

# Numerical study of sensitivity enhancement in a photonic crystal microcavity biosensor due to optical forces

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**Abstract:** Photonic crystal microcavity biosensors can detect single biomolecules, but reliance on diffusion from microfluidic flow for particle delivery limits the minimum detectable particle concentration. Here the particle equation of motion is solved to find the sensitivity enhancement due to optical forces. The enhancement is examined for a range of parameters, including input optical power, fluid flow rate, device quality factor, and particle size.

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## 1. Introduction

Detection of biological molecules is necessary in diverse fields, including basic biology, clinical diagnostics, biosecurity, and food and environmental safety [1]. Established biosensing methods tend to be costly, complex, and time-consuming, and so an intensive effort is underway to leverage advanced microfabrication technology to create labs-on-a-chip that can reduce cost and complexity for the user. Several groups have demonstrated on-chip optical biosensors capable of sensitive detection of sub-micrometer particles. Label-free optical biosensing methods and platforms include surface plasmon resonators [2–4],

whispering-gallery-mode resonators [5,6], interferometric methods [7,8], optical fiber-based methods [9], and photonic crystal resonators [10–14].

In this paper, the sensing platform considered is a two-dimensional photonic crystal (PhC) optical resonator fabricated in a silicon-on-insulator (SOI) substrate. PhCs are structures with periodically-varying refractive index. This periodicity can create an interference phenomenon that forbids propagation through the crystal for a range of optical frequencies. This range of frequencies is called the photonic bandgap (PBG). A waveguide for light within the PBG can be formed by introducing a line defect in the PhC, and a resonator can be formed by introducing a point defect [15].

Typical 2D PhCs on SOI are produced by etching a lattice of air holes in the silicon layer, or by forming the inverted structure, an array of rods. The defects can consist of missing, shifted, enlarged, or shrunken holes. In 2D PhC resonators, light is confined in the in-plane direction by the PBG and out-of-plane by total internal reflection (TIR). The use of silicon as the device layer medium offers two advantages over other platforms: the microelectronics industry has made possible very precise nanofabrication in silicon, and the high refractive index contrast between silicon and the fluid-filled holes produces a wide PBG.

The optical mode of a 2D PhC resonator has a volume on the order of a cubic wavelength or smaller. This tight optical field confinement makes the resonant wavelength very sensitive to local refractive index changes, especially inside the defect hole [11,14–16]. When biomolecules venture near the resonator they cause the resonant wavelength to detectably shift. Chemical functionalization can be used to selectively bind a target biomolecule upon contact with the sensor surface. Particles that are not targeted will not bind, reducing the likelihood of a false positive [17]. 2D PhC resonators have been used as a platform for detection of a single monolayer of protein [10], of a single polystyrene bead [11], and of human papillomavirus (HPV) [13]. Additionally, resonator designs have been modified to allow for multiplexed, error-corrected detection with resonators in series [12]. There is a great diversity of 2D PhC designs that have been employed for sensing analytes in bulk or small numbers of discrete particles. For more information, the reader should consult a more exhaustive review [18].

For ease of use and device portability, an input sample should be delivered to the biosensor using microfluidics, on-chip streams of fluid driven by pressure or electrokinesis [19]. The microfluidic channel layer can be fabricated on top of the photonic device layer. In order for detection to occur, particles flowing above the sensor must diffuse down to the sensor surface, near the resonator. Over time, particles would surely come into contact with the sensor, but detection must occur within a few minutes, at most, in a practical device.

Sheehan and Whitman showed that it is this reliance on diffusion that limits the minimum analyte concentration  $n_{min}$  that can be detected in a given time [20]. They used the biosensor geometry to determine the rate of particle incidence on the sensor, and ultimately  $n_{min}$  as a function of experiment time. Further improvements in sensitivity will require creative approaches to overcome this diffusion limit. In one example, particle adsorption onto non-sensing areas was blocked using hydrogel nanoparticles [17]. In this work, optical forces are examined as a method for directed, rather than random, particle transport to the sensing region.

In recent years researchers have shown that optical forces near waveguides are capable of transporting particles [21–23], and resonators are capable of trapping and storing particles [24–30]. Previous numerical studies have investigated optical potential well parameters like well depth and trap stiffness [31], and the orbits of particles bound to spherical microresonators [32]. However, no work has yet been done to rigorously quantify the impact of optical forces on metrics of detection. Building on the authors' previous work [33], here the trajectories of particles are calculated from first principles when those particles are subjected to optical and fluidic forces, as well as Brownian motion. The particle trajectory calculations are used to determine the minimum concentration detectable by the sensor,  $n_{min}$ . Its

dependence on optical power and flow speed are determined in several device configurations, and the ultimate limits of the device are explored at optical powers far exceeding those reasonably available in the lab.

## 2. Methods

The combined photonic and microfluidic system considered here is depicted in Fig. 1. A point defect in a PhC is introduced by removing several holes and adding a larger hole. Resonant light tunnels into and out of the PhC resonator using traditional ridge waveguides that abut the PhC. A microfluidic channel runs over the top of the device in order to transport particles near the resonator. The surfaces near the resonator are chemically functionalized to bind the target particles upon contact [12,13]. It is assumed that functionalization is local, so that the incoming particle concentration is not depleted by binding to channel walls upstream.

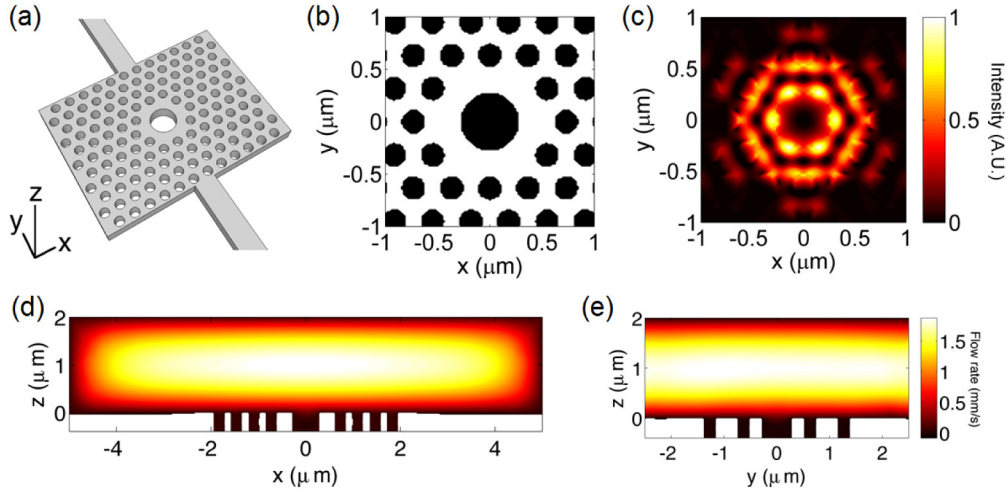


Fig. 1. (a) Schematic of a large-defect photonic crystal cavity. (b) Enlarged image of defect and (c) optical mode on resonance over area depicted in (b). Fluid flow profile in (d) cross-section and (e) profile. Channel has dimensions  $10 \times 2 \mu\text{m}^2$ . Photonic crystal has lattice constant  $a = 366 \text{ nm}$ , holes have radius  $0.3a$ , and the defect has radius  $0.75a$ . The silicon slab's thickness is  $317 \text{ nm}$ , and the surrounding fluid is water ( $n = 1.33$ ).

Particle motion is modeled using the Langevin equation [34]

$$m_p \ddot{\mathbf{x}}_p(t) = \mathbf{F}_{\text{drag}}(\mathbf{x}_p(t)) + \mathbf{F}_{\text{opt}}(\mathbf{x}_p(t)) + m_p \mathbf{n}(t). \quad (1)$$

$m_p$  is the particle mass,  $\mathbf{x}_p$  its position, and  $\mathbf{F}_{\text{drag}}$  and  $\mathbf{F}_{\text{opt}}$  are the fluid drag and optical forces.  $\mathbf{n}(t)$  is a noise term used to model Brownian motion. The effects of gravity and buoyancy are negligible. To determine the particle trajectories, the fluid drag force and the optical force are mapped out, and then the particle differential equation [Eq. (1)] is solved using the Runge-Kutta algorithm [35]. Each step of the computational method is briefly described below.

### 2.1 Fluid drag force

The fluid drag force is mapped out over the simulation domain using an approximate expression, the Khan-Richardson force,

$$\mathbf{F}_{\text{KR}} = \pi r_p^2 \rho_p (\mathbf{u} - \dot{\mathbf{x}}_p) \left| \mathbf{u} - \dot{\mathbf{x}}_p \right| \left( 1.84 Re_p^{-0.31} + 2.93 Re_p^{0.006} \right)^{3.45}. \quad (2)$$

Here  $r_p$  is the particle radius,  $\rho_b$  is the background fluid density,  $\eta$  is the dynamic viscosity,  $\mathbf{u}$  is the fluid velocity, and the particle Reynolds number is given by

$$Re_p = \frac{2r_p \rho_p |\mathbf{u} - \dot{\mathbf{x}}_p|}{\eta}. \quad (3)$$

$\mathbf{F}_{KR}$  is more accurate than the Stokes force, which is typically used. Like the Stokes force, it is the result of a Taylor series expansion of the fluid drag coefficient for small Reynolds numbers [36], but  $\mathbf{F}_{KR}$  contains more terms than Stokes' force. It assumes unbounded flow, but it provides an accurate approximation of the fluid drag force in a microfluidic channel.

The fluid velocity  $\mathbf{u}$  is the input to Eqs. (2) and (3), so to calculate  $\mathbf{F}_{drag}$   $\mathbf{u}$  must be found. This is accomplished via finite element modeling using COMSOL Multiphysics. Pressure-driven laminar flow and conditions of no slip are assumed at the channel walls. The fluid velocity component in the direction of fluid flow is plotted in Figs. 1(d) and 1(e), where an average fluid velocity of 1 mm/s is imposed at the channel input. The flow velocity approaches zero at the channel boundaries due to the no slip condition. This condition fails only when the fluid density is so low that the average molecule velocity has significant variation over one mean free path, which is not the case with water [37].

To ensure convergence of COMSOL's numerical solution, the fluid velocity at various points throughout the volume was monitored as the solution was recalculated with progressively finer grid. When the calculated result varied by less than 1% after successive grid refinements, the solution was considered converged. COMSOL uses an adaptive grid meshing, with smaller spacing near smaller geometrical features. When converged, the smallest grid spacing was 10 nm near PhC holes. Towards the center of the microfluidic channel grid spacing was much larger, so the overall computation times was a relatively short 10-20 minutes.

The maximum fluid velocity is limited to  $\sim 10^{-2}$  m/s in these simulations. Typical channels are fabricated by bonding molded polydimethylsiloxane (PDMS) to the device surface. At velocities higher than  $10^{-2}$  m/s, the pressure in a channel of these dimensions will be too great for the channel layer to remain attached to the silicon surface. Thus, attention is restricted to velocities of  $10^{-2}$  m/s and lower.

## 2.2 Optical force

An approximate expression for the time-averaged optical force  $\langle \mathbf{F}_{opt} \rangle$  can be found by treating the particle as a point dipole [38]:

$$\begin{aligned} \langle \mathbf{F}_{opt} \rangle = & \frac{\pi}{3} a_p^3 (\epsilon_p - \epsilon_m) \epsilon_0 \Re[\alpha] \nabla |\mathbf{E}_0(\mathbf{r})|^2 + \frac{4\pi}{3} a_p^3 (\epsilon_p - \epsilon_m) \epsilon_0 \frac{\sigma}{c} \langle \mathbf{S}(\mathbf{r}) \rangle \\ & + \frac{4\pi i}{3} a_p^3 (\epsilon_p - \epsilon_m) \epsilon_0 \sigma c \nabla \times \langle \mathbf{L}(\mathbf{r}) \rangle \end{aligned} \quad (4)$$

$\epsilon_p$  is the relative permittivity of the particle,  $c$  is the speed of light in vacuum,  $\mathbf{E}_0$  is the incident electric field,  $\langle \mathbf{S} \rangle = \frac{1}{2} \Re[\mathbf{E}_0 \times \mathbf{H}_0^*]$  is the time-averaged Poynting vector, and  $\langle \mathbf{L}_s \rangle = \frac{\epsilon_0}{4i\omega} \mathbf{E}_0 \times \mathbf{E}_0^*$  is the time-averaged spin density of a transverse electromagnetic field. The particle polarizability  $\alpha$  is calculated using [39]

$$\alpha_0 = 3V \frac{\epsilon_p - \epsilon_m}{\epsilon_p + 2\epsilon_m} \quad (5a)$$

$$\alpha = \frac{\alpha_0}{1 + i n_p^3 k_0^3 \alpha_0 / (6\pi)}. \quad (5b)$$

$n_p$  is the particle refractive index and  $k_0$  is the free-space wavevector. The scattering cross-section is  $\sigma = k_0 \Im[\alpha] / \epsilon_0$ .  $\Re$  and  $\Im$  denote the real and imaginary parts of the enclosed quantities. This expression is general for small dielectric or metal particles, as it depends on the particle relative permittivity.

The optical force is the sum of three terms. The first term is the gradient force, and it attracts particles to regions of high optical intensity. The second term is the scattering force, and it is due to the transfer of momentum to the particle from scattered photons. The third term is the spin force. The spin force is significant when the electromagnetic field has non-uniform helicity [38].

If the surrounding fluid is water ( $n_b = 1.33$ ), then the resonant wavelength of the device depicted in Fig. 1(a) is  $\lambda_0 = 1561$  nm. The optical intensity at resonance is plotted in Fig. 1(b). The electric and magnetic fields are obtained by three-dimensional finite-difference time-domain (FDTD) simulations using the program FDTD Solutions developed by Lumerical Solutions, Inc [40]. The electric and magnetic fields are calculated on a  $20 \times 20 \times 20$  nm<sup>3</sup>.

As in the finite element calculation of the fluid velocity field, the FDTD calculations were performed on increasingly finer grid spacings until there was less than 1% variation in calculated quantities. The FDTD simulation was performed on four processor nodes in parallel, and required approximately ten hours of computation time with the chosen grid spacing and a computational region of  $5 \times 4 \times 2$   $\mu$ m<sup>3</sup>.

An important figure of merit for optical biosensors is the resonator's quality factor  $Q = \lambda_0 / \Delta\lambda_{FWHM}$ , where  $\Delta\lambda_{FWHM}$  is the full-width at half-maximum of the resonance [15]. Resonators with a narrower bandwidth, and thus larger  $Q$ , are capable of sensing smaller refractive index changes. The resonator discussed in this study has a modest quality factor  $Q \sim 500$  when the cladding material is water. The authors have fabricated devices of similar or higher  $Q$  [10–12], and  $Q$  factors of more than  $10^6$  have been demonstrated in 2D PhC resonators on SOI [41]. Thus, it is expected that the performance achieved in this study could be improved with a higher- $Q$  cavity.

### 2.3 Brownian motion

The effect of Brownian motion is included in Eq. (1) using the random thermal force  $m_p \mathbf{n}(t)$ . Thermal forces are treated as a Gaussian white noise process [42]. At each time step, a normally distributed random number  $G_i$  is generated for the  $i^{th}$  vector component of the thermal force. The normal distribution has zero mean and unit variance. The  $i^{th}$  force component at this time step is then given by  $m_p n_i(t)$ , where

$$n_i(t) = G_i \sqrt{\frac{\pi S_0}{\Delta t}}. \quad (6)$$

$\Delta t$  is the time step duration. Accurate modelling of Brownian motion requires  $\Delta t$  shorter than the particle relaxation time  $\tau_p = m_p / (6\pi\eta r_p)$ . The spectral intensity of the Gaussian white noise process is given by  $S_0 = 12k_B T \eta r_p / m_p^2$ .  $k_B$  is the Boltzmann constant and  $T$  the temperature. For statistical accuracy, 100 simulations are run for each particle initial position.

### 2.4 Trapping and detection metrics

To evaluate the sensing enhancement due to optical force-assisted transport, trapping and detection are characterized using the minimum detectable concentration  $n_{min}$ . To find  $n_{min}$ , trajectories are calculated for particles released upstream of the resonator, with initial positions spanning the channel cross-section. For each initial position, 100 particle trajectories are calculated. The induced redshift from each trajectory is calculated to first order using [15]

$$\delta\lambda = \frac{\lambda_0}{2} \frac{\int d^3\mathbf{r} \Delta\epsilon(\mathbf{r}) |\mathbf{E}(\mathbf{r})|^2}{\int d^3\mathbf{r} \epsilon(\mathbf{r}) |\mathbf{E}(\mathbf{r})|^2} \quad (7)$$

where  $\lambda_0$  is the unperturbed free space wavelength,  $\Delta\epsilon$  is the perturbation in the relative permittivity due to the particle at its final position,  $\epsilon$  is the unperturbed relative permittivity, and  $\mathbf{E}$  is the electric field.

The average redshift induced by a single particle released from position  $(x,y)$  is stored in the function  $\overline{\delta\lambda}(x,y)$ . The total number of particles released from  $(x,y)$  in a time  $t$  is given by  $J_z(x,y)t dxdy = nu_z(x,y)t dxdy$ , where  $J_z$  is the z-component of the particle flux,  $n$  is the particle concentration, and  $u_z$  is the z-component of the fluid velocity. Thus, the total redshift as a function of time is given by

$$\Delta\lambda(t) = nt \int_{CS} \overline{\delta\lambda}(x,y) u_z(x,y) dxdy \quad (8)$$

or, if the detection threshold is  $\Delta\lambda_{th}$ , the minimum detectable concentration in a time  $t$  is given by

$$n_{min}(t) = \frac{\Delta\lambda_{th}}{t \int_{CS} \overline{\delta\lambda}(x,y) u_z(x,y) dxdy}. \quad (9)$$

### 3. Results and discussion

#### 3.1 Particle trajectories

The first results simply depict particle trajectories in the vicinity of the defect. These are plotted in Figs. 2(a) and 2(b). A plotted trajectory gives the average position of the particles at various time steps. Particles are released two micrometers upstream of the resonator at various heights above the channel floor. They are assumed to be latex particles of refractive index 1.41 and radius 50 nm. Fluid flows at an average rate of 0.01 m/s, parallel to the input waveguide.

These figures show that optical forces induce capture of particles with initial position up to ~600 nm from the channel floor, provided they are located in the center of the channel when upstream of the optical resonator.

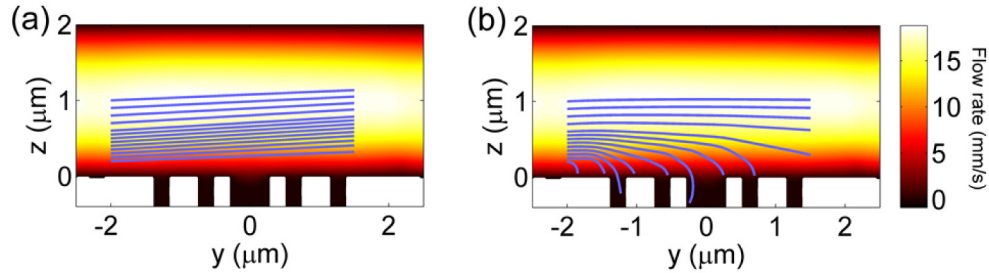


Fig. 2. Trajectories of particles in a microfluidic channel ( $10 \times 2 \mu\text{m}^2$  cross-section) near a photonic crystal resonator optically pumped at (a) 0 W and (b) 100 mW. Particles have refractive index 1.41 and radius 50 nm. Background medium is water.

#### 3.2 Minimum detectable concentration and the impact of Brownian motion

Better quantification of trapping and detection requires mapping out trajectories throughout the channel and calculating the detection metric  $n_{min}$  using Eq. (9). This was performed for average flow velocity  $10^{-3}$  m/s (parallel to input waveguide) at various optical powers, and

the results are plotted in Fig. 3. For comparison,  $n_{min}$  is also plotted there when Brownian motion is left out of the particle equation of motion.

When the device is unpumped, the minimum detectable concentration is  $3.4 \times 10^8$  particles/mL. This decreases to  $7.2 \times 10^7$  particles/mL when the device is pumped with 100 mW coupled into the input waveguide, which is a reasonable optical power that can be achieved in the lab with an Erbium doped fiber amplifier. This shows that, for this combination of flow rate and optical power, optical pumping can enhance device sensitivity by a factor of 4.7.

At higher optical powers, optical trapping dominates particle transport, and there is little effect from diffusion. This can be seen in Fig. 3, as  $n_{min}$  with and without Brownian motion converge for higher optical powers; at high optical powers the optical forces reliably trap all of the particles that might have diffused to the surface. Additionally, the optical forces can reach particles that would otherwise have a low probability to diffuse to the surface.

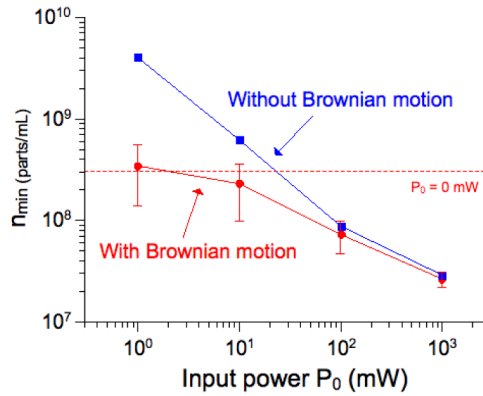


Fig. 3. Minimum detectable concentration  $n_{min}$  with and without Brownian motion included in the equation of motion. Average fluid flow rate  $U_0 = 10^{-3}$  m/s and flow is parallel to input waveguide. The dashed horizontal line gives  $n_{min}$  for zero input power when Brownian motion is included. Particles are latex beads of refractive index 1.41 and radius 50 nm. Experiment runtime is assumed to be one hour.

### 3.3 Dependence on experimental conditions

In order to better understand the limits of trapping and detection in these devices, simulations also were performed at optical powers that cannot reasonably be used in a laboratory. Nonlinear optical effects are ignored in this idealized case as a first order determination of the limits of optical trapping. Suggestions are later made for greatly reducing the input optical power required in order to achieve the same effect.

Simulations were performed at various flow rates and optical powers and processed assuming two different experimental condition related to experiment runtime. In the constant-time case, at each flow rate, fluid is allowed to flow for one hour. In the constant-volume case, at each flow rate, a given volume 7.2 nL is allowed to flow past the sensor. 7.2 nL corresponds to average fluid velocity of  $10^{-4}$  m/s flowing in a  $10 \times 2 \mu\text{m}^2$  channel for one hour. The results for the first condition are plotted in Fig. 4(a), and results for the second condition are plotted in Fig. 4(b). Flow is parallel to the input waveguide.

Under both experimental conditions,  $n_{min}$  initially decreases as the optical power increases because the optical force is proportional to the input power. However,  $n_{min}$  increases for very high powers because particles instead collect at an “optical hot spot” located upstream of the resonator. Figure 4(c) depicts the optical force in the downward direction at the surface of the PhC, and it is evident that there is a buildup of optical intensity at the effective index discontinuity where the input waveguide abuts the PhC. Flow is parallel to the waveguide and, as seen in Fig. 2, particles that contribute most to the redshift come from directly

upstream of the resonator. If instead they are trapped at the front of the PhC, then detection will be inhibited. Thus,  $n_{min}$  increases for very high optical powers.

The dependence of  $n_{min}$  on fluid velocity is subtler. When the experiment is conducted under conditions of constant time [Fig. 4(a)], the lowest achievable  $n_{min}$  occurs at the highest fluid velocity. When the fluid volume is held constant [Fig. 4(b)], the absolute minimum of  $n_{min}$  is identical across all fluid velocities, though for higher fluid velocities it occurs at higher optical powers.

To understand this, first consider the case of constant volume. In this case, the total number of particles that flows past the sensor is the same for each fluid velocity. In the flow regime

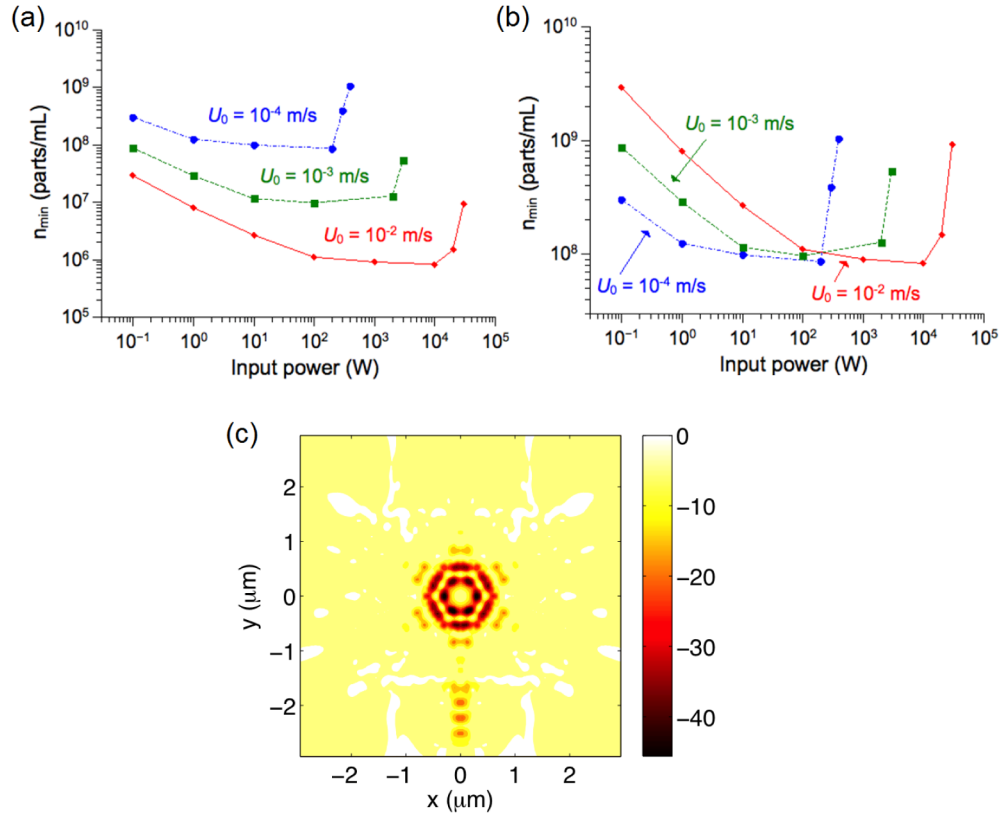


Fig. 4. Minimum detectable concentration  $n_{min}$  under flow conditions of (a) constant flow time of one hour and (b) constant volume of 7.2 nL allowed to flow over sensor. (c) Optical force in the  $z$ -direction. Scale is in pN. Particles are latex beads of refractive index 1.41 and radius 50 nm. Flow is parallel to input waveguide.

considered here the Navier-Stokes solution for this microchannel is linear in fluid velocity. In the absence of optical forces and Brownian motion, at a faster flow rate a particle will traverse the same trajectory more quickly. When optical forces are included, the same trajectories again can be traversed at various flow rates if the optical force scales linearly. Therefore, as flow rate increases, the same number of particles can be trapped and detected by simply linearly increasing the optical force. This is why in Fig. 4(b) the curve for  $n_{min}$  has the same shape for each flow rate, but is shifted to increasing optical powers with increasing fluid velocity.

With this explanation it is simple to understand the results of the constant time condition [Fig. 4(a)]. The curves of  $n_{min}$  are shifted to lower concentrations with increasing fluid

velocity because, when the run time is held constant, the total number of particles that flows past the sensor is proportional to the fluid velocity. When more particles contribute to the overall redshift, that redshift is larger.

### 3.4 Dependence on device orientation

The results of the previous section showed an absolute minimum of  $n_{min}$  due to particle trapping at the waveguide-PhC interface. It is worth considering whether this can be corrected simply by rotating the device to be perpendicular to the direction of flow. Then, particles directly upstream of the resonator will not be trapped short of detectable positions. These simulations were performed, and the results are given in Fig. 5.

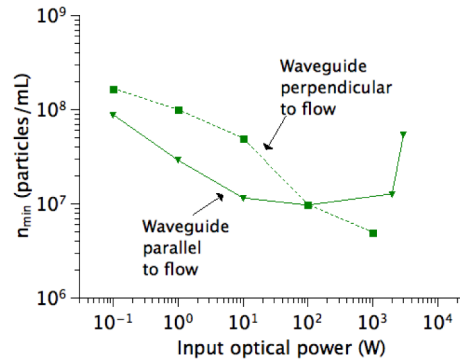


Fig. 5. Comparison of  $n_{min}$  between flow parallel and perpendicular to input waveguide. Average flow rate is  $10^{-3}$  m/s, particles are latex beads of refractive index 1.41 and radius 50 nm.

These results prove that particle trapping prior to the resonator inhibits detection for optical powers higher than 100 W. However, at lower powers there is a lower  $n_{min}$  for case of parallel device alignment. Further work should be done to determine the cause, but it is possible that, with parallel flow and low optical power, the input waveguide attracts particles without bringing them into contact with functionalized surfaces. Then particles are concentrated in initial positions upstream of the resonator ideal for later trapping and detection.

### 3.5 Dependence on particle size

The dependence of  $n_{min}$  on particle radius was also studied here. The range of particle radii studied was quite limited (50 – 100 nm), though relevant to similarly sized viruses like HPV and HIV [43]. The particle sizes were bound by computation time: The optical force in Eq. (4) is only valid for particles much smaller than the wavelength, so particles with radius larger than 100 nm were not considered. The equation could be extended to this domain by integrating the force density, similarly calculated, over the particle volume at each particle position, or by using the Maxwell stress tensor [33], but this would add significant computation time. The lower limit of particle size is again defined by the minimum time step. Trajectory calculations of particles significantly smaller than 50 nm would require significantly smaller time steps in accordance with the discussion on simulation of Brownian motion above.

Regardless, interesting results can be obtained by calculating  $n_{min}$  for a small range of particle sizes, as in Fig. 6. To understand the results, first consider the data for zero input optical power. Smaller particles undergo greater displacement due to Brownian motion, as modelled in Eq. (6). For this reason, Brownian motion is more likely to transport and bind smaller particles near the resonator. When particles are transported to the resonator by diffusion alone,  $n_{min}$  improves with decreasing particle size. At the same time, the optical

force defined in Eq. (4) increases linearly with particle volume. For a fixed non-zero optical power,  $n_{min}$  improves with increasing particle size. Taken together, the optical force-induced enhancement in  $n_{min}$  improves dramatically with increasing particle size.

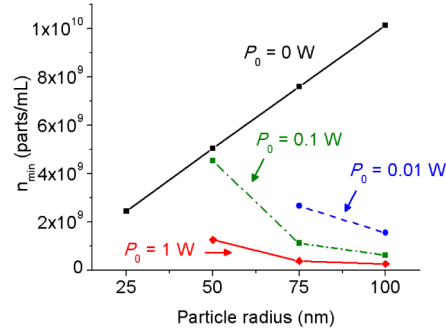


Fig. 6. Dependence of  $n_{min}$  on particle radius for various optical powers. Average flow rate is  $10^{-4}$  m/s, particles are latex beads of refractive index 1.41 and radius 50 nm.

### 3.6 Dependence on device $Q$ -factor

For this study, a modest  $Q$ -factor of  $\sim 500$  was used. No effort was dedicated here to  $Q$ -factor optimization: A device similar to one used in previous experiments [11] was simulated and a resonant mode was chosen. Nevertheless, some comments can be made regarding the impact of higher  $Q$  cavities.

A cavity with higher  $Q$  would lead to greater buildup of electromagnetic energy stored in the cavity. This would cause an increase in the magnitude of the electric field, and thus also the optical force. If the  $Q$  factor could be increased by a factor of ten without otherwise changing the shape of the resonant mode, then the magnitude of  $|\mathbf{E}|^2$  would similarly increase by a factor of ten. Alternatively, an order of magnitude less optical power could be input in order to generate a mode with the same stored energy. As previously mentioned,  $Q$ -factors higher than  $10^6$  have been demonstrated in silicon PhC resonators [41]. Thus, it is reasonable to expect that  $Q$ -factor optimization could shift  $n_{min}$  results above to much lower and more reasonable optical powers.

## 4. Conclusions

The optical forces near on-chip optical devices has been a subject of interest for the last several years, but little effort has been done to quantify the impact of these forces on the detection limits of optical biosensors. This work studied the application of optical forces to biosensing by calculating the trajectory of sub-micrometer particles subjected to fluidic and optical forces.

Trajectory calculations were used to determine the minimum nanoscale particle concentration required for detection in a given time. With the device geometry chosen, enhancement in  $n_{min}$  was negligible for practical optical powers on the order of 1-10 mW. However, simulations afforded the ability to operate at optical powers unattainable in the lab, and resulting enhancements increased. At a flow velocity of  $10^{-3}$  m/s, 100 mW of input power could generate a modest enhancement factor of 4.7.

Impractically large optical powers demonstrated that for a given flow velocity there is an optimal pump power when flow is parallel to the input waveguide. At high input powers, particles are undetectably trapped in an “optical hot spot”, where the input waveguide abuts the photonic crystal. When a fixed fluid volume flows over the sensor, the resulting optimal  $n_{min}$  is a fixed value for all flow velocities. The optical power necessary to achieve this optimal  $n_{min}$  increases linearly with increasing flow velocity. If, instead of flowing a fixed volume, the particle solution is allowed to flow for a fixed time, then for a given input optical

power it is found that the fastest flow rates lead to the lowest minimum detectable concentration. At faster flow rates, more particles have an opportunity to interact with the resonator and become trapped and detected. This increase in available particles outweighs the lower likelihood that an individual particle will be trapped at higher flow rates.

$n_{min}$  did not continue to improve with increasing input power because, upstream of the resonator, particles could be undetectably trapped in an “optical hot spot” where the input waveguide abuts the photonic crystal. As power increased, more particles accumulated here to the detriment of detection. There is no such limitation on enhancement when flow is perpendicular to the waveguide, but in this case performance is worse at low powers. It may be that when flow is instead parallel to the input waveguide, there is some build-up of particle concentration due to optical forces above the waveguide, in initial positions that lead to favorable trapping trajectories.

Finally, there is hope that the enhancements in  $n_{min}$  demonstrated here even for absurd optical powers could be realized with device optimization, or when applied to larger particles.  $Q$ -factors many orders of magnitude higher than the  $Q \sim 500$  are achievable, which would lead to much higher buildup of the electric field in the resonant mode for a given input power. In turn, this would lead to an increase in the optical force through its dependence on the magnitude of  $|\mathbf{E}|^2$ . This merits further study. Enhancement also increased for larger particle size because the optical force increased while diffusion became a less effective transport mechanism. Thus, optical force-directed transport provides greater benefit to the detection of larger particles.