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Rectangular-cavity resonances enhanced absorption in metallic-nanoshelled 2D rod arrays and 3D photonic crystals

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Abstract. A metallic-nanoshelled rectangular dielectric rod is proposed to flexibly enhance and tune the structural absorption. Due to the ultra-small thickness of the metallic-nanoshells, electromagnetic (EM) waves can penetrate into the rods and rectangular cavity resonances can be formed. At the cavity resonances, the strong EM wave–matter interaction results in an enhancement in the structural absorption by more than one order of magnitude. By stacking the nanoshelled rods, a three-dimensional (3D) woodpile photonic crystal with both the rectangular cavity resonance and the photonic band gap effect is realized. As a result, the structural absorption of the nanoshelled 3D photonic crystal is significantly enhanced to ∼99.99% at the resonant wavelength.

Metallic nanostructures [1], ranging from metallic nanoslits [2, 3] to three-dimensional (3D) metallic photonic crystals (MPCs) [4, 5], have been extensively studied for their intriguing properties such as enhanced transmission [2], resonant absorption [1], [6–8] and strong field enhancement [9]. Most of the unique features of the metallic nanostructures are induced by either the collective plasmonic effects [6, 9, 10] or the optical cavity resonances [3, 11]. For example, metallic spherical nanoshells [1, 6] have been well investigated for their strong

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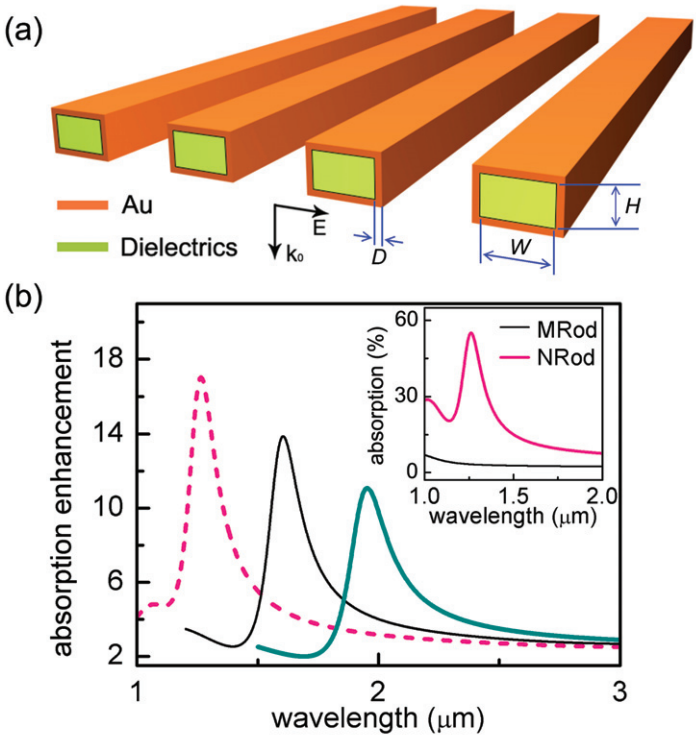

Figure 1. (a) Schematic diagram of an array of rectangular NRods consisting of dielectric cores (with height H, width W, refractive index n and infinite length) and gold nanoshells (with a thickness D). The NRods are periodically separated by a distance a. (b) Absorption enhancement of NRods compared with pure MRods under $H = 300$ nm (dashed line), 400 nm (solid thin line) and 500 nm (solid thick line). Other simulation parameters: $W = 400$ nm, $D = 15$ nm, $a = 800$ nm and $n = 1.56$. Inset: absorption spectra of an MRod and an NRod with the same geometrical parameters.

absorption caused by localized plasmon modes [10]. However, one problem of those ultra-small nanoparticles is that the field enhancement area is concentrated close to the surface of the nanoshells (<10 nm), where the fluorescence quenching effect occurs and limits the applications to plasmon-enhanced fluorescence [11]. On the other hand, by utilizing the optical cavity modes, field enhancement of a large volume [11] and the strong structural absorption have been realized in large-scale nanoshells [11] and 3D MPCs [5, 12, 13]. However, the absorption enhancement and tunability are less appealing and the structures are difficult to integrate into solid-state nano-devices.

Here we propose to enhance and tune the structural absorption by employing a rectangular cavity resonance in a nanoshelled rod (NRod), which consists of a dielectric rectangular rod coated by a gold nanoshell, as shown in figure 1(a). Compared with the 'external' cavity formed within the dielectric spacer between the metallic rods of the 3D MPCs [5, 12, 13], the rectangular cavity within our NRods is an optical 'internal' cavity, which is much simpler in geometry and more flexible in tunability. Moreover, our NRods facilitate the resonances of higher-order cavity modes and the peak absorption can be enhanced by more than one order of magnitude compared with that of pure metallic rods (MRods). More importantly, by

integrating the NRods into a 3D woodpile photonic crystal, the structural absorption at the resonant wavelength is further enhanced to ∼99.99%, which is not applicable to conventional 3D MPCs [14].

Figure 1(a) shows the schematic diagram of our simulations. Linearly polarized light is incident on an array of parallel NRods from the top. The light polarization is perpendicular to the NRods, which have a width of W, a height of H and a shell thickness of D. The key factor to introduce the optical internal cavity is the shell thickness. In our NRods, the small thickness of the metallic nanoshells ($D < 50$ nm) allows the penetration of the electromagnetic (EM) waves into the rods. Therefore, with the cavity boundaries naturally provided by the rectangular nanoshells, certain resonances can be formed. To confirm the existence of the cavity resonances, the transmission, reflection and absorption properties of the NRods (and all the other structures in this paper) are calculated in three dimensions with the frequency domain solver of a CST software package. In the numerical calculations, we use the plane wave excitation performed with a Gaussian pulse. To meet the convergence criterion, an adaptive tetrahedral mesh refinement system is activated for the finite element meshing during the running of the frequency domain solver. In such a system, after the initial meshing of the first pass, multiple passes (with improved meshing) will be run until the sufficient scattering parameters convergence criterion is satisfied. For simplicity, we consider the nanoshell material as gold with optical properties described by the Drude model with epsilon infinity $\varepsilon_\infty = 1$, plasma frequency $f_p = 2172$ THz and relaxation time $\tau = 27.4$ fs [12].

As shown in the inset of figure 1(b), there is a big difference in the absorption spectra between an NRod and an MRod (the MRod has the same geometrical parameters as the NRod except that the dielectric part of the NRod is replaced by pure gold). At certain resonant wavelengths (λ_c), the absorption of the NRod is enhanced by more than ten times compared with that of the MRod, which results from the strong EM wave–matter interaction at the cavity resonances. Moreover, this enhancement in absorption is extremely sensitive to the structural parameters. Figure 1(b) shows that λ_c shifts towards shorter wavelengths and the absorption enhancement grows as the rod height is decreased. The linear relationship between λ_c and the rod height is further demonstrated in figure 2(a), where the rod width is kept unchanged. We also confirm that λ_c changes linearly with the refractive index of the embedded dielectrics inside the NRod (not shown). These linear relationships are consistent with the formula of a rectangular cavity resonance, i.e. $m\lambda_c = 2nH + \Delta\varphi(\lambda_c)$ [15][4], where m is the order of the resonance and $\Delta\varphi(\lambda_c)$ is the extra phase shift at wavelength λ_c induced by the metallic nanoshells. This formula is somewhat like the model of a planar Fabry–Perot (FP) cavity. In fact, our simulations show that when the rod width is simply increased, the value of λ_c decreases correspondingly and finally approaches the resonant wavelength of an FP cavity that has the same height H but an infinite width, as shown in figure 2(b). This indicates that the left side and right side metallic shells of the rod (separated by the dielectric rod width W) provide an additional confinement of

[4] For a dielectric rectangular cavity with a length of L_x, a width of L_y and a height of L_z, the cavity resonant frequency satisfies $f_{lpm} = (c/2n)\sqrt{(l/L_x)^2 + (p/L_y)^2 + (m/L_z)^2}$, where n is the refractive index and the three subscripts $\{lpm\}$ designate a TE standing wave pattern in the cavity. In the case of $p = 0$ and $L_x = \infty$, the resonant wavelength becomes $\lambda = 2nL_z/m$. When the dielectric rectangular cavity is coated with a metallic nanoshell, an additional phase shift is induced. Therefore, the cavity resonant wavelength λ_c in NRods with height H can be written as $m\lambda_c = 2nH + \Delta\varphi(\lambda_c)$, where the wavelength-dependent $\Delta\varphi$ is determined by the thickness of the nanoshells as well as the width of the NRods.

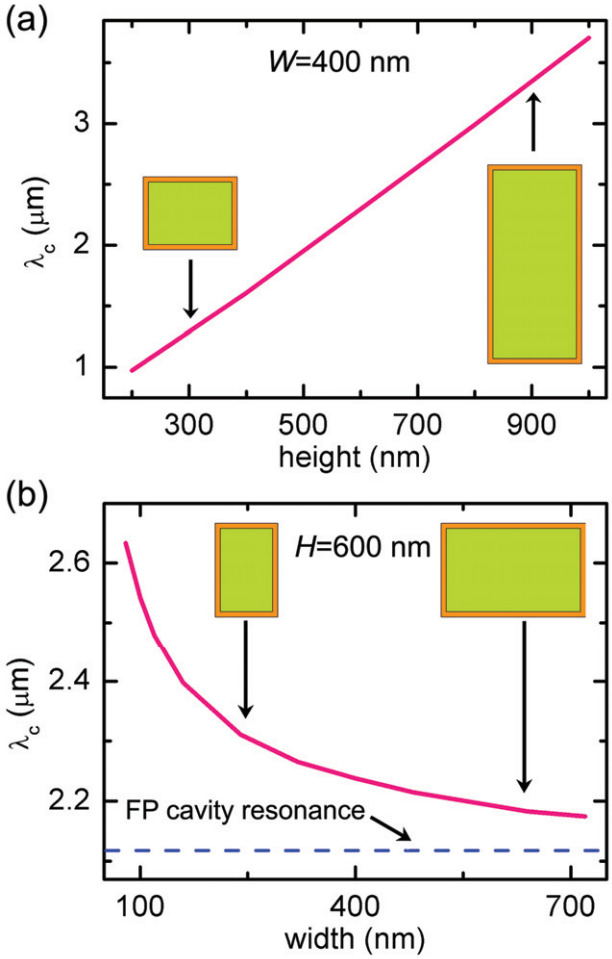

Figure 2. Resonant wavelength (λ_c) as a function of the rod height (a) and rod width (b). The relative geometries of the cross-sections of the rods are depicted in the insets. It is shown that when the rod width is simply increased, λ_c approaches the resonant wavelength of an FP cavity with $H = 600\,\text{nm}$ and $W = \infty$.

the penetrated EM waves and induce a positive $\Delta\varphi$. Therefore, simply changing the rod height, the rod width or the dielectric refractive index of the NRods offers great flexibility to tune the enhanced absorption channel.

In addition, based on the cavity resonance formula, it is expected that multiple orders of resonance can be formed inside the NRods. Our simulation, as illustrated in figure 3 (left), indeed shows multiple enhanced absorption peaks, where the simulated E-field distributions inside the rod unambiguously confirm the standing cavity modes in the propagation direction (as shown in figure 3 (center and right)). It should be mentioned that the thickness of the metallic shell also influences the position of λ_c (through mediating the value of $\Delta\varphi$, not shown). However, as mentioned earlier, the shell thickness is the key factor to induce the enhanced absorption and its value should be always less than 50 nm. If it is too large, no light can penetrate into the NRod and no cavity resonance can be coupled. For example, when $D > 60\,\text{nm}$, the NRod acts exactly as an MRod and the corresponding enhancement factor drops close to 1.

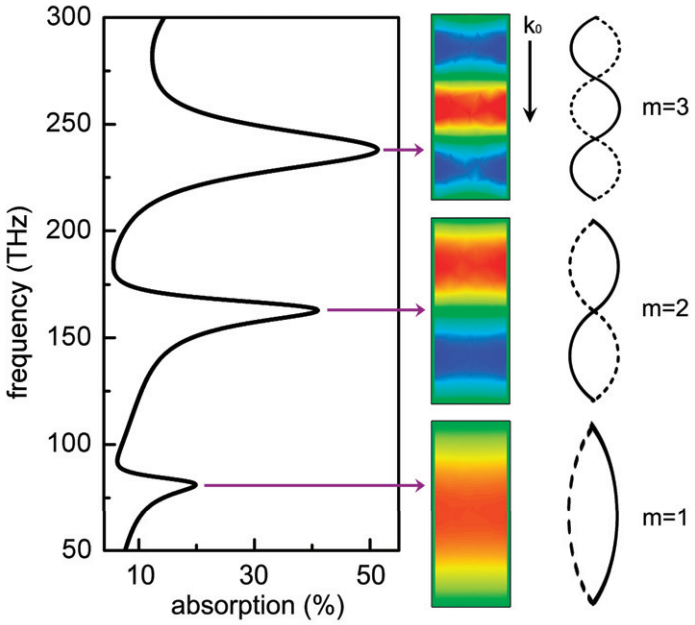

Figure 3. Absorption spectrum (left) and internal E-field distribution at the resonant frequencies (center) of NRods. (Right) Schematic diagram of the cavity resonances at corresponding orders of the resonances. Simulation parameters: $W = 400\,\text{nm}$, $H = 1000\,\text{nm}$, $D = 15\,\text{nm}$, $a = 1000\,\text{nm}$ and $n = 1.56$.

One straightforward application of the NRods is the utilization of the NRods as building blocks to stack 3D nanoshelled photonic crystals (NPCs), as shown in the schematic of diagram 4(a). In such a scheme, the rectangular cavity of NRods could offer 3D NPCs novel properties beyond the conventional photonic band gap effects. As shown in the inset of figure 4(b), due to the cavity resonance of the NRods, a sharp 'dip' appears in the band edge region of a four-layer 3D NPC, where the slow light effect takes place [14]. As a result of the combination (of the cavity resonance and the band edge effect [14]), the structural absorption of the 3D NPC is increased to ∼99.99% (figure 4(b)), which is significantly enhanced compared with that of a 2D NRod array and a 1D thin film. Moreover, this nearly 100% absorption in the 3D NPC is much higher than the band-edge-enhanced absorption of a 3D gold MPC (∼49% in our calculation with structural geometrical parameters the same as those of the NPC) and that of the published 3D tungsten MPCs (<60%) [14].

In conclusion, we have theoretically demonstrated an NRod to flexibly enhance and tune the structural absorption. By employing an ultra-thin metallic nanoshell, rectangular cavity resonances with multiple orders can be formed, which enhance the absorption of the NRod by more than one order of magnitude. Furthermore, by stacking the NRods into 3D, a nearly 100% absorption can be achieved in a woodpile NPC. The investigated absorption enhancement and tunability, as well as the higher-order mode excitation, provide the feasibility to explore NRods as a candidate for potential photonic devices such as nanoscale sensors, efficient radiation sources and solar cell systems [8]. Experimental realization of the NRods and NPCs could be through coating the easy-to-fabricate dielectric structures with metallic nanoshells by employing chemical approaches such as the chemical vapor deposition method [16] or the electroless deposition method [17].

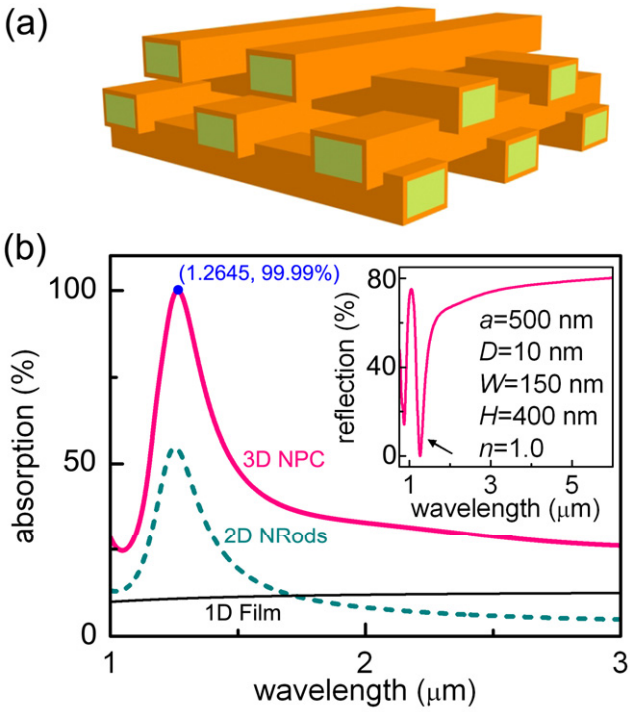

Figure 4. (a) Schematic diagram of a four-layer 3D photonic crystal formed by stacking 2D NRods (figure 1(a)) into a woodpile geometry. The adjacent layers are rotated by 90° and separated by a distance H. Between every other layer, the NRods are shifted relative to each other by $a/2$. In following simulations, the incident light is linearly polarized perpendicular to the first-layer rods. For simplicity, the rod length in simulations is infinite in each layer. (b) Absorption spectra of a 1D film (with thickness D), 2D NRods and a 3D NPC. Inset: calculated reflection spectrum of the 3D NPC in 4(b). The arrow indicates a rectangular-cavity-resonance-induced dip near the band edge region of the NPC. Calculation parameters are shown in the inset, which are chosen to match the optical cavity resonance with the photonic band edge.

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