



## Invited Paper

## Titanium nitride nanoparticles as an alternative platform for plasmonic waveguides in the visible and telecommunication wavelength ranges

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## ARTICLE INFO

## Article history:

Received 15 November 2017

Received in revised form 12 March 2018

Accepted 12 April 2018

Available online 17 April 2018

## Keywords:

Nanoparticle

Titanium nitride

Surface plasmon polariton

Plasmon waveguide

Refractory plasmonics

## ABSTRACT

We propose to utilize titanium nitride (TiN) as an alternative material for linear periodic chains (LPCs) of nanoparticles (NPs) which support surface plasmon polariton (SPP) propagation. Dispersion and transmission properties of LPCs have been examined within the framework of the dipole approximation for NPs with various shapes: spheres, prolate and oblate spheroids. It is shown that LPCs of TiN NPs support high-Q eigenmodes for an SPP attenuation that is comparable with LPCs from conventional plasmonic materials such as Au or Ag, with the advantage that the refractory properties and cheap fabrication of TiN nanostructures are more preferable in practical implementations compared to Au and Ag. We show that the SPP decay in TiN LPCs remains almost the same even at extremely high temperatures which is impossible to reach with conventional plasmonic materials. Finally, we show that the bandwidth of TiN LPCs from non-spherical particles can be tuned from the visible to the telecommunication wavelength range by switching the SPP polarization, which is an attractive feature for integrating these structures into modern photonic devices.

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## 1. Introduction

Plasmonic nanoparticles (NPs) are one of the cornerstones of modern science and technology due to an almost uncountable number of applications [1]. The uniqueness of the NPs originates from their ability to support localized surface plasmons (LSPs) which enables strong confinement of electric fields at scales much smaller than the wavelength of the incident radiation. Strong enhancement of local fields is vital for a wide variety of possible applications such as surface enhanced Raman spectroscopy [2], upconversion [3], biomedicine [4] and solar energy harvesting [5].

Arrays of non-touching NPs enable nanoscale electromagnetic energy transfer via propagation of so-called surface plasmon

polaritons (SPPs) [6,7] which paves the way for utilization of nanostructures in chemical sensing [8–11], nanoantennas [12,13] and nanosized waveguides [14–19]. Propagation of SPPs is usually considered in 1D or 2D arrays of NPs from conventional plasmonic materials: Ag [6,15,16,20–24] and Au [17,18,25,26]. Various types of technological aspects such as disorder [15,20], polydispersity [15] impact of the substrate [21,27,28], thermal effects [29] have been thoroughly considered so far. However, high Ohmic losses and consequent overheating of metal NPs lead to strong suppression of the LSPs [30] and, as a result, significant attenuation of the SPP. Moreover, the SPP frequencies lie mostly in the visible or near infrared ranges, while integration with CMOS-compatible devices requires bandwidth of LPCs to lie within the telecommunication wavelength range. These drawbacks make it unlikely that LPCs of plasmonic NPs can be utilized as a tool for efficient guiding of electromagnetic energy over distances of several hundred nanometers for applications in highly integrated optical devices operating below the diffraction limit of light [31].

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There are some strategies to deal with strong attenuation of SPPs. For example, utilization of non-spherical NPs can lead to nondecaying propagation of SPPs in LPCs in homogeneous media [32] or to minimization of SPP suppression due to interaction with the dielectric substrate [27]. However, inevitable Ohmic losses in metals and consequent overheating of NPs represent a more complicated problem to deal with. The temperature dependent optical properties of noble metals [30,33–36] imply strong suppression of LSP resonances at high temperatures, which is of crucial importance for SPP propagation. Finally, chemical instability, inability to dynamically adjust optical properties [37] limit successful implementations of Ag and Au LPCs of NPs in photonic devices.

Recent progress in plasmonics, however, indicates a way to overcome drawbacks of conventional noble metals by using so-called alternative plasmonic materials [38,39]. Numerous materials have been benchmarked against conventional Ag and Au in terms of local field enhancement [40] and refractory behavior [41,39,42]. Metal transition nitrides, particularly, titanium nitride (TiN) have been considered as most promising material from this perspective [43–46]. TiN thin films and NPs have a great potential in photodetection [47], solar energy harvesting [48], sustainable energetics [49], nonlinear optics [50,51], and biomedicine [52]. The position of the LSP resonance peak of a single TiN NP lies in the near infrared region [46] which is a vital feature for utilization of TiN NP arrays in photonic devices operating at telecommunication wavelengths [53,54]. Finally, low-cost large area fabrication [55], thermal stability [56] are important advantages of TiN which immediately enable its wide practical implementation.

In this paper, we propose to utilize TiN for waveguiding applications in LPCs of spherical and spheroidal NPs. TiN optical properties provide an opportunity to shift the SPP frequency to telecommunication wavelengths, while the TiN refractory behavior could potentially resolve issues with strong SPP suppression at high temperatures.

## 2. Model

### 2.1. Dipole approximation

A substantial part of theoretical and experimental studies of electromagnetic properties of metal nanostructures are based on the dipole approximation (DA) [15,16,21,23,57–62]. This approximation is quite simple yet efficient for accurate description and prediction of optical properties of plasmonic nanostructures. The applicability of DA is, however, strictly limited by the geometry of the structure [63,64]: the distance between the NPs in a periodic array should be significantly larger than the size of the NPs. For example, in the case of nanospheres, the center-to-center distance between neighboring NPs should exceed the NP diameter by the factor of 1.2 and 1.4 for transverse and longitudinal polarization of incident irradiation, respectively, as shown in Ref. [65]. Otherwise, it is necessary to take into account quadrupole [65] or higher order interaction for an adequate description of the electromagnetic properties of such structures.

Although the dipole approximation serves as a well-known approach, extensively described in literature, in this section we provide a general formalism for the convenience of the Readers. Let us consider an LPC of  $N$  identical NPs whose centers are located at points  $x_n = (n-1)h$ , where  $h$  is the center-to-center distance, and  $n = 1, \dots, N$ . We consider LPCs located in a homogeneous environment with dielectric permittivity  $\varepsilon_h$ . Assume that the LPC is excited by an external monochromatic electric field  $\mathbf{E}_n^{\text{ext}} = \mathbf{E}^{\text{ext}}(x_n)$  (time dependence  $\exp(-i\omega t)$  is omitted in all expressions, here  $\omega$  is the frequency of the incident field). In this case, the dipole moments  $\mathbf{d}_n$

**Table 1**  
Temperature-dependent optical constants for TiN [70].

	23 °C	400 °C	800 °C
$\varepsilon_\infty$	7.86981	6.50246	4.87685
$\omega_p$ , rad/fs	11.21219	11.37931	11.47047
$\Gamma_D$ , rad/fs	0.39501	0.56213	0.80521
$\omega_{L,1}$ , rad/fs	9.86939	11.76819	15.9342
$\gamma_1$ , rad/fs	2.15736	1.80793	2.78026
$\omega_{0,1}$ , rad/fs	6.18342	6.47208	7.17094
$\omega_{L,2}$ , rad/fs	2.28396	4.03393	3.52391
$\gamma_2$ , rad/fs	1.32176	3.08411	2.76507
$\omega_{0,2}$ , rad/fs	3.06892	2.93219	2.79545

induced in each NP are coupled to each other and to the external field via the following coupled dipole equations:

$$\frac{1}{\alpha} \mathbf{d}_n - \sum_{m \neq n}^N \hat{G}_{nm} \mathbf{d}_m = \mathbf{E}_n^{\text{ext}}, \quad (1)$$

Here  $\alpha$  is the polarizability of the NP,  $\hat{G}_{nm}$  is the Green's tensor which describes the electric field at  $x_n$  point created by a point dipole located at the  $x_m$  point. Explicit expressions for the Green's function can be found elsewhere [15,16].

In this paper, we consider three different shapes of NPs: spheres, prolates and oblate spheroids. The quasistatic polarizability of NPs with these shapes is defined by the following expression:

$$\alpha_0 = \frac{4\pi}{V} \frac{\varepsilon_p - \varepsilon_h}{\varepsilon_h + L(\varepsilon_p - \varepsilon_h)}, \quad (2)$$

where  $V$  is the volume of the NP,  $\varepsilon_p$  is the dielectric permittivity of the NP material,  $L$  is a static depolarization factor [66].

For NPs with dimensions much smaller than the wavelength of the incident illumination, retardation effects should be taken into account [67,68]. Moreover, a so-called dynamic correction [69] to the polarizability of spheroidal NPs has to be introduced for an adequate description of its electromagnetic properties. Thus, the polarizability  $\alpha$  takes the form:

$$\alpha = \alpha_0 \left[ 1 - \frac{k^2}{l_E} D \alpha_0 - i \frac{2k^3}{3} \alpha_0 \right]^{-1}, \quad (3)$$

where  $\alpha_0$  is defined by Eq. (2),  $D$  is a dynamic geometrical factor [69],  $k = \sqrt{\varepsilon_h} \omega / c$  is the wave number,  $c$  is the speed of light in a vacuum,  $l_E$  is the length of the semiaxis of the NP along which the electric field is applied. Static  $L$  and dynamic  $D$  depolarization factors for prolate and oblate spheroids can be found with well-known expressions [66,69] which are not provided in this paper. For spherical NPs:  $L = 1/3$  and  $D = 1$ .

Finally, the TiN dielectric permittivity can be described by the Lorentz oscillator model [70]:

$$\varepsilon_p = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\Gamma_D \omega} + \sum_{j=1}^2 \frac{\omega_{L,j}^2}{\omega_{0,j}^2 - \omega^2 - i\gamma_j \omega}, \quad (4)$$

where  $\varepsilon_\infty$  describes high energy interband transitions outside the probed energy spectrum,  $\omega_p$  is the plasma frequency,  $\Gamma_D$  is the Drude relaxation constant,  $\omega_{L,j}$ ,  $\omega_{0,j}$ , and  $\gamma_j$  describe the Lorentz oscillator strength, energy, and damping, respectively. Temperature-dependent constants entering Eq. (4) are represented in Table 1.

### 2.2. Dispersion properties

Dispersion relations are one of the most important properties which quantify the ability of LPCs from metal NPs to support SPP propagation. There are various approaches to estimate dispersion

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