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Inverse design of dielectric nanostructures for optical trapping

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ABSTRACT

Optical trapping in nanostructures has usually been achieved utilizing the strong field gradients of plasmonics resonances. However, given the inherent optical losses in metals to heat dissipation, their use can prove detrimental to biological trapping settings and can affect other trapping properties. Dielectric nanostructures do not suffer these intrinsic losses, but it remains challenging to design dielectric structures with strong field gradients. In this work, we use inverse design by topology optimization to design a dielectric nanostructure that confines light to trap nanoparticles in air. The obtained trapping potential is deep enough – with a trapping depth below -10 k_BT – to overcome thermal fluctuations.

Keywords: Inverse design, topology optimization, nanophotonics, optical trapping, dielectrics, near-field optics

1. INTRODUCTION

In recent years, the field of nanophotonics and nano-optics has gained significant attention thanks to advancements in design and fabrication techniques, which have enabled increased and novel functionalities of optical and photonic components. More particularly, the development of inverse design has facilitated the design of complex devices to achieve desired functionalities. Inverse design can explore design parameter spaces with many design variables to optimize target Figures of Merit (FOM), going beyond traditional trial-and-error based design principles. One of main methods in inverse design is topology optimization (TO), a gradient-based design optimization method widely used in the design of optical applications to minimize (maximize) a target FOM.[1] This optimization method is widely used in the design of optical applications, and has recently been applied to optimize the geometry of plasmonic nanostructures for optical trapping applications.[2] In optical trapping applications, the strong field gradients associated with plasmonic resonances can be utilized to achieve stable trapping of nanoscopic particles. However, metallic structures are lossy at optical frequencies, which can potentially make the trap heat up, resulting in adverse effects for the trapping environment and the trapped species.[3] Thus, near-lossless dielectric nanostructures based on strong field confinement mechanisms have been proposed to achieve stable trapping of nanometer-sized particles.[4] In our previous work[5] we used TO to inverse design near-lossless dielectric devices for omnidirectional gradient force optical trapping. In this work, we further study the validity of the dipole approximation for the inverse designed cavity presented in,[5] and show its robustness to different particle choices.

2. RESULTS

For spherical particles with a radius (R_{sph}) much smaller than the wavelength of light (λ), $R \ll \lambda$, we may apply the dipole approximation. In this approximation, the trapping potential (U) seen by a dipole-like particle can be described as,[6]

$$U(\mathbf{r}) = -\frac{\alpha_{\text{R}}}{4}\left[\mathbf{E}^*(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r})\right], \tag{1}$$

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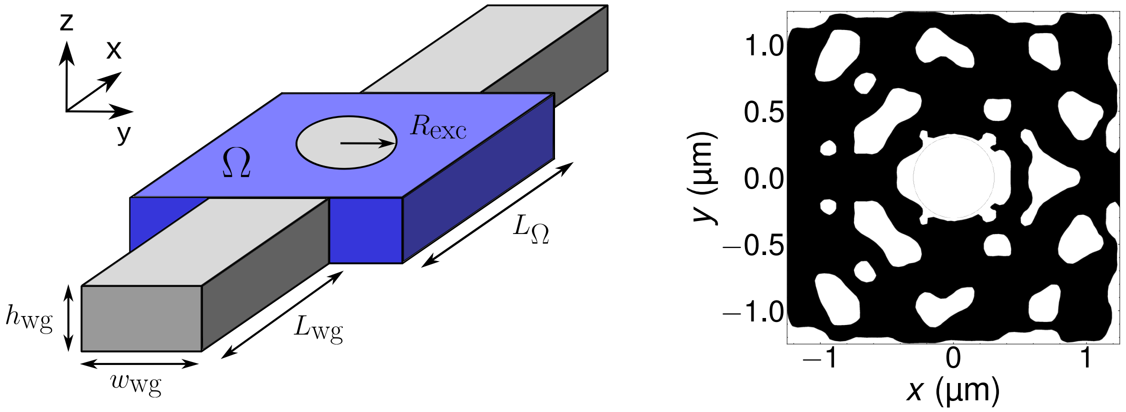
where $\mathbf{r}$ denotes the spatial coordinates, α_R denotes the real part of particle's polarizability, and $\mathbf{E}(\mathbf{r})$ denotes the complex electric field. As detailed in,[5] to find a device that supports an omnidirectional trapping potential in the dipole approximation picture, we minimize the difference of the electric field distribution in an optical cavity with respect to a reference three-dimensional Gaussian field. The electromagnetic simulation of the optical cavity system is performed in the domain in Figure 1a, where a silicon waveguide (gray), with a refractive index $n_{\mathrm{Si}} = 3.48$, width $w_{\mathrm{wg}} = 275$ nm and height $h_{\mathrm{wg}} = 400$ nm, is excited with the fundamental mode. The waveguide transmits the mode to the square design region Ω (in blue), with length $L_\Omega = 2.5$ µm and a cylindrical exclusion region with a radius $R_{\mathrm{exc}} = 300$ nm. The material in exclusion region is fixed to air, allowing it to act as the central cavity region. The remaining material distribution in the design domain is optimized to obtain the Gaussian-like electric field distribution that results in an omnidirectional trapping potential inside the exclusion region. For an excitation in the near infrared with a wavelength $\lambda = 1550$ nm, the optimization yields the two-dimensional design projection in Figure 1b, where white denotes air and black silicon. The optimized design is then extruded in the z direction. The geometry of this device is able to achieve an omnidirectional trapping potential with a depth below -10 $k_B T$ for an excitation with an input power of $P_{\mathrm{in}} = 15$ mW, and a spherical particle with a radius $R_{\mathrm{sph}} = 15$ nm and refractive index $n_{\mathrm{sph}} = 2$. The design is the result of a combination of couplers and mirrors that help, guide, confine, and shape the field in the cavity. Further details about the trapping potential and trapping forces for the inverse designed cavity can be found in our recent publication.[5]

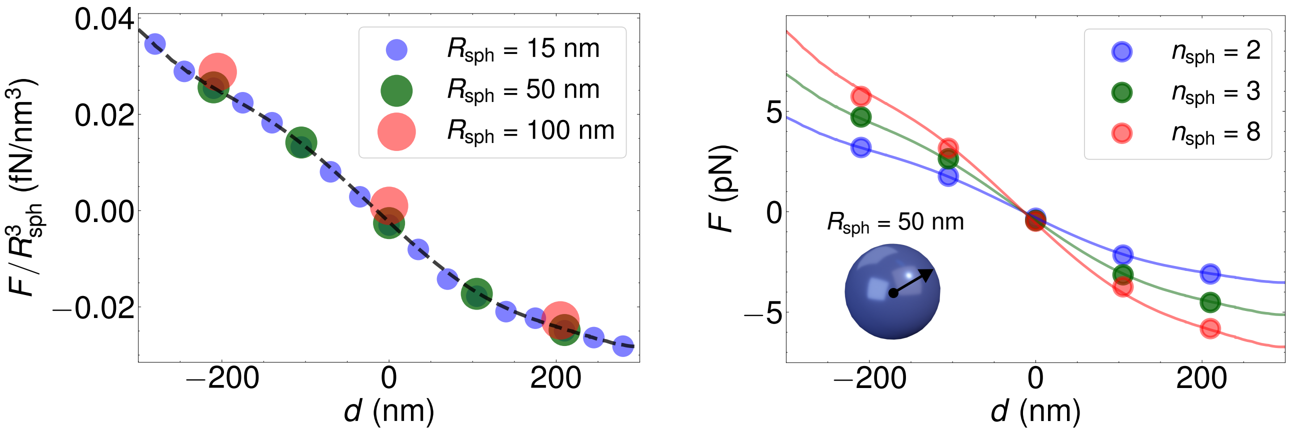


(a) Sketch of the simulation and design (Ω) domains.

(b) Optimized design for the design domain (Ω).

Figure 1: Simulation setup and optimized design. The optimized design is projected onto the design domain Ω, which is extruded in the z axis.

In the results presented in,[5] it is shown that the dipole approximation holds for spherical particles with a radius of $R_{\mathrm{sph}} = 15$ nm and refractive index $n_{\mathrm{sph}} = 2$. Here, we test the limits of the dipole approximation by changing the size and material of the spherical particle. Following Equation 1, the inverse designed device is expected to work for particles much smaller than the wavelength of light (λ), and sufficiently small index contrast with respect to the background medium (air). Thus, in Figure 2 we investigate the validity of the dipole approximation by studying the effects of varying the particle size and the refractive index. First, in Figure 2a, we study the effects of placing spherical particles with a refractive index $n_{\mathrm{sph}} = 2$ and different radii, at different positions along the x axis in the cavity region shown in Figure 1b. Then, we compare the optical force calculated through the Maxwell stress tensor (MST) calculation[6] (data points) to the empty-cavity dipole approximation picture (dashed line), by normalizing the force by particle volume. We observe that for particles with radii $R_{\mathrm{sph}} \in \{15\ \mathrm{nm}, 50\ \mathrm{nm}\}$ much smaller than the wavelength ($R_{\mathrm{sph}} \ll \lambda$), the dipole approximation holds. However, for particles with radii $R_{\mathrm{sph}} = 100\ \mathrm{nm}\,(\sim 0.06\lambda)$ comparable to wavelength, the MST force calculation starts to deviate from the dipole approximation. We expect this effect to get accentuated for larger sphere radii. In Figure 2b we study the effect of varying the refractive index for the spherical particle with a radius $R = 50$ nm, by comparing the empty-cavity dipole approximation (lines) and the MST calculation (data points). The results show that for low refractive index values $n_{\mathrm{sph}} \in \{2, 3\}$, the dipole approximation and the MST calculation agree well, as the data points lie on top of the curves, but as we increase the refractive index to larger values $n_{\text{sph}} = 8$, some data points in the MST calculation start to deviate from the dipole approximation picture. Similar to Figure 2a we expect the two calculations to further deviate for larger values of the refractive index of the particle.



(a) Normalized force for different particle radii (R_{sph}). (b) Force for different particle refractive indexes (n_{sph}).

Figure 2: Testing the validity of the dipole approximation by comparing the empty-cavity picture (lines) with the MST calculation (data points) for the inverse designed cavity. In (a) we set the refractive index of the particle to $n_{\text{sph}} = 2$ while we vary the radius and compare the force normalized to particle volume. In (b) we compare the force while keeping the radius at $R_{\text{sph}} = 50$ nm and varying the refractive index.

The discrepancies between the dipole approximation and the MST calculation for larger particle radii and refractive indexes are potentially caused by the local field changes induced by the changes in the refractive index, which cannot be captured in the empty-cavity picture. Moreover, these refractive index changes can cause that the cavity mode changes resonance frequency, effectively modifying the response of the cavity for the excitation wavelength. Nevertheless, the results in Figure 2 show the robustness of the omnidirectionally trapping inverse designed cavity, through the agreement of optical force calculations for the dipole approximation picture utilized in the TO framework and the MST calculations, for particles with radii smaller than $R_{\text{sph}} \leq 100$ nm and refractive indexes smaller than $n_{\text{sph}} \leq 8$. More results related to the optimized cavity[5] will be presented at the SPIE Optics + Photonics 2024 conference.

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