(ld, 0, t) + E_{0\alpha}(0, ld, t) \right) \quad (4)$$

The Eq. (4) describes the dipole-type coupling between the arranged nanospheres (Fig. 2). As one can see,

all the terms of the Eq. (4) are “dimension-sensitive” values, i.e. they rigidly depend on the geometric parameters of such waveguides.

Let us analyze “behavior” of the electric field of propagating plasma oscillations caused by an external source of the field at the frequency range near the resonance of a given system of nanoparticles. Then let it be: $F = \omega_{0\alpha}(1 + \phi/\omega_{0\alpha})$, where it is true: $\phi/\omega_{0\alpha} \ll 1$. Then one can get: $F^2 - \omega_{0\alpha}^2 \approx 2\phi\omega_{0\alpha}$.

After that, when solving this Eq. (4) using the Fourier transformation with the corresponding boundary conditions and nearby the resonance frequencies, one can obtain the following equations concerning the electric field strength $E_\alpha(ld, a, t)$ of the travelling plasmon wave:

$$\begin{cases} E_z(ld, a, t) = 2\omega_{p,h}^2 E_{0z}(0,0) \cdot b_{0z}(\varphi) \cdot \left[1 + \left(\frac{\omega_p a}{\omega_{p,h} c \sqrt{3}} \right) \frac{\partial}{\partial t} \right] [\cos(u_{0z}l - Ft - \delta_{0z}(F)) + \cos(u_{0z}l + Ft + \delta_{0z}(F))] \\ E_x(ld, a, t) = -\omega_{p,h}^2 E_{0x}(0,0) \cdot b_{0x}(\varphi) \times \\ \times \left[1 + \left(\frac{\omega_p a}{\omega_{p,h} c \sqrt{3}} \right) \frac{\partial}{\partial t} + \left(\frac{\omega_p a}{\omega_{p,h} c \sqrt{3}} \right)^2 \frac{\partial^2}{\partial t^2} \right] [\cos(u_{0x}l - Ft - \delta_{0x}(F)) + \cos(u_{0x}l + Ft + \delta_{0x}(F))] \end{cases}, (5)$$

Here:

- $E_{0\alpha}(0,0)$ – the amplitude of the electric field strength oscillations at that node of the nanoscale metallic chain where the external source of the field is located;
- $b_{0\alpha}(\phi) = 1/\sqrt{(\omega_{0\alpha}^2 - F^2)^2 + 4F^2/\tau_0^2}$;
- $u_{0\alpha}$ is a value of the range: $0 \leq u_{0\alpha} \leq 2\pi$;
- $\delta_{0\alpha}(F) = \text{arctg}\left(\frac{2F}{\tau_0 \cdot (\omega_{0\alpha}^2 - F^2)}\right)$.

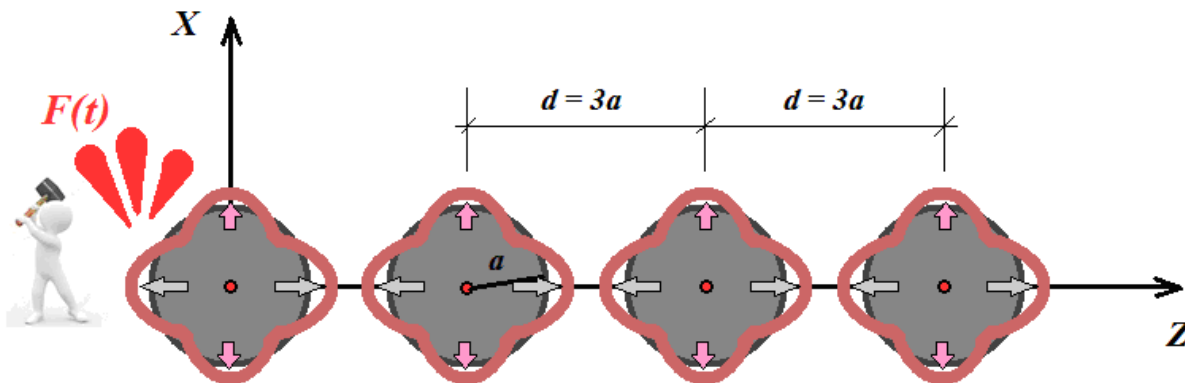


Figure 2. The illustration of surface plasma oscillations propagation along a linear array made up of spherical metallic nanoparticles. The process is based on the dipole-type coupling between the arranged nanospheres.

2. Obtained Results and Discussion

Based on the above theory, the author calculated the attenuation of the signal in the form of plasmon waves passing along a nanoscale waveguide made up of a 1D-array of spherical metal nanoparticles. Presented results were obtained within the RPA modeling framework based on the following input data: the matter of the waveguide is one of the noble metals (Au, Ag, Cu); the radius $a = 25$ nm; the distance between the nanosphere centers $d = 75$ nm; the surrounding medium for the nanoparticles – vacuum ($\epsilon_h = 1$) and SiO_2 ($\epsilon_h = 3.8$) [25]. To quantify the signal losses in such waveguides it is usually used well known decibel scaling to express the ratio of two values of the electric field strengths quantity: $A_a = 20 \lg(E_{1\alpha}/E_0)$ dB. In this formula: E_0 stands for the value of electric field strengths of the signal generator (the “reference field”); $E_{1\alpha}$ stands for the value of electric field strengths at the remote point (the field under study). Note: usually this value is measured in “dB/500 nm” units.

The table below (see Table 1) shows the results of calculations of the attenuations rates of the plasmon waves that travel along the described above metal nano-chains made of silver spherical nanoparticles.

The linear Attenuation Rate calculated for the plasmon waves in Au/Ag/Cu-waveguides in different media(radius $a = 25$ nm; center-to-center distance $d = 75$ nm; $T^\circ = 300$ K)

Medium	Linear Attenuation Rate of the Plasmon Waves (dB/500 nm)					
	metal: Au		metal: Ag		metal: Cu	
	Longitudinal A_z , dB/500 nm	Transverse A_x , dB/500 nm	Longitudinal A_z , dB/500 nm	Transverse A_x , dB/500 nm	Longitudinal A_z , dB/500 nm	Transverse A_x , dB/500 nm
vacuum, $\epsilon_h = 1$	3.2	7.9	3.1	7.3	17.0	24.0
SiO ₂ , $\epsilon_h = 3.8$	3.3	8.7	3.2	7.4	17.3	25.0

The presented results show the sensitivity of the modeling functions to certain changes (variations) of the basic parameters of the mentioned waveguide as the input data for the corresponding computational procedures.

By comparing the current results with the results of other researchers for the same case (Ag, $a = 25$ nm, $d = 75$ nm, longitudinal wave travelling in vacuum), one can see a good agreement with the obtained data. Judge for yourself: 1) attenuation for the signal intensity was 3 dB/500nm (see p. R16 358 of [3]); 2) it was found optimum guiding conditions, which corresponds to 2.4 dB/500nm [26].

Conclusion

Calculations of damping values for propagating of surface plasma oscillations (plasmon-polariton waves) that travel along nano-sized waveguides of great length are performed. It is considered the case when an external electric field source will be placed amongst such ensemble of nanoparticles, and the source can create the external alternating electric field with its frequency of F near the plasmon resonance of the given ensemble.

The obtained results – the linear attenuation rates of the plasmon waves – are presented in Table 1: these data are in good agreement with similar results of other authors. In addition, such proximity of the results suggests that different theoretical approaches (considerations) and different computational routines lead to similar results. It is evident, that the material of the surrounding medium may influence of on the damping rate of the electric field strength of the travelling plasmon excitation.

These calculated values of the attenuation rate of plasmon waves can indicate a high efficiency of this described above method of transmitting EM-energy along such waveguides. The author believes that such nanoscale waveguides can be successfully used for subwavelength transmission lines within integrated optics circuits.

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