Journal of Quantitative Spectroscopy & Radiative Transfer 191 (2017) 1–6

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

# Thermal limiting effects in optical plasmonic waveguides

A.E. Ershov [a,b,c], V.S. Gerasimov [b], A.P. Gavrilyuk [a,b], S.V. Karpov [b,c,d], V.I. Zakomirnyi [b,e], I.L. Rasskazov [f,*], S.P. Polyutov [b]

[a] Institute of Computational Modeling, Federal Research Center KSC SB RAS, 660036 Krasnoyarsk, Russia
[b] Institute of Nanotechnology, Spectroscopy and Quantum Chemistry, Siberian Federal University, Krasnoyarsk 660041, Russia
[c] Siberian State Aerospace University, 660037 Krasnoyarsk, Russia
[d] Kirensky Institute of Physics, Federal Research Center KSC SB RAS, 660036 Krasnoyarsk, Russia
[e] Royal Institute of Technology, Stockholm SE-100 44, Sweden
[f] The Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

ARTICLE INFO

*Article history:*
Received 8 September 2016
Received in revised form
21 December 2016
Accepted 17 January 2017
Available online 21 January 2017

*Keywords:*
Plasmon resonance
Optical plasmonic waveguide
Surface plasmon polariton
Thermal effects

ABSTRACT

We have studied thermal effects occurring during excitation of optical plasmonic waveguide (OPW) in the form of linear chain of spherical Ag nanoparticles by pulsed laser radiation. It was shown that heating and subsequent melting of the first irradiated particle in a chain can significantly deteriorate the transmission efficiency of OPW that is the crucial and limiting factor and continuous operation of OPW requires cooling devices. This effect is caused by suppression of particle's surface plasmon resonance due to reaching the melting point temperature. We have determined optimal excitation parameters which do not significantly affect the transmission efficiency of OPW.

Published by Elsevier Ltd.

## 1. Introduction

Optical plasmonic waveguides (OPW) in the form of plasmonic nanoparticle chains [1–5] attract significant attention in recent years due to their applicability to transmit modulated and spatially-localized optical radiation by means of surface-plasmon polaritons (SPPs). This interest is associated with vast majority of applications of such chains, particularly in sensing [6–9], nano-antennas [10,11] or creation of nanoscale optical integrated functional elements for new types of computing devices operating at optical frequencies at a scales much smaller than the radiation wavelength [12–14] and so on.

The influence of disorder [15–17], waveguide geometry [18–20], particles' shape [21–24] on OPW optical properties were investigated in details in recent years. The effect of a dielectric or metallic substrate on transmission [25,26] and dispersion [27,28] properties of OPW which is of primary importance for practical application of plasmonic chains has been also considered. In most studies, the only one, for example, the leftmost (first) nanoparticle in the chain is excited by external radiation [15–17,25,26]. Obviously, such excitation will be accompanied by heating of both the particles and surrounding medium. Heating of nanoparticles by laser radiation was studied in recent works [29–31]. However, these studies did not take into account the effect of heating on the optical properties of nanoparticles and *vice versa*. Earlier, in Ref. [32], the model of optodynamical effects in resonant domains of plasmonic nanoparticle aggregates was presented. This model takes into account light-induced changes of inter-particle forces as well as the permittivity of a particle material which occur in high intensity pulsed laser radiation. Further studies made it possible to consider the effect of heating of the particle metal core on the quality factor of surface plasmon resonance and to develop the improved version of the optodynamical model [33,34]. It was shown that heating of particles and subsequent melting significantly affect their resonant properties. Therefore, we can conclude that such complementary phenomenon will obviously affect the transmission properties of the OPW.

The approach to the description of heat exchange between nanoparticles and the environment [32,33,35] is also applicable to the case of a single laser pulse with a duration much shorter than the thermodynamic equilibrium establishing time. However, these models disregard the effect of substrate on OPW which may play the role of the cooling device. Therefore, in our work, we have developed the thermodynamic model which takes into account heat exchange between OPW nanoparticle, surrounding environment and substrate as well as the temperature dependence of the particle optical properties.

To the best of our knowledge, there is a lack of data on the

* Corresponding author.
*E-mail addresses:* karpov@iph.krasn.ru (S.V. Karpov), il.rasskazov@gmail.com (I.L. Rasskazov).

http://dx.doi.org/10.1016/j.jqsrt.2017.01.023
0022-4073/Published by Elsevier Ltd.

effect of heating of nanoparticles in OPW on its transmission properties. Therefore, the goal of our paper is to study the changes of OPW transmission properties associated with heating and melting of nanoparticles comprising the chain.

## 2. Model

Consider the simplest case of a linear chain consisting of $N=11$ identical spherical Ag nanoparticles with a radius $R=8$ nm. Nanoparticles are arranged equidistantly in the medium with $\varepsilon^{H} = 1.78$ over the surface of the quartz substrate (see Fig. 1). The distance between the centers of the neighboring particles is $h=24$ nm. The gap between OPW surface and substrate is set to 0.5 nm.The particle size is assumed to be much smaller than the wavelength of incident radiation $R \ll \lambda$ and $h \leq 3R$. Therefore, selected geometrical parameters provide the validity of the dipole approximation [15–17,21–23] which will be used in our calculations.

### 2.1. Electromagnetic interactions in the OPW

We consider a local excitation of the OPW particles, which can be experimentally implemented by using, for example, a near-field optical microscope tip. The external field $\mathbf{E}_n = \mathbf{E}(\mathbf{r}_n)$ applied to the $n$th particle located at $\mathbf{r}_n$ can be described as follows:

$$\mathbf{E}_n = \mathbf{E}_0 \exp(i\mathbf{k}\mathbf{r}_n). \tag{1}$$

Here $|\mathbf{k}| = 2\pi\sqrt{\varepsilon^{H}}/\lambda$ is the wave vector, $\mathbf{E}_0$ is the amplitude of the electric component of the electromagnetic field.

Assume that the only $n=1$ nanoparticle interacts with an external field so that $\mathbf{E}_n = 0$ for $n \neq 1$. In this case, the dipole moment $\mathbf{d}_n$ induced on the $n$th particle can be described by the coupled dipole approximation:

$$\mathbf{d}_n = \varepsilon_0 \alpha_n \left[ \mathbf{E}_n \delta_{n1} + \sum_{m=1}^{N} \hat{\mathbf{G}}(\omega; \mathbf{r}_n, \mathbf{r}_m)\mathbf{d}_m \right], \tag{2}$$

where $\alpha_n$ is the dipole polarizability of the $n$th particle, $\delta_{n1}$ is Kronecker delta, $\hat{\mathbf{G}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ is the $3 \times 3$ Green's interaction tensor describing the electric field produced at $\mathbf{r}_n$ by electric dipole (oscillating with frequency $\omega$) located at $\mathbf{r}_m$. For OPW on substrate, the Green's interaction tensor is defined as follows:

$$\hat{\mathbf{G}}(\omega; \mathbf{r}_n, \mathbf{r}_m) = \hat{\mathbf{G}}_{\text{free}}(\omega; \mathbf{r}_n, \mathbf{r}_m) + \hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_m), \tag{3}$$

where $\hat{\mathbf{G}}_{\text{free}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ and $\hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ are Green's tensors that describe electric field in a homogeneous environment and reflected from the substrate, correspondingly. Expression for $\hat{\mathbf{G}}_{\text{free}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ is well-known and can be found elsewhere. Tensor $\hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ can be written in the form of a Fourier integral [36–38]. Calculation of this integral represents quite complicated task.

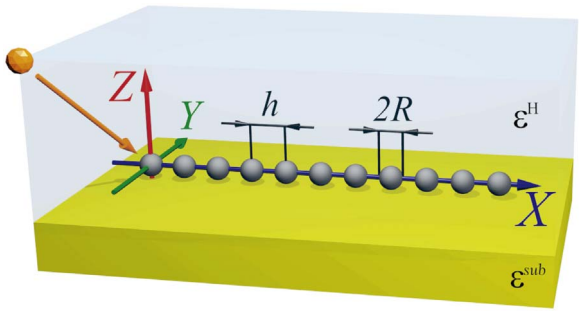


**Fig. 1.** Schematic illustration of the of OPW geometry used in numerical simulations.

In some cases, the integrals of $\hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$ can be evaluated along an appropriate integration path using a Gauss-Kronrod quadrature [39] or via analytical short-distance expansions [40]. However in this work, we use a purely numerical approach to compute $\hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_m)$. Specifically, we compute the Fourier integral numerically by discretization. Finally, it should be noticed that summation in (2) runs over all indices, but the term $\hat{\mathbf{G}}_{\text{free}}(\omega; \mathbf{r}_n, \mathbf{r}_n) = 0$ by definition.

An expression for the dipole polarizability for $n$th nanoparticle in homogeneous environment, which takes into account the radiation reaction correction, has the form [41]:

$$\alpha_n^{-1} = \left[\alpha_n^{(0)}\right]^{-1} - \frac{i}{6\pi}|\mathbf{k}|^3, \tag{4}$$

where $\alpha_n^{(0)}$ is so-called bare or Lorenz-Lorentz quasistatic polarizability of the particle. Self-interaction of $n$th nanoparticle with field reflected from substrate is described by $\hat{\mathbf{G}}_{\text{refl}}(\omega; \mathbf{r}_n, \mathbf{r}_n) \neq 0$.

In our work, we take into consideration the fact that a particle can be in the melting process. Thus, the nanoparticle is considered as a core-shell nanosphere with a solid core and a liquid shell. Therefore, the $\alpha_n^{(0)}$ can be described as follows [42]:

$$\alpha_n^{(0)} = 4\pi R_n^3 \times \frac{\left(\varepsilon_n^{L} - \varepsilon^{H}\right)\left(\varepsilon_n^{S} + 2\varepsilon_n^{L}\right) + f_n\left(\varepsilon_n^{S} - \varepsilon_n^{L}\right)\left(\varepsilon^{H} + 2\varepsilon_n^{L}\right)}{\left(\varepsilon_n^{L} + 2\varepsilon^{H}\right)\left(\varepsilon_n^{S} + 2\varepsilon_n^{L}\right) + 2f_n\left(\varepsilon_n^{S} - \varepsilon_n^{L}\right)\left(\varepsilon_n^{L} - \varepsilon^{H}\right)}. \tag{5}$$

Here $R_n$ is radius of the $n$th particle, $\varepsilon_n^{S}$ and $\varepsilon_n^{L}$ are the temperature and size dependent permittivities of the particle material in the solid and liquid state, respectively, $f_n$ is the mass fraction of solid material in the particle. The expression (5) takes into account the extreme cases of completely solid ($f_n = 0$) and fully liquid particles ($f_n = 1$). The full description of $f_n$ will be given below. It should be noticed that Ag nanoparticle keeps its spherical shape even in the fully liquid state due to extremely high values of surface tension. Therefore, the expression (5) is valid for any values of $f_n$.

Permittivities $\varepsilon_n^{S}$ and $\varepsilon_n^{L}$ take into account finite size effects [43]:

$$\varepsilon_n^{S,L} = \varepsilon_{\text{tab}}^{S,L} + \frac{\omega_{\text{pl}}^2}{\omega(\omega + i\Gamma_0)} - \frac{\omega_{\text{pl}}^2}{\omega(\omega + i\Gamma_n)}, \tag{6}$$

where $\omega$ is the electromagnetic field frequency, $\varepsilon_n^{S,L}$ is the permittivity of the solid or liquid material of the particles, $\varepsilon_{\text{tab}}^{S,L}$ is the corresponding tabulated experimental values for bulk at the temperature of 300 K for solid material [44] and at the melting point for liquid one [45], $\Gamma_0$ is the time dependent bulk electron relaxation constant for corresponding temperature, $\omega_{\text{pl}}$ is the plasma frequency of the particle material, $\Gamma_n$ is the temperature and size dependent electron relaxation constant of a particle:

$$\Gamma_n = \Gamma_0\left(T_n^{\text{ion}}\right) + A\frac{v_F}{R_n}. \tag{7}$$

Here $v_F$ is the Fermi velocity. The value of $A$ is taken to be unit in most of cases [42]. However, the relaxation processes depend on the state of particle surface and on other factors. The dependence of the relaxation constant for bulk material $\Gamma_0(T)$ on the temperature can be approximated by the following expression [46]:

$$\Gamma_0(T) = bT + c, \tag{8}$$

where $b$ and $c$ are the linear dependence coefficients obtained by linear approximation of the experimental data [47]. Detailed analysis of this model will be published elsewhere.

To describe the transmission properties of OPW we use the transmission coefficient [15,22,20]:

$$Q_{\text{tr}} = \frac{|\mathbf{d}_N(t)|}{|\mathbf{d}_1(t=0)|}, \tag{9}$$