Design of nanoslotted photonic crystal waveguide cavities for single nanoparticle trapping and detection

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We design and numerically simulate an on-chip photonic device that integrates both optical manipulation and detection functionalities for a single nanoparticle or macromolecule. A unique combination of a photonic crystal waveguide cavity and a nanoslot structure leads to a ~1300 times enhancement of the optical gradient trapping force compared with a conventional waveguide trapping device. Numerical simulations indicate that the designed device is capable of stably trapping a single nanoparticle inside the nanoslot cavity, and thus provides an ideal platform for single particle detection and analysis using cavity-enhanced spectroscopic technologies. © 2009 Optical Society of America

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Optical trapping is ideally suited for manipulating living cells, virus particles, and even DNA molecules as a contactless and nondestructive tool. To date, most research on optical micromanipulation has focused on laser beam free-space trapping [1]. However, it has been demonstrated that the optical force arising from an evanescent field can also be used to trap particles at the interface between two media. The use of an integrated planar waveguide for on-chip particle manipulation [2–4] has the advantage of dramatically decreasing the system footprint, possibly enabling massively parallel handling of particles. However, waveguide optical trapping often requires large input power owing to the low evanescent field intensity, a major roadblock toward its applications. The gradient optical force decreases fast when scaling down the particle size, as it varies with the cube of the radius. Therefore, trapping particles smaller than 100 nm in diameter is difficult using either free-space optics or evanescent trapping configurations, as high laser powers are needed. In addition, that the focused spot of laser beam is comparatively large limits our ability to position trapped particles precisely.

In this Letter, we propose and numerically verify a near-field trapping design utilizing nanoslotted waveguide photonic crystal (PhC) cavities [5]. Resonant enhancement of optical fields effectively reduces the power required for stable trapping; trapping by a standing wave inside the resonator also eliminates the traveling-wave scattering forces [6,7]. Further, introduction of a nanoslot structure in the PhC cavity takes advantage of the large electric-field discontinuities at dielectric boundaries and results in significant field concentration and enhancement [8]. We show that such a cavity-based trapping device is capable of single nanoparticle trapping, and that the nanoslot cavity device setting is also ideal for single nanoparticle detection, given the strong cavity-enhancement effect and the ultrasmall interrogation volume.

The proposed waveguide PhC structure consists of a 1D hole array in a silicon-on-insulator (SOI) photonic wire waveguide, as shown in Fig. 1. The refractive indices of the silicon and silicon dioxide are taken as 3.46 and 1.45, respectively. The hole array period, a, is 420 nm and the radius of the holes is 100 nm. A PhC cavity with a length $a_d = 930$ nm is formed between two linear hole arrays. A third-order resonant mode confined in the cavity, near a wavelength of 1.55 μm, exhibits an enhanced field intensity, which peaks in the center of the cavity. Tapered boundary regions with locally varied hole spacing are used to reduce the impedance mismatch between the Bloch mode and the waveguide mode. The refractive index of the Bloch mode can be calculated from $n = \lambda/2a$, and is 1.84 for our design. The refractive index of the waveguide mode is found to be 2.26 using numerical simulations with a mode solver. In our simulations, each tapered region consists of four holes with radii of 96, 92, 88, and 84 nm. The spacing between the holes is also adjusted locally to maintain a constant r/a ratio in the tapered regions. Compared with a conventional PhC cavity design with an abrupt disruption of the periodicity, such a tapered cavity design minimizes out-of-plane radiative loss of the cavity mode and improves the cavity Q factor from 130 to 1850 (Fig. 2) [9].

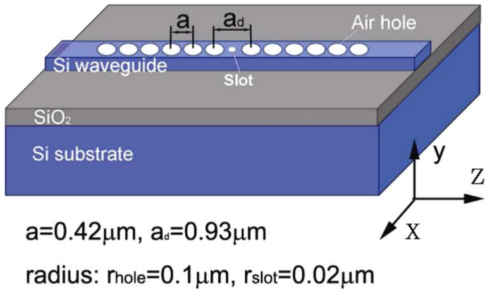

Fig. 1. (Color online) Schematic illustration of a nanoslot waveguide photonic crystal cavity.

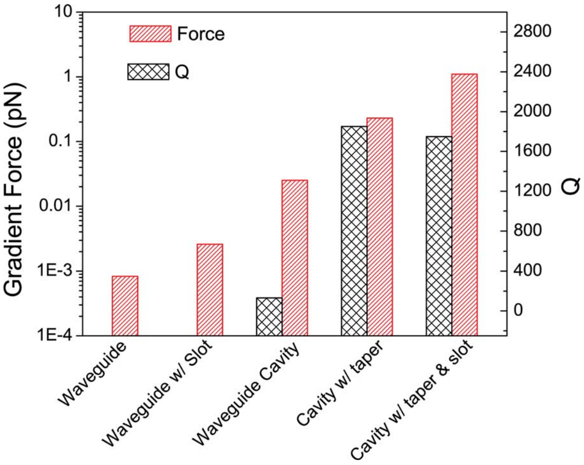

Fig. 2. (Color online) Cavity Q factor and corresponding optical gradient force along the y axis in a waveguide, a waveguide PhC cavity, a waveguide PhC cavity with a taper only, and a waveguide PhC cavity with both a taper and a nanoslot.

To further increase the field enhancement, beyond that provided by resonant cavity enhancement, we incorporate a nanoslot structure to leverage the large-field discontinuities at high-index-contrast dielectric boundaries. In our simulation, a nanoslot is formed by introducing a 20 nm radius hole in the center of the cavity, as schematically illustrated in Fig. 1. Figure 3 plots the E_x field component on an x–y plane cross section through the nanoslot. It is clear that the nanoslot contributes to high optical field localization. As we discuss further in this Letter, this subwavelength confinement of high field intensity should make possible optical trapping and detection of single nanoparticles with sizes down to a few tens of nanometers.

We perform 3D finite-difference time-domain simulations to determine the field distribution in this structure when the nanoparticle position is varied. The power input to the waveguide is taken as 5 mW. Numerical simulations predict that 18% of the incident power is transmitted through the device. A polystyrene particle (refractive index $n=1.59$) with a radius of 10 nm is used in our simulations. It is assumed that the medium above the device is water ($n=1.33$). The gradient force along the y axis is calculated by integrating the Maxwell stress tensor over the particle surface. From Fig. 2, it can be seen that introducing a nanoslot into the waveguide enhances the gradient force by ~3 times. The optical gradient force for the PhC cavity structure is ~30 times larger than that of the waveguide-only device. A further ninefold enhancement of trapping force is obtained by incorporating the tapered structure due to the increased cavity Q factor. The introduction of the nanoslot also leads to a further fivefold enhancement of the trapping force by confining the high field intensity in the nanoslot. The decrease of the Q factor from 1850 to 1750 arises from the cavity mode experiencing increased scattering loss due to the nanoslot. In these simulations, the particle is located on the surface of the waveguide at the entrance to the nanoslot (Fig. 1). This position is also employed for the simulations not incorporating the nanoslot or cavity. At this position, the field gradient and optical force have their maximal values. The particle position is denoted "above slot" in the inset of Fig. 5.

The gradient forces for a particle at different positions in the nanoslot are also simulated using the Maxwell stress tensor approach. Figure 4 shows the potential profile along the y direction, calculated by integrating the trapping force along the y axis. Here the zero potential is defined as when the particle is at an infinite distance from the nanoslot. In practice, the zero potential point is taken as 2 μm from the waveguide surface, since the exponential decay of the fields in the y direction means that there is negligible error in assuming this. The dramatic enhancement of optical force leads to a trapping potential >10 kT even for particles with sizes down to 10 nm (comparable with that of a single protein or DNA molecule), which should allow the stable trapping of a single macromolecule inside the nanoslot cavity despite the presence of Brownian motion. Optical damage to the trapped molecule is estimated from the field intensity obtained from the simulation. The field intensity at the center of the nanoslot is 2.4 TJ/($\mathrm{m}^2\cdot\mathrm{s}$), found us-

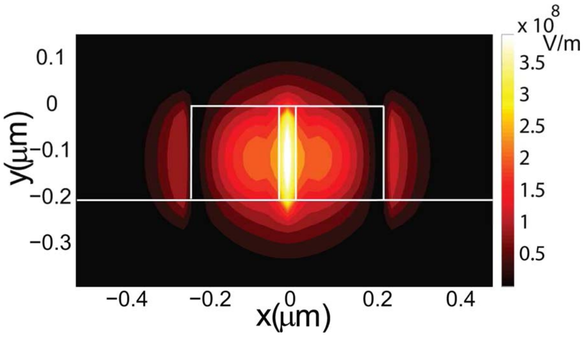

Fig. 3. (Color online) E_x field distribution in the plane $z=0$, showing strong field confinement in the nanoslot.

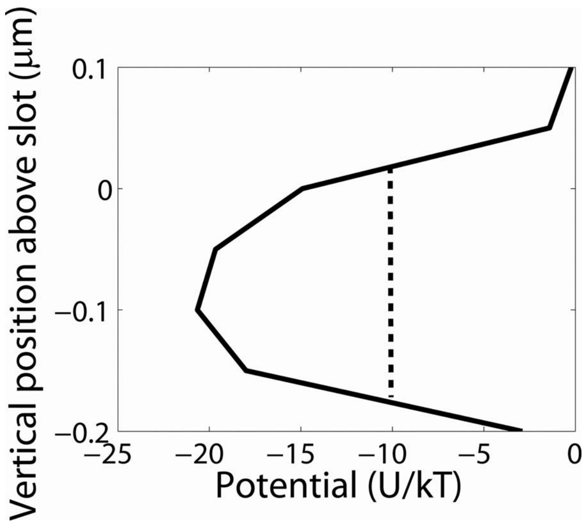

Fig. 4. Trapping potential well along the y axis normalized to kT. The dashed line indicates the criterion of stable trapping (trapping potential >10 kT). The potential is calculated by integrating the work done by the optical force on a nanoparticle with a refractive index of 1.59 and a radius of 10 nm.

ing $I=c\cdot(\varepsilon\cdot|E|^2+\mu\cdot|H|^2)/2$. A dose of 204 TJ/m^2 is required for detectable damage in DNA according to a previous study [10]. Therefore, DNA could be trapped in the center for about 3 s before optical damage becomes significant. In addition, if we take into account the Brownian motion of the trapped molecule, the molecule effectually samples the field distribution inside the nanoslot, resulting in reduced optical damage compared with the estimation based on the peak field value in the slot center.

We also quantitatively evaluate the field perturbation and the resulting resonant modification due to trapping of a single particle/molecule inside the nanoslot cavity for *in-situ* single particle detection [11]. Our results indicate that the optical trapping cavity also serves as a highly sensitive particle detection device suitable for rapid manipulation and analysis of particles/molecules. The resonance peak shifts 0.5 nm after trapping of a single nanoparticle in the center of slot, as shown in Fig. 5. The majority of the optical mode energy is confined to a small region, meaning that even a small modification of the refractive index profile inside the cavity can lead to a large change of the cavity resonance frequency.

In summary, we have designed a waveguide photonic crystal cavity structure for nanoparticle manipulation and detection. Numerical simulations indicate that the device is capable of trapping nanoparticles with radii down to 10 nm with a low input power of 5 mW. Tapered boundary regions and a nanoslot contribute to strong light confinement in a subwavelength spot (~40 nm in our simulation). The high field intensity in the nanoslot enhances the optical force ~1300 times compared with a conventional channel waveguide. Importantly, the cavity trapping device also offers an ideal setting for characterization of the trapped particle/molecule using cavity-enhanced optical techniques. We foresee that this device can potentially become a versatile platform technology for single-molecule, virus, or nanoparticle manipulation; detection; and other lab-on-a-chip applications [12].

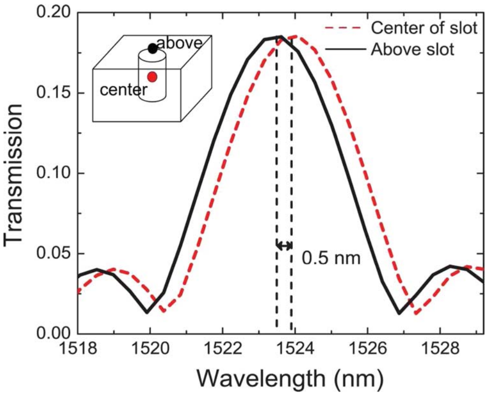

Fig. 5. (Color online) Transmission spectra with a nanoparticle centered above the nanoslot. The high field concentration inside the nanoslot leads to the large 0.5 nm resonance spectral shift.

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12. After acceptance of this Letter, we learned that related work has been submitted by Sudeep Mandal, Xavier Serey, and David Erickson (Cornell University, Ithaca, NY), who are preparing a paper to be called "Nanomanipulation using silicon photonic crystal resonators."