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Dielectric nanopatterned surfaces for subwavelength light localization and sensing applications

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In this paper we present a theoretical study of dielectric nanostructures capable for localizing light in subwavelength volumes. These are arrays of Si nanoparticles on top of reflecting substrates, which can be properly designed to sustain resonances that confine light outside the particle, near the surface, resulting in increased sensitivity of the resonance wavelength to the refractive index of the surrounding medium. A sensor based on this concept could be advantageous in applications where losses, typical for metallic plasmonic sensors, are unwanted.

1. Introduction

Subwavelength confinement of light in nanoparticle arrays is a very challenging topic and important for a plethora of applications such as light harvesting [1] high resolution microscopy [2], or even optical encoding [3]. Engineering surfaces that can confine light have attracted lot of attention over the last years, and a lot of effort has been devoted in the study of metallic [4–7], and dielectric [8,9] nanoparticle arrays on top of a substrate. In such structures, the nanoparticles in the array act as resonators for the electromagnetic (EM) field, and the interactions between them generate a very rich optical response. The main difference between metallic and dielectric nanoparticles is that the first are characterized by the particle-plasmon excitations which are collective oscillations of the EM field and the free electrons of the metal, that localize light near the surface of the particle, while, on the other hand, dielectric particles support the so called Mie resonances, localizing the field mainly inside them [10]. Structures that contain metallic nanoparticles are for this reason privileged in sensing applications, because the confinement of the EM field outside the surface of the particles leads to increased sensitivity of the plasmonic resonance frequency to the surrounding medium [11,12]. Unfortunately, there is an unavoidable loss of energy due to the Joule-heating effect on the metals. To overcome this problem, there have been proposals to replace metals in a wide range of applications [13–18]. In Ref. [19], strongly absorbing surfaces are designed with weakly absorbing dielectric materials. The concept is simple: a Si sphere array is placed on top of a Bragg stack that acts as a mirror, and a careful design of the geometry leads to resonant absorption. Following a similar concept, we can obtain the formation of a resonant state between the Bragg mirror and the periodic arrangement of Si scatterers, that minimizes reflectance and localizes the EM field in the surface of the Si particles, opening the way for all-dielectric sensors [20]. Similar guided mode resonance filters were proposed several years ago [21]. The optical response is simulated with our implementation of layer multiple scattering method [22,23], which is an efficient and exact electromagnetic solver. In all cases considered, dispersive materials are described using realistic optical constants tabulated in the literature [24, 25].

2. Results and discussion

We consider a square array of Si spheres on top of a Bragg multilayer as shown in Fig. 1. The sphere array has a lattice constant $a = 370$ nm, while the diameter of the Si spheres is $2r = 130$ nm. The Bragg multilayer consist of five TiO_2(50 nm)/SiO_2(100 nm) bilayers, supported by a semi-infinite TiO_2 substrate with refractive indices $n_{SiO_2} = 1.46$, $n_{TiO_2} = 2.50$. Between the array and the Bragg stack, a 135 nm thick SiO_2 spacer, interposes. The surrounding medium is water ($n_{env} = 1.33$). This geometry supports various resonant modes under normal incidence of light, which are shown in Fig. 2a. Without the sphere array, this surface would be an almost total reflector for light incident normally, in the spectral region under consideration (Bragg band gap). The presence of the periodic array allows the excitation of the waveguide slab modes [4], leading to a very rich optical spectrum with multiple resonances as shown in Fig. 2a. The Mie resonances of the Si particles are responsible for the drops found around 545 and 565 nm. While there are several slab modes of the multilayer stack that are weakly excited due to presence of the periodic array, and are responsible for the small sudden drops in reflectivity close to 491 and 504 nm. Moreover, there exist collective resonances due to the diffraction coupling [26–28] between the particles in the array, which depend on the lattice constant and periodicity that are outside the wavelength window considered here. The zero-reflectance, pointed out with arrow in Fig. 2a,

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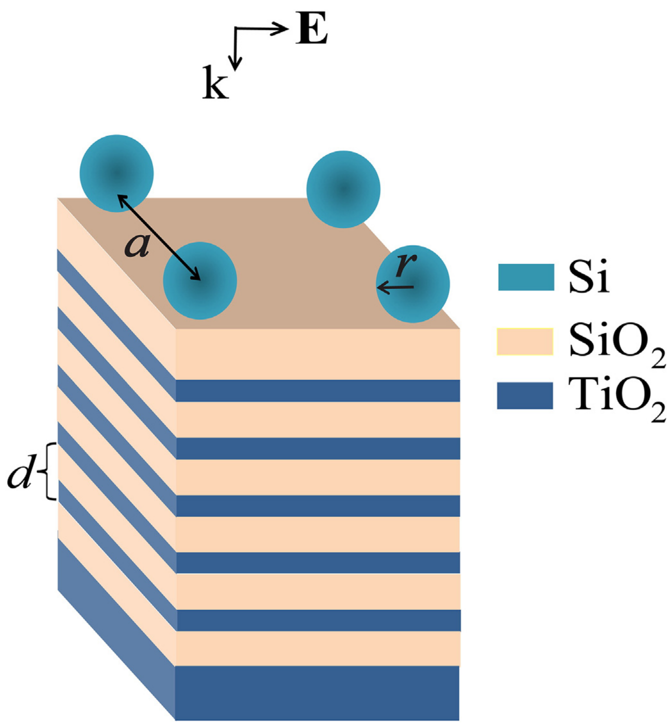

Fig. 1. Schematic of a square array (a = 370 nm) of Si spheres ($2r$ = 130 nm) on top of a Bragg multilayer consisting of five TiO_2(50nm)/SiO_2(100nm) bilayers (the thickness of each layer is given in the parenthesis). The structure is supported by a semi-infinite TiO_2 substrate, while the top side is water.

is a result of a guided mode resonance formed between the Bragg mirror and the high-refractive-index particle array [20]. As a result, the electric field is concentrated outside the Si particles. This can be seen by the corresponding field profile (Fig. 2b), where the field is mainly confined on the top surface of the Si sphere, and only a small amount penetrates inside the Bragg multilayer. By its nature, this resonance does not crucially depend on the particle's exact shape.

By changing slightly the refractive index of the surrounding medium, we observe a shift in the resonant wavelength (λ_{res}), depicted with the gray line in Fig. 2a. As expected, the field concentration on the surface of Si particles, results in strongly localized EM field, and increased sensitivity of the resonance position upon variations of the refractive index of the surrounding medium [12]. Our calculations show that similar structures with a rectangular lattice or arrays of cylinders have similar modes in their spectra with strong field enhancement, comparable to metallic nanoparticle structures. On the contrary, the slab modes that guide light mostly inside the inner stack layers, or particle-Mie resonances that confine light inside the spheres, do not vary with small changes in the refractive index of the surrounding medium n_{env}.

In Fig. 3 we see the linear dependence of the resonance wavelength (λ_{res}) versus the refractive index of the surrounding environment (n_{env}). The slope of this line is termed as sensitivity ($S = \Delta\lambda/\Delta n$), which in this case is equal to 200 nm/RIU (Refractive Index Unit). Another quantity used to describe the sensing capability of a sensor, taking into account the full width at half maximum (FWHM) of the resonance, is the Figure Of Merit (FOM), which is defined as FOM = S / FWHM. In our case, FWHM = 3.3 nm, which gives a FOM as high as 61. These quantities indicate that this, all dielectric sensor, is very competitive to plasmonic sensors [29].

As already discussed, the role of the reflecting substrate is essential for the formation of the resonant state under consideration, and we can assume that a metallic film could replace the Bragg mirror. In Fig. 4a we see the schematic of a structure similar to that of Fig. 1, but the Bragg mirror is substituted by a Ag film separated from the Si sphere array by a SiO_2 spacer of thickness 110nm. The choice of the metal is not of particular interest, as long as it plays the role of a reflector, and no plasmonic excitation is required. In Fig. 4b we see with black line the reflectivity, under normal illumination, in water (n_{env} = 1.33), while with gray line we assume a glucose solution with n_{env} = 1.34. The slight change in n_{env} causes a shift in the resonance close to 520 nm, while the other one, close to 545 nm, remains unchanged. This behavior is clarified if we consider the nature of each resonance. Fig. 4c shows the field profile for the resonances pointed out with arrow (λ_{res} = 520 nm), while the other resonance (545 nm) is a particle (Mie) resonance, almost confined inside the particle. As already discussed, λ_{res} is sensitive to changes of the environment medium (n_{env}). This dependence is shown in Fig. 4d, while the slope is somewhat higher than that of Fig. 3, obtaining a sensitivity S = 265 nm/RIU. The corresponding FOM = 88, indicates a very high sensoric capability of the structure. In this way, very thin, low-loss, nanopatterned surfaces can be designed. By replacing Si spheres with cylinders with the same radius = 65 nm, and height = 130 nm, the resonance under consideration is shifted close to 540 nm, while the calculated sensitivity is S = 206 nm/RIU. Of course further optimization could tune the position of the resonance and increase the sensitivity of the cylinders.

For the square lattice of Fig. 4a, under normal incidence of light, polarizations along the x and y axis have identical spectrum. For a rectangular lattice though, with a_x = 370 nm and a_y = 380 nm the

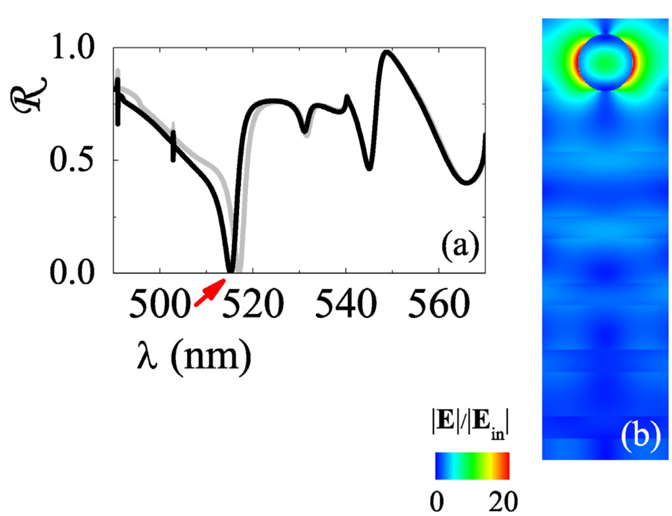

Fig. 2. (a) Reflectivity spectrum for the structure of Fig. 1 under normal incidence of light, inside water (black line) with index of refraction n_{env} = 1.33, and inside a glucose solution with n_{env} = 1.34 (gray line). (b) Field profile for normally incident light at the resonant wavelength pointed out with arrow in (a).

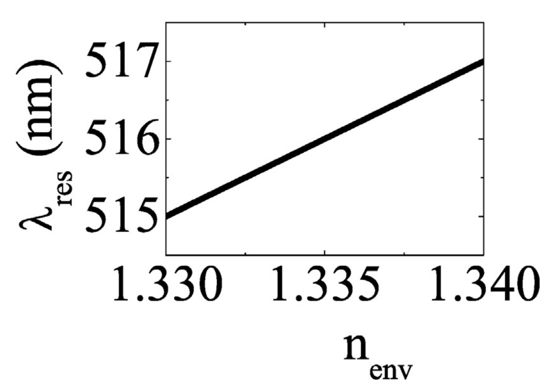

Fig. 3. Shift of the resonant wavelength (λ_{res}), pointed out with arrow in Fig. 2(a), to changes of the refractive index of the surrounding environment medium (n_{env}). The slope is equal to the sensitivity S.