Monte Carlo simulation of light scattering from diatom frustules of *Gomphoneis sp.*

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Monte Carlo simulation of the light scattering pattern from diatom frustules of the species *Gomphoneis* was attempted by implementing Mie theory in conjunction with a subroutine which accounts for size distribution among the diatoms. A biotechnical procedure was followed in preparing the samples of diatom frustules which were used as samples for scattering measurements required for validating the simulations.

INTRODUCTION

In recent years, a tremendous amount of research has been done to understand the nature of electromagnetic scattering by spherical and nonspherical particles [1-3]. In addition to experimental and theoretical studies on light scattering by particulate matter, several groups have tried to simulate light propagation in scattering media [4-8]. Such Monte Carlo methods of solving the light scattering problems due to particulate matter have been proving to be a very successful tool in verifying experimental observations obtained by use of the different investigating instruments as well as lending support and improving the current theoretical models.

In this work we report the development of a program coded in C language for Monte Carlo simulation of light scattering from diatom frustules of *Gomphoneis species* and comparison of these simulations with experimental observations and theoretical predictions. The technique involved generation of light scattering intensity values as a function of scattering angle for a particular size and shape of diatom frustules. In case of simulation, the scattering intensity at each angle was represented by average of non-uniform random values generated by Monte Carlo method and computed on the basis of Mie theory. A normal size distribution was considered on the basis of images obtained by scanning electron microscope. The experimental observations of scattered light intensity from the diatom frustules were obtained using a designed and fabricated laser-based setup incorporating sixteen silicon detectors to monitor the scattered light [9].

DIATOMS

Diatoms are a group of single celled photosynthetic micro alga found in both fresh water and marine environment. Diatoms are unicellular structures with the protoplasts enclosed in an amorphous silica cell wall called frustules, consisting of two valves joined together by a girdle.

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These structures in the diatom frustule range from micrometer to nanometer scales. These naturally synthesized 3D nanostructured materials are of great importance in recent research in nanotechnology from various points of view, which includes its morphology, mechanical properties, optical, and electrical properties. Researchers are reporting the potential application of diatom frustules in optoelectronics, biophotonics, gas sensor, filtration and targeted drug delivery. Out of the over 200 000 species of these photosynthetic algae with world wide distribution, our work here focuses on the light scattering properties from the particular *Gomphoneis species* of diatoms which is found locally in water in Assam, India. A sample (20 ml) of water containing diatoms was centrifuged at 6000 rpm for 15 minutes to allow sedimentation of the heavy diatom particles. The precipitate was suspended in 1 ml of distilled water and washed. The "WC" media proposed by Guillard and Lorenzen (1972) was used with slight modifications to culture the diatoms using the prepared sample as inoculum [10]. The solid culture plates were incubated at 22°C under white fluorescent light in a B.O.D. incubator (Narang Scientific Works, New Delhi) for 14 days. For the liquid culture, all the growth nutrients were dissolved in 1000 ml of sterile water and the media was autoclaved before inoculation with environmental samples.

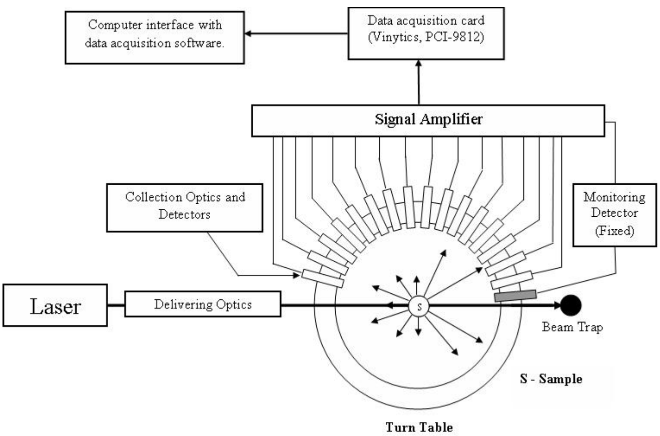

Figure 1. Experimental setup.

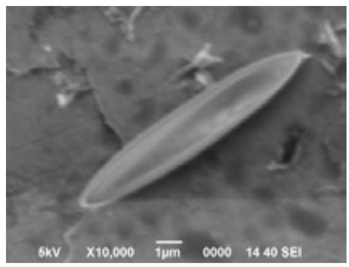

Figure 2. SEM micrograph of *Gomphoneis sp.*

EXPERIMENTS AND SIMULATION

The schematic diagram of the experimental setup is shown in Fig. 1. The setup consisted of a laser source, controlled sample holders, photodetector arrangements, data acquisition systems, and associated instrumentation. In this experiment we used a He-Ne laser source with 632.8 nm wavelength and an output power of 2 mW. The diameter of the beam cross-section was 2 mm and the distance between the source and the scattering centre was 250 mm. The laser light was scattered by a sample of fresh water diatoms suspended in water and placed at the scattering centre by a mechanical arrangement. The scattered light intensity was sensed by 16 static Si detectors (BPW34) having large sensitive area (7.5 mm^2) mounted on a circular disc and were connected to a high gain, low noise amplifier circuit. The amplified signals were interfaced to a dedicated data acquisition system (Vinytics, PCI-9812) for data recording. The whole array of 16 detectors could be rotated simultaneously about an axis perpendicular to the plane of the circular disc. Readings were in steps of 1° from an angle of 10° to 170° and each detector was separated from the next one by an angle of 10°.

The simulation process involved the generation of uniform random numbers and then forcing the uniform random numbers into a non-uniform pattern governed by Mie-theory (using it as a probability distribution function) by using the Inverse transformation method. Fig. 3 gives the algorithm for such a process. The photons in the simulation program were shared unequally among the diatoms of different size which were governed by a normal size distribution function. Finally, this simulated plot for the phase function of the Mueller matrix was compared with the experimental and theoretical plots.

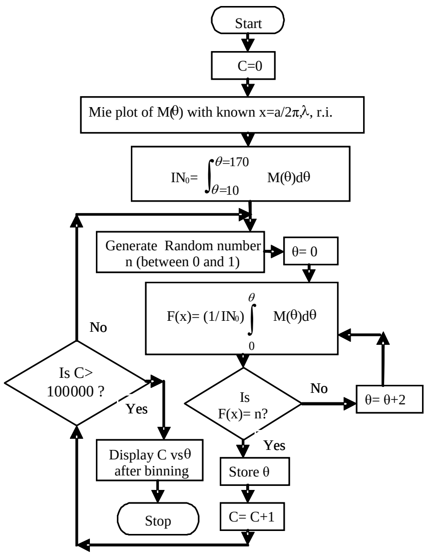

Figure 3. Simulation flowchart.

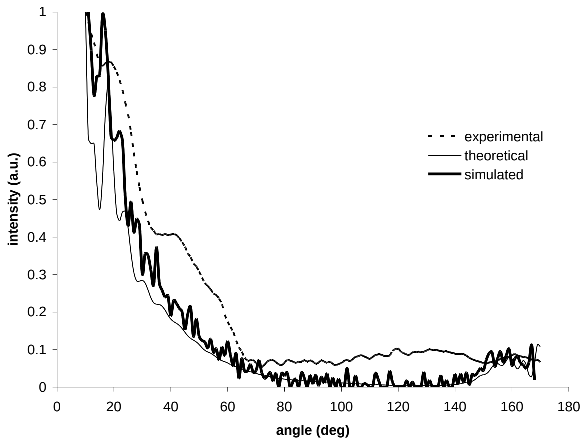

Figure 4. Plot of intensity vs. angle.

RESULTS AND DISCUSSION

Figure 4 shows the simulated plot superposed on the experimental and theoretical plot (Mie theory) obtained for diatom frustules of *Gomphoneis species* with a length of around 7 μm. Normal size distribution with a standard deviation of 5 % was considered for simulation. The simulation results are fairly consistent with the theoretical predictions for the diatoms. However, there is a noticeable deviation of both the simulated and theoretical plots from the experimental plot. One of the reasons for this discrepancy is because of the inadequacy of Mie theory in case of diatom structures with a very high asphericity aspect ratio. Moreover, the non-uniformity of the surface of these diatom frustules also plays a role in this discrepancy. Yet, it can be seen from Fig. 4 that the simulated plot tends more towards the experimental results in comparison to the theoretical plot especially in the forward scattering region between 10° and 60°.

Although it is difficult to simulate for diatoms with very complex structures using current theories alone, a combination of different techniques will be tried in the future for further investigations of more complex diatoms.

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