Optimization and Modeling of an Energy Harvesting Optical Micropropeller for Microfluidic Applications

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Optimization and Modeling of an Energy Harvesting Optical Micropropeller for Microfluidic Applications

An honors thesis presented to the College of Nanoscale Science and Engineering, University at Albany, State University of New York & SUNY Polytechnic Institute in partial fulfillment of the requirement for graduation with honors in Nanoscale Engineering, completion of Capstone project, and graduation from The Honors College.

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Abstract

The design and materials optimization of a optical micropropeller comprised of silver nanorods on a fused silica substrate was developed. A combination of surface plasmon resonance, thermophoretic and convective forces enable rotation of the micropropeller in an aqueous environment. This work aims to eliminate the dependence of optical micropropellers on the requirement for a light source by relying on a blackbody radiation energy harvesting principle. This energy harvesting principle is able to plasmonically excite noble metal nanorods of a specific aspect ratio at specific wavelengths that correspond to an ambient temperature. By investigating the dependence of the aspect ratio and the micropropeller’s optical and thermal responses at a specific wavelength, an optical micropropeller can be developed that can operate in low temperature environments without external sources. The forces from the Poynting vector caused by electric field generation and the force from the convective current were found to be possible in a 50°C aqueous environment. The forces acted in the same direction, presenting the possibility that enough torque could be generated to facilitate rotation.
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Introduction

Surface plasmon resonance (SPR) is an excitation of all free electrons within the conduction band, which leads to an in-phase oscillation [1]. The incoming light induces a dipole in the electron with respect to the core of the nanoparticle and the electrons oscillate around the metal nanoparticle (Figure 1). The frequency of this oscillation is dependent on the shape, size, dielectric constant, and other optical constants of the material and the surrounding medium [1-4]. This phenomenon traditionally occurs in noble metal nanostructures such as gold (Au), silver (Ag), and copper (Cu).

![Figure 1. Model of the oscillation that occurs during surface plasmon resonance [2]](image)

While SPR traditionally relies on an incident light source for this electron excitation, Karker et al. [5-6] showed that plasmonically active materials could be excited using spectral radiance from black bodies (thermal radiation). Using lithographically patterned nanorods, Karker et al. performed high temperature gas sensing relying solely on thermal energy harvesting, eliminating the need for an external incident light source [5-6]. Currently, this thermal energy harvesting principle has only been shown to be effective at temperatures of 300˚C or higher, severely limiting its use to high-temperature applications. Theoretically, however, this principle should be able to hold at lower temperature values by adjusting the necessary parameters, expanding its capabilities for integration into devices other than high-temperature MEMS devices.

One such application, are optical micropropellers. Current optical micropropellers suffer from requiring an incident light source to function. This poses limitations for its integration into environments where optics are not easily implementable or may cause unwanted interference. Micropropellers have potential applications as mechanical transducers and actuators, energy conversion, and in vivo biological manipulation and detection [7]. The device’s ability to create optical rotation allows for applications beyond just a micropropeller. They have potential applications in lab-on-a-chip systems where it can act as a fluid stirring bar. Coupled into plasmonic lab-on-a-chip systems specifically, they could perform both stirring and field enhancement for sensing and biomedical diagnostics. Additionally, the rotation principle relies on thermophoretic and convective forces [8] that produce significant heat generation. This heat generation could be used in conjunction with its potential as a micromixer for catalyzing localized chemical reactions using heat [9].

In order for this optical micropropeller coupled with energy harvesting to have practical application, a lower operating temperature needs to be achieved. By adjusting the aspect ratio of the nanorod and the nanorod material itself, the operating temperature of the energy harvesting micropropeller can be brought to temperatures as low as 37˚C.
Materials and Methods

Simulation of Metallic Nanoparticles using a Boundary Element Method

All modeling of the plasmonic properties of the micropropeller was performed using a MATLAB MNPBEM toolbox for the simulation of metallic nanoparticles (MNP), using a boundary element method (BEM) [10]. Material information regarding the wavelength-dependent refractive index and extinction coefficient was derived of a combination of parameters determined by Rakic et al. [11] and Hagemann et al. [12]. This allowed for modeling of the micropropeller between 1 and 248 µm for gold, silver, and copper.

The model was built using the same MNPBEM toolbox. The substrate that comprised of the body of the micropropeller was built to be 4 µm long, 200 nm wide, and 100 nm thick. The nanorods were chosen to have a 40 nm diameter and be 800 nm in length. Two nanorods were placed on opposite sides of the substrate with one sitting on top of the substrate and one sitting below the substrate (Figure 2).

Figure 2. 3D model of optical micropropeller built for simulations

A spectrum for each plasmonic material was gathered on a YSZ substrate in a water matrix. The scattering cross section of the micropropeller was gathered for each material from 1000 to 20000 nm. A similar procedure was conducted but modulating the substrate material instead, keeping the rod material the same for each simulation.

The last set of simulations done using the MNPBEM toolbox plotted the field lines of the electric field enhancement of the rod on the substrate. For these simulations, only one rod was
modeled on a layer structure to attain a qualitative plot of the electric field enhancement of the rod with a 15-\(\mu\text{m}\) wave.

**COMSOL Multiphysics Simulation Software and Computational Fluid Dynamics**

A qualitative assessment of the heat transfer and fluid dynamics affecting the micro-propeller was performed using COMSOL Multiphysics Simulation Software and the Computational Fluid Dynamics module. Time-dependent simulations were performed to observe the affects of micro-propeller composition and dimensions on thermal diffusion and fluid flow.

Due to limitations regarding the physics modules and toolboxes available for the COMSOL license, the micro-propeller was scaled up to the centimeter length scale. This scaling factor was chosen because the applied boundary conditions and parameters would, when applied to examples from the COMSOL model gallery, successfully replicate the demonstrated results. This scaling factor combined with the unknown quantity of heat generation due to optical absorption also required assumptions to be made about the nature and amount of heat transfer occurring at the metal nanorods. For computational simplicity, an overall power output of 0.5 watts over a total rod volume of 2.56 mm\(^3\) was applied to all simulations.

To qualify these assumptions, it was necessary to determine the turbulent or laminar nature of the flow regime and verify that our scaling factor does not change the physics applicable to the original micron scaled design of the micro-propeller. To do this, the Grashof number was calculated. The Grashof number for vertical flat plates is given by (1) below.

\[
Gr = \frac{g\beta\Delta T L^3}{\nu^2}
\]  

(1)

where \(\beta\) is the thermal expansion coefficient, \(\Delta T\) is the temperature difference, \(g\) is gravitational acceleration, \(L\) is the characteristic length-scale of convection, and \(\nu\) is the kinematic viscosity of the fluid. This dimensionless number is a ratio of buoyancy to viscous forces and is used to determine the tendency of a system towards turbulence. When the Grashof number is above \(10^8\) the boundary layer is turbulent. Since the calculation for Grashof number in the micro-scale case and the centimeter-scale case were both below \(10^8\), the flow was found to be laminar [13].

Time dependent, non-isothermal, laminar flow was modeled. The propeller was constructed within a rectangular (20 cm x 30 cm x 10cm) volume for the water. Open bounds were applied at the walls for laminar flow while a non-slip layer of glass insulated the floor on which the propeller rested. The ceiling of this volume was modeled to be a slip boundary exposed to atmospheric pressure with an external natural convection heat flux term of 2 W/m\(^2\). The walls of the fluid volume were placed at a sufficient distance from the propeller to set temperature boundary conditions of fluid infinitely far away at 20\(^\circ\)C.

**Determination of Nanorod Aspect Ratio**

Prior to modeling, the proper aspect ratio of the nanorods needed to be determined that would give the desired response at around 37\(^\circ\)C. To do this, the wavelength of light that would be akin to the spectral radiance of the environment at 50\(^\circ\)C was found. 50\(^\circ\)C was chosen as opposed to
37°C for the sake of simplicity in calculations. Using Plank’s law modified for nanorod geometries (2):

\[
U(\lambda) = \frac{8\pi h v^3}{c^3 \left( \exp \left( \frac{hc}{\lambda kT} \right) - 1 \right)}
\]

Where h is Plank’s constant, c is the speed of light in a vacuum, k is the Boltzmann constant, \( v \) is the frequency, and \( T \) is the temperature of the heated body [5]. Using (1), an energy vs. wavelength profile of radiant heat energy at a specific temperature, 50°C, was found. The energy vs. wavelength profile indicated a peak position of the broad peak at around 15 \( \mu \)m (Figure 3). The peak, however, is rather broad indicating that there is a large wavelength range that the spectral radiance emits that can possibly excite the plasmonic material.

![Figure 3. Energy vs. Wavelength profile for the spectral radiance at 50°C](image)

The aspect ratio can be determined from the wavelength. Karker et al. plot the longitudinal plasmon peak wavelength as a function of the nanorod aspect ratio based on experimental samples and data extrapolation (Figure 4) [5]. Since the peak position determined using (2) above was not included in the plot, the data was extrapolated to around 15 \( \mu \)m. In keeping with the trend of the plot in Figure 4, the aspect ratio that would exhibit a 15-\( \mu \)m longitudinal peak position would be 1:60.
Figure 4. Longitudinal plasmon peak wavelength vs. nanorod aspect ratio for previously deposited samples as well as predicted plasmon peak positions obtained through linear extrapolation of the experimental data points from Karker et al. [5]

An aspect ratio of 1:60 leaves little room for scaling down due to resolution limits of current fabrication technologies. The e-beam method employed by the Carpenter lab yields a minimum rod diameter of around 40 nm. This means that abiding by the 1:60 aspect ratio determined above limits the rod size to a minimum of 2.4 μm in length. This micropropeller technology could not be adapted to any environment below that minimum size, severely limiting its application potential.

The absorption cross-section of a gold nanorod can be plotted to find a smaller aspect ratio that should still absorb the proposed 15-μm spectral radiance. From the Lorenz-Mie theory, the absorption cross section is given by (3):

$$
\sigma_{abs}(\omega) = \frac{V}{3c} (\varepsilon_m)^3 \sum_{i=1}^{3} \frac{(Y_i + 1)^2}{(\varepsilon_1 + Y_i \varepsilon_m)^2 + \varepsilon_2^2} \frac{\omega \varepsilon_2}{\omega}
$$

Where V is the particle volume, c is the speed of light in a vacuum, $\varepsilon_m$ is the matrix dielectric constant, $Y_i$ is the shape factor for the $i$th axis (which is directly proportional to the aspect ratio), $\omega$ is the resonant peak frequency, and $\varepsilon_1$ and $\varepsilon_2$ and the real and imaginary parts of the dielectric function of the metal, respectively [5]. Plotting the cross section as a function of the resonant peak frequency determined that this aspect ratio had a non-zero absorption cross section at around 15 μm and well into longer wavelengths. This meant that the nanorods created with a 1:20 aspect ratio may absorb at the proposed temperature.

As mentioned above, the standard nanorod fabrication technique utilized by the Carpenter lab can yield nanorod diameters down to only about 40 nm. Thus, the nanorods chosen for modeling had this 40-nm diameter and a length of 800 nm to satisfy the aspect ratio conditions.
Specific Aims

To determine whether or not the micropropeller design presented could rotate under the defined conditions, two separate modeling methods were applied. Within both sets, optimization of the design was necessary to determine what would enable the best rotation. As such, two aims were set up as standards of success for this project.

**Aim 1. Model the optical properties of the micropropeller for optimization of rod and substrate material. Provide proof of concept.**

For this design to be most effective, the best rod material and substrate material needed to be found that would enhance the plasmonic properties of the micropropeller. The rod materials tested were gold, silver, and copper because of their well-characterized plasmonic properties. In order for these simulations to be most effective, the wavelength dependent refractive index and dielectric constant need to be provided to the toolbox. Many materials have not been plotted out far enough into the IR range to be used reliably for simulations aside from copper, silver, and gold. Determining which one has the best scattering cross section at the defined wavelength range will determine which one would be best to be plasmonically excited in the proposed conditions.

The substrate material must be modified because it will modify the energies of the plasmon modes of the nanorod [13]. So for these simulations, three different classes of materials were chosen to determine which would be best. In this case, the substrate material determined may not be the “best,” but determining the family of materials that will allow for future, more focused, optimization down the line.

Silicon was chosen as a metallic substrate for simulation. Si is the most widely used substrate material for MEMS devices. Most MEMS fabrication is done using standard lithography and processing techniques on Si wafers, its universal applications in MEMS devices makes it a good substrate material to test on. A main disadvantage of Si is that it is not biocompatible nor biostable [15], which would severely limit this micropropellers potential as an *in vivo* bio-MEMS component.

Yttrium-stabilized zirconia (YSZ) was chosen as a ceramic substrate for simulation. YSZ is highly used in the Carpenter lab as a material for embedding Au nanoparticles for plasmonic-based sensors [16-18]. Additionally, YSZ is a desirable material because of its biocompatibility, mechanical strength, chemical stability, and wear resistance [19]. A major drawback of using YSZ is that it is susceptible to corrosion [20] and low temperature hydrothermal degradation (aging) [21].

The final material, a simple fused silica substrate, was chosen because of it’s common use in microfluidic MEMS. Silica-based devices are popular in the creation of microfluidic systems because of their good insulating properties and high resistance to mechanical stress, surface stability, and solvent compatibility [22]. Silica-based microfluidics have been used in biological applications [23], demonstrating their biocompatibility. Additionally, silica glass is effectively opaque at wavelengths above 3.5-4 µm [24]. So the silica substrate can be treated much like the Si and YSZ substrates without having to take into account any plasmonic excitation on the backside of the rod.

In addition to determining the optimal rod and substrate material to use, a proof of concept needs to be drawn from the results. By plotting the electric field lines of the micropropeller, the
direction of the electric field over the rods can be modeled. From these electric field lines, inferences can be made about the direction of the electromagnetic force acting upon the rod that may substantiate the claim that the micropropeller can rotate using thermal energy harvesting at 50°C.

**Aim 2. Model the natural convection behavior of the micropropeller for further optimization. Provide proof of concept.**

The thermophoretic force generated by the plasmonics of the rod is also essential for rotation. By modeling the convective current that can occur in the device, the micropropeller could have two forces contributing to the torque of the device. The principle of this force relies on the creation of a temperature gradient. Plasmonically excited materials will create this temperature gradient through heat generation, resulting in thermophoretic and convection forces [8]. To maximize these forces, the substrate material and the rod material need to have opposing thermal properties to create a larger gradient. The substrate would optimally have a low thermal conductivity, $k$, and a high heat capacity, $C_p$. The rod material needs to have a high thermal conductivity and a low heat capacity.

Using the optimized materials determined from Aim 1, thermal and velocity profiles can be generated for the micropropeller. These profiles with further illustrate whether or not the rod can rotate and the proposed conditions, providing further proof of concept. Additionally, the thermal profiles provide further optimization opportunity. The design for the optical properties may not be an optimal design when coupled with thermal properties.

**Results and Discussion**

**Optimizing Rod Material**

The nanorods sitting on either side of the micropropeller needed to be optimized to determine which material would be best to create a strong electric field for torque. For this, a strong peak or set of peaks in the mid-IR would be ideal for the optical micropropeller. Copper, silver, and gold were chosen as the possible rod materials for optimizing because of their well-characterized plasmonic properties. Rakic et al. [11] and Hagemann et al. [12] mapped out the wavelength-dependent refractive index properties of all three noble metals from 1 µm to 248 µm. This data was used for the simulations to generate simulated spectra from 1000 to 20000 nm (Figure 5).
In order for a 1:20 aspect ratio to be substituted for a 1:60, the rod material needs to have a signal out at 15 µm. The micropropeller with gold nanorods (Figure 5a) only has a peak at around 8000nm for the x-polarized light and a ~7750nm peak for y-polarized light. At longer wavelengths, the scattering cross section of the micropropeller exhibits no signal. It will not induce an electric field out at 15 µm and, therefore, exhibit no rotation in that environment. As such, a micropropeller outfitted with gold nanorods would not be desirable for this design given the intended environment.

A micropropeller with copper nanorods gives a large peak at around 13 µm that extends much farther into the IR (Figure 5b). The 1:20 copper nanorods will be plasmonically enhanced by a 15-µm wave as well as longer wave fronts. Since a 15-µm wave corresponds to a temperature of only about 50°C, longer wavelengths would relate to even lower temperatures. Based on the modeled spectrum in Figure 5b, copper nanorods could induce an electric field at these lower temperatures since the scattering cross section is still strong beyond it’s peak value at 13 µm.

While silver does not have a distinct peak in the mid-IR, it does show promise for electric field enhancement at 15 µm and beyond (Figure 5c). The magnitude of the scattering cross section, which denotes the probability of a scattering even occurring, is higher than the copper spectrum. Additionally, unlike copper, the spectrum beyond 15 µm is not decreasing. The increase in the silver
spectrum indicates that there may be another peak beyond the modeled range. The silver nanorod micropropeller has the potential of plasmonic enhancement at 50°C and lower based on Figure 5c, indicating that it would be the best suited rod material for energy-harvesting micropropeller applications.

Optimizing Substrate Material

Figure S1 shows the scattering cross section of the micropropeller when the Ag nanorods are placed onto a Si substrate. The nanorods still have a non-zero scattering cross-section at 15µm and beyond, meaning plasmonic enhancement can occur at those mid- to far-IR wavelengths even on a Si substrate. Further investigation of the behavior of the plasmon resonance of the Ag nanorods on a Si substrate can be found in Figure S2. Here, the field enhancement lines for a single Ag nanorod on a Si layer are plotted for the plane 40 nm above the rod. The field enhancement lines travel away from the rod on the right side and into the rod on the left side. From modeling the field enhancement at father distances from the rod, it was found that the electric field induced from the 15-µm wave travels from the right side of the rod to the left.

A similar analysis was performed for the micropropeller when the Ag nanorods are placed onto a YSZ substrate (Figure 5c). The spectra for Si and YSZ are similar in shape, but Si has a much higher scattering cross section at lower wavelengths. That does not matter for the mid-IR excitation needed, so a better comparison can be made through the electric field map of a Ag nanorod on YSZ (Figure S3) as compared to Si. The shape of the electric field maps is the same as Figure S2 for Si. However, based on the color scale bars of both plots, the intensity of the electric field generated by a Ag nanorod on YSZ is larger than that of Si by a factor of 2.

YSZ, however, was not the optimal material. The fused silica glass substrate showed the best optical properties of the three materials. The spectrum for the micropropeller with a fused silica substrate (Figure 6) is similar in shape to Figure 5c. The scattering cross section scale of Figure 6 is greater than that of Figure 5c, meaning a greater scattering probability for a fused silica substrate than a YSZ substrate.

Figure 6. Scattering cross section of the micropropeller with Ag nanorods on a fused silica substrate
The field enhancement on the rod under a glass layer substrate (Figure 7) showed the same field pattern as it did on a Si and YSZ substrate. Much like how the value of the field lines for YSZ was greater than Si, the value of the field lines for the fused silica was greater than YSZ and Si. The field intensity was increased by a factor of 4 compared to Figure S2 and a factor of 2 when compared to Figure S3.

![Figure 7](image_url)

Figure 7. Field enhancement of a single Ag rod on a fused silica layer 40nm above the surface of the rod with a) the whole rod, b) the left edge of the rod, and c) the right edge of the rod

The electric field travels from one end of the nanorod to the other. Based on this electric field and knowing that the induced magnetic field will be normal to the electric field, an inference about the Poynting vector can be made. The Poynting vector refers to the electric flux density of a field and is proportional to the force caused by electromagnetic fields. So, based on how the electric field curves from the right edge of the rod, over the rod, to the left edge of the rod (Figure 7), the Poynting vector on the rod is oriented down towards the substrate [25]. Even though this is modeling only one rod, the same electric field direction and resulting Poynting vector can be assumed. The rods are far enough apart from one another and separated by a substrate that the plamonics of the rods will not interfere with one another. As such, the micropropeller illustrated in Figure 2 will have a Poynting vector pointed into the substrates on both sides, allowing an
asymmetric force to be generated on the micropropeller. The micropropeller should then spin counterclockwise in the X-Y plane based on the plasmonic enhancement of the nanorods.

**Thermal Properties of Substrate Materials**

Upon initial investigation of each material in the optimization process, some conclusions about which materials well have the best thermal properties can be made. As stated in the Specific Aims, the best rod material will have a high thermal conductivity and a low specific heat capacity. From inspection of Table 1 below, the best rod material would be likely Ag. Ag has the highest value for the thermal conductivity and the second lowest value for specific heat capacity among the three rod materials. While Au has the lowest specific heat capacity, it also has the lowest thermal conductivity.

A similar look at the substrate materials will give a similar idea of which will have the better thermal properties. For the substrate, the thermal conductivity needs to be low with a high specific heat. This would mean that either glass or YSZ would be the best materials for the substrate.

**Table 1.** Comparison of the thermal conductivity and specific heat capacity of each material, unless otherwise specified, constants taken directly from the COMSOL Multiphysics Modeling software

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal conductivity W/mK</th>
<th>Specific Heat Capacity J/kg°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>314</td>
<td>126</td>
</tr>
<tr>
<td>Ag</td>
<td>406</td>
<td>223</td>
</tr>
<tr>
<td>Cu</td>
<td>385</td>
<td>386</td>
</tr>
<tr>
<td>Si</td>
<td>159</td>
<td>712</td>
</tr>
<tr>
<td>YSZ</td>
<td>2.2 [26]</td>
<td>400 [27]</td>
</tr>
<tr>
<td>Fused silica</td>
<td>1.4</td>
<td>730</td>
</tr>
</tbody>
</table>

The thermal properties of the micropropeller with Ag nanorods and varying substrate materials are shown below in Figure 8. To maximize torque on the rod, there needs to be maximum asymmetry in the rod. So the thermal properties of the micropropeller should show two distinct nodes for this asymmetry. The fused silica glass substrate will give two distinct temperature nodes on either side of the micropropeller (Figure 8a-b). These temperature nodes are apparent in both the thermal and isothermal profiles of the micropropeller. YSZ gives two distinct temperature nodes in its thermal profile (Figure 8c), but some blending of the nodes occurs in the isothermal plot towards the center of the rod (Figure 8d). The Si substrate is by far the worst substrate material. There are no distinct temperature nodes in the micropropeller for both the thermal and isothermal temperature profiles (Figure 8e-f). Since Si's thermal conductivity is two orders of magnitude larger than YSZ or fused silica (Table 1), its value is much closer to the thermal conductivity of Ag. The properties of fused silica show advantages over YSZ as well. The thermal conductivity of fused silica is lower than YSZ and the specific heat capacity is higher. This means that of the two, fused silica would be the better substrate material to promote thermophoretic and convection forces on the micropropeller.
There is, however, a problem that was identified with the design used for the optical properties. The substrate is too thin, which allows the temperature gradient to bleed through to the backside. This inhibits the asymmetric thermophoretic and convective forces needed for rotation of the micropropeller. Some further design optimization was needed for the thickness of the substrate to maximize the asymmetry of the forces on the propeller. Because of the relatively long length of the substrate compared to the length of the nanorods, there is likely little to no optical interference between the two rods. Meaning that increasing the thickness of the substrate will have no effect on the optical properties of the micropropeller and the optical data will still hold.
Optimization of Substrate Thickness for Velocity Enhancement

All simulations for thickness dependence of the velocity profile were performed using the previously determined optimized materials. The nanorod material was set to be Ag and the substrate material used was fused silica. To eliminate the bleeding of the temperature gradient through the substrate, the dependence of the thermally generated force on the rod on substrate thickness was established. Using a temperature gradient as the driving force, velocity profiles of the micropropeller were generated (Figure 9).

![Figure 9](image)

Figure 9. Velocity profile of micropropeller with a) a substrate thickness of 1 mm and b) a substrate thickness of 2.5 mm. Plots of the velocity lines on either side of the micropropeller for one rod with c) a substrate thickness of 1 mm and d) a substrate thickness of 2.5 mm.

Figure 9c-d exhibit the velocity lines that develop from the thermal gradient on either side of the nanorod. For torque to occur, the velocity pushing down on the rod needs to overcome the velocity on the other side of the rod. Increasing the substrate thickness by 250% greatly increases the magnitude of the velocity pushing down on the micropropeller and decreases the magnitude of the velocity pushing up on the micropropeller (Figure 9a-b).

Plotting the difference in the fluid velocities on either side of the edge of the micropropeller as a function of thickness (Figure 10), an almost linear relationship is observed. A 250% increase in the thickness of the substrate correlates to an approximately 25% increase in the net fluid velocity difference on each edge of the micropropeller. Increasing the thickness of the substrate material will allow greater net velocities on either side of the rod to induce rotation, to a certain extent. Increasing the thickness too much will add unnecessary weight that the force would be unable to rotate the massive structure.
Based on the velocity profiles of Figure 9b, there are two net directions on either side of the micropropeller that point in opposite directions. This correlates to an asymmetrical force on either side of the micropropeller that will initiate rotation. The micropropeller, based on the velocity profiles, will enable the micropropeller design in Figure 2 to rotate in the X-Y plane. This coincides with the theoretical rotation caused by the electromagnetic force on the micropropeller determined previously. These two forces coupled together prove that there are forces generated from energy harvesting at 50°C that will enable rotation of an optical micropropeller without the use of a light source.

Conclusion

In this study, an energy harvesting optical micropropeller was successfully modeled. Through the coupled use of an MNPBEM toolbox and COMSOL, the optical and thermal profiles of the proposed design of the micropropeller were found. Using the optical data, the rod and substrate materials were optimized to create the greatest plasmonic enhancement that would lead to the greatest electric field enhancement. It was determined that the best noble metal nanorod material to use was Ag and the optimal substrate material was fused silica glass. The thermal data supported this choice for rod and substrate material.

The electric field generated by surface plasmon resonance was determined for a single Ag nanorod on a fused silica layer. Based on the direction of the electric field lines, it was determined that there is an electromagnetic force pointing down on the rod into the substrate. By process of
symmetry, this will occur on either side of the rod. Since the forces on either side are pointed in opposite directions, this will create an asymmetrical force that allows the rod to spin.

The thickness of the substrate material was found to have an effect on the thermal properties of the micropropeller and subsequently the fluid velocity generated by the temperature gradient. A plot of the net velocity as a function of the substrate thickness found an almost linear relationship to the percent fluid velocity difference on the micropropeller and the thickness. The velocity profiles found for the micropropeller show that the thermophoretic and convective forces on the micropropeller will push it in the same direction as the electromagnetic force. The two forces can combine constructively to increase the overall torque on the micropropeller and thus proves that rotation is possible for an energy harvesting optical micropropeller for microfluidic applications.

Future Work

Quantitative modeling of the plasmonic properties of the micropropeller will enable determination of whether or not this device produces enough torque to overcome its weight and rotate. In order for this modeling to be feasible, the absorption cross section of the micropropeller would need to be determined, something that was not included in the MNPBEM toolbox. The absorption cross section would be beneficial for another reason. Current modeling only outputs the scattering cross section of the micropropeller, but that does not give the whole picture. Determination of the total extinction cross section, which is composed of absorption and scattering cross sections, gives the summation over all electric and magnetic multipole oscillations [28]. This would provide more accurate plasmonic data on top of what has already been collected.

One of the major limiting factors of this current work is the limitation of COMSOL’s Computation Fluid Dynamics package. Because it cannot model at the micron scale, an accurate picture of the behavior of the temperature gradients cannot be achieved. Within reason, the scaled up version of the micropropeller provides and general idea of the thermal properties of the design. With a microfluidics package on COMSOL, the temperature and velocity profiles of the micropropeller can be found to underscore the initial data found above.

Even with the 1:20 aspect ratio discussed, the size of the device is still limited. By investigating plasmonic materials that absorb in the IR, such as some metal oxides and plasmonic ceramics [29-30], the aspect ratio limitation may be completely eliminated. In addition, other geometries could be tested to see which ones will shift the plasmon peaks into the IR bands better. Nanorods were studied because of the linear dependence on the peak position vs. aspect ratio determined by Karker et al. [5], but optically induced rotating devices have been made using alternative geometries such as light mills [31] and nanoantennas [8].

Individual Contributions

MATLAB MNPBEM modeling was done by Jacqueline Elwood for materials agreed upon by both members of the group. COMSOL modeling was performed by Jerry Shih after determination of optimal materials for the micropropeller.
References

Supplemental Material

Figure S1. Scattering cross section of the micropropeller with Ag nanorods on a Si substrate

Figure S2. Field enhancement of a single Ag rod on a Si layer 40nm above the surface of the rod with a) the whole rod, b) the left edge of the rod, and c) the right edge of the rod
Figure S3. Field enhancement of a single Ag rod on a YSZ layer 40nm above the surface of the rod with a) the whole rod, b) the left edge of the rod, and c) the right edge of the rod