Investigating the morphology of an optically trapped particle using Mie scattering

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Abstract. Microscopic polystyrene particles suspended in water are trapped by optical tweezers and we determine their diameter using Mie scattering theory. A near infrared laser is used to form the optical trap near the focus by a high numerical aperture lens. The particles have a higher refractive index than the surrounding medium and the focused light creates a strong gradient force which traps the transparent, dielectric particles. The trapped particle is illuminated with broadband white light. Mie scattered light from the particle is collected in the epi-direction by a microscope objective and measured with a spectrometer. Due to internal reflections, specific wavelengths resonate within the spherical cavity. These resonances are commonly referred to as whispering gallery modes, or morphologically dependent resonances. These resonances are measured in the spectrum of the Mie scattered light. By comparing the wavelength of these resonance peaks to theoretical simulations, we can precisely determine the diameter of the particle in the trap. Here, the analysis of these measurements will be discussed.

1. Introduction

Mie scattering theory can be used to determine an individual particle's diameter and refractive index [1, 2]. Studying an individual particle negates ensemble averaging and one is able to probe local changes in the sample's diameter and refractive index. To study the individual particle, it is isolated and trapped using the optical tweezers system. Here, a polystyrene bead suspended in water is optically trapped using an optical tweezers [3]. The optical trap is created by focusing light tightly with a high numerical aperture lens. The ray diagram description of optical trapping forces in figure 1 shows the refraction of light by a particle with a higher refractive index than the surrounding medium. The change of momentum that the light experiences creates a net force towards the focus of the light. This is the gradient force and is proportional to the gradient of the electric field. A tighter focus provides a stronger gradient force to create a stable trap.

Once a particle is isolated by the optical tweezers, white light illuminates it and Mie scattering from the particle is used to determine the particle's diameter and refractive index, approximated here by the Cauchy expression [1],

$$n = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \tag{1}$$

When broadband white light is incident on the spherical particle, specific wavelengths will be resonant within the sphere. These resonant modes are known as whispering gallery modes and correspond to the peaks seen on the spectrum of the scattered light. The positions of these

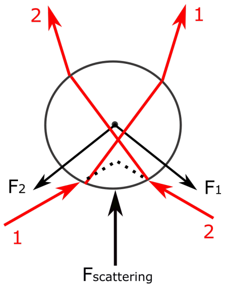

Figure 1. Rays 1 and 2 are refracted by the particle and result in a net gradient force towards the focus of the light. Due to the tight focusing of the light, the gradient force is larger than the scattering force, creating a stable optical trap.

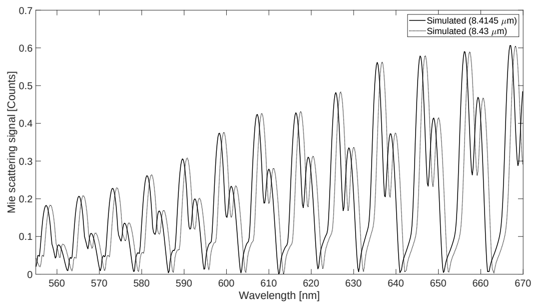

Figure 2. Simulated spectra for the scattering of light from a polystyrene particle in water shows a difference in the peak positions between particles with a diameter of 8.4145 μm (solid) and 8.43 μm (dotted).

peaks can be calculated using Mie theory [4]. Mie theory solves Maxwell's equations for a plane wave incident on a spherical particle. By solving these equations and including the boundary conditions of the sphere, the spectrum of the scattered light is simulated, (figure 2).

Using this technique, for a similar sample of polystyrene particles, Jones, King and Ward [1] determined the refractive index within ± 0.0005 and the particle radius within ± 0.4 nm. In comparison, optical imaging yields a limited lateral resolution on the order of approximately 167 nm using a NA of 1.5 at 500 nm [5]. Combined with optical trapping, the Mie scattering technique described here is not limited to polystyrene particles. It can also be used to spatially manipulate and study individual aerosol droplets [6, 7] which is useful in climate studies. For similar sized water droplets, accurate sizing of the droplets was demonstrated to within ± 2 nm [4].

2. Methodology

The optical trap is constructed based on the Thorlabs Optical Tweezers Module (OTKB/M), figure 3. The trapping laser (975 nm) is focused into the sample by a high numerical aperture microscope objective, (NA 1.25, 100X oil immersion objective). The samples used here are polystyrene particles (diameter 8.9 μm ± 0.66 μm) suspended in water. The trapped particles are imaged in transmission with a white light LED. A condenser lens (NA 0.4, 10X air objective) collects the light and the image is formed on a CMOS camera. Light from the white light LED scatters from the trapped particle and is collected in the epi-direction by the NA 1.25 objective lens. This scattered light is measured with a spectrometer (Ocean Optics USB4000) with a spectral resolution of 0.2 nm. The integration time for collecting the spectrum of the scattered light was 5 ms and averaged over 10 measurements. To reduce background noise in the spectrum of the scattered light, an aperture is introduced and imaged into the trapping plane. This reduces the scattering from the water surrounding the particle and ensures that the majority of the scattered light is from the trapped particle.

We simulate the Mie scattering for various particle diameters and refractive index iteratively as described by Jones, King and Ward [1]. The software used here allows the user to select the refractive index of a sphere and the size parameter. Given the refractive index of water [8], it computes total scattering, total extinction and angular distribution of the scattered light. The LabVIEW vi was written by Dr AD Ward, STFC and the Dynamic Link Library by Martin Fierz [9].

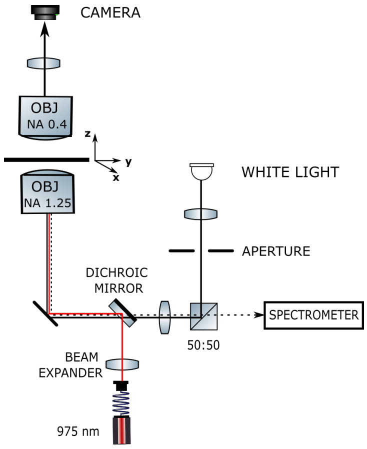

Figure 3. The trapping laser is focused by a high numerical aperture objective (OBJ NA 1.25). The sample is illuminated by a white light LED and imaged on a CMOS camera. The back scattered white light from the trapped particle is measured using a spectrometer.

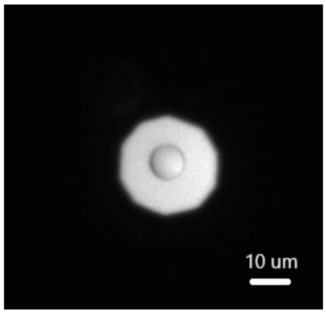

Figure 4. A polystyrene particle is trapped in water using the optical tweezers system and imaged on a CMOS camera as shown here. An aperture is also imaged into the trapping plane to reduce scattering from water and increases signal to noise ratio in the measured spectrum.

3. Results and discussion

We demonstrated optical trapping of polystyrene particles suspended in water, figure 4. Limiting the illumination to the particle by imaging an aperture onto the trapping plane, reduces the background in the acquired spectrum.

The Mie resonances from the trapped particle are measured with the spectrometer, figure 5. To compare these measurements to simulated Mie scattering from a polystyrene particle in water with varying diameters, the residual background is removed. First, the scattering of white light from water was subtracted, after which the remaining background was removed by fitting a polynomial to the minima in the spectrum and dividing the spectrum by the polynomial, normalising the background.

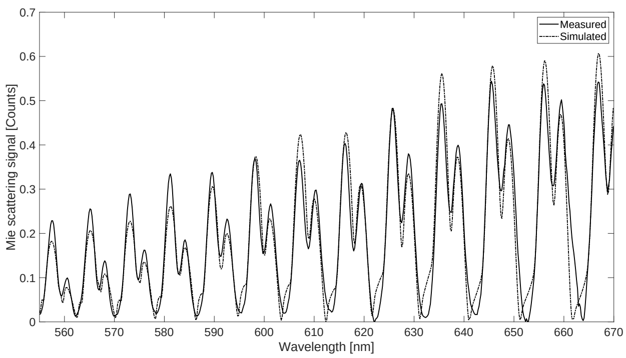

Figure 5. The measured Mie resonance structure (solid line) from an optically trapped polystyrene particle suspended in water is compared to simulated scattering (dotted line) for a particle with diameter 8.4145 μm.

To determine the particle diameter and refractive index, the simulated spectrum is varied iteratively by adjusting the diameter and refractive index until it best represents the measurement. Peak positions are used to compare the spectra, because the signal to noise is better for the peaks than the valleys.

As a starting point, representative refractive index values for polystyrene are used to initially to estimate the particle's diameter. Using the chosen refractive index values, the diameter is found that results in the simulation best matching the measured spectrum. This is used as the initial diameter of the particle.

Using this estimated particle diameter the refractive index is then adjusted until individual peaks of the simulated and measured spectrum overlap optimally in wavelength. The refractive index required for the individual peaks to align are recorded and a dispersion curve for this particle diameter is plotted. The Cauchy equation is fit (using MATLAB's Trust Region algorithm [10]) and the root mean square error (RMSE) from the fit is indicated in table 1 as an estimate of the uncertainty on the refractive index of the polystyrene particle.

The estimated particle diameter is then varied by 1 nm increments and the process is repeated. Figure 6 shows the RMSE for various particle diameters used for particle 1. The minimum RMSE from the quadratic fit indicates a particle diameter of 8.4145 μm ± 0.0001 μm. This corresponds to the diameter and refractive index that best describes the measured experimental scattering. The refractive index dispersion for this particle diameter is obtained from a fit resulting in a $R^2 = 0.9807$ (bead 1 in figure 7),

$$1.583 + \frac{2806}{\lambda^2} + \frac{3.817 \times 10^8}{\lambda^4} \tag{2}$$

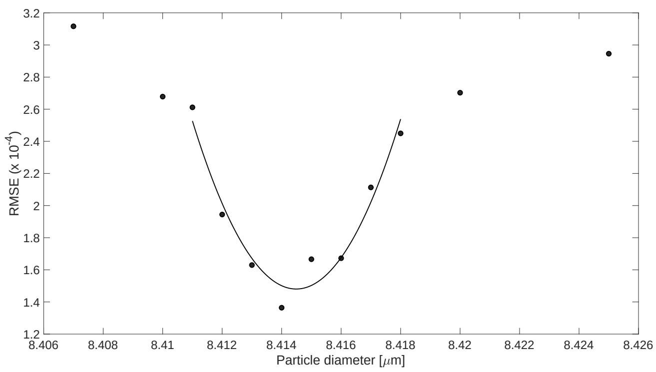

Figure 6. The refractive index dispersion is fit using the Cauchy relation and the resulting root mean square error (RMSE) of the fit is shown here for various particle diameters. The minimum of the quadratic fit to the RMSE values corresponds to a particle diameter of 8.4145 μm ± 0.0001 μm.

This protocol described above was repeated for three similar polystyrene particles and the results are summarised in table 1. The technique is highly sensitive and able to distinguish between the refractive indices of individual particles. The refractive index dispersions for the three particles are plotted in figure 7. The average for this limited sample size is also shown.

This work was done under the assumption that the particles can be treated as spherical particles (in order for the Mie theory to apply conveniently). Non-spherical deformities in the particle shape will lead to splitting or broadening of the peaks, which was not observed. The uncertainty in the measurement is a result of the absolute spectral resolution, the accuracy of the calibration of the spectrograph, and the signal to noise.

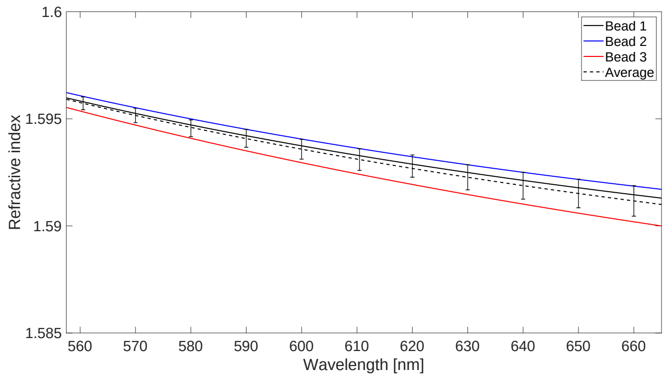

Figure 7. A plot of the refractive index dispersion for three polystyrene particles suspended in water along with their average. The standard deviation at selected wavelengths is also shown.

Table 1. Three polystyrene particles were trapped in water and investigated for their individual diameter and refractive index. The table shows their diameter and Cauchy terms A, B and C representing the refractive index of the individual particles.

Particle	Diameter [μm]	A	B [nm^2]	C [nm^4]	RMSE	R^2
Particle 1	8.4145 ± 0.0001	1.583	2806	3.817×10^8	1.48×10^{-4}	0.9807
Particle 2	8.4035 ± 0.0001	1.584	2484	4.088×10^8	0.99×10^{-4}	0.9842
Particle 3	8.4267 ± 0.0004	1.578	4964	1.508×10^8	3.85×10^{-4}	0.9273

4. Conclusion

In this work, an optical tweezers system was used to trap micron-sized polystyrene particles suspended in water. By doing so, individual particles could be targeted to determine their diameter and refractive index using Mie theory. An existing methodology was adapted to determine these properties from the spectrum of back scattered white light from a trapped particle. The spectrum showed strong resonance peaks that were compared to simulated Mie resonance spectra. The peak positions were used to determine the particle's diameter and refractive index using an iterative protocol. The diameter of the micron sized particles was determined with an uncertainty of less than a nanometer. In addition, it was demonstrated that the technique is sensitive to changes in the refractive index per individual particle. The technique described here can be used to study trapped water droplets in, air expanding this work to aerosol studies.

Acknowledgments

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