CHAPTER VII

CONCLUSIONS AND FUTURE DIRECTIONS

This thesis provides a detailed description of computational light scattering studies of highly irregular interstellar dust (graphite, fayalite and their mixtures) and atmospheric aerosol analogue (silica) samples supported by experimental simulations with a laboratory light scattering setup. A computational technique based on four different software packages is developed to compute and calculate light scattering properties of irregularly shaped particles.

The light scattering properties of dust analogue particles dispersed in both shapes and sizes were considered in which a number of complex 3D shapes (not provided with original DDSCAT) were generated externally. Several theoretical models have been developed to study the nonspherical particulate matter samples by generating various target geometries and using their combinations for computations. The efficiency and validity of the computational techniques are verified and established using laboratory measurements with analogue samples at three laser wavelengths, namely 543.5 nm, 594.5 nm and 632.8 nm. A laboratory light scattering setup has been modified to study and measure the light scattering parameters of small particulate matter (in the form of analogue samples of atmospheric aerosol and interstellar dust) in the Optoelectronics and Photonics Research Laboratory, Tezpur University, India. This setup can measure the values of phase function $F_{11}(\theta)$, and degree of linear polarization $-F_{12}(\theta)/F_{11}(\theta)$, over the scattering angle range from 10° to 170° in steps of 1° and 5° respectively. The instrumental errors are calculated by conducting 100 sets of experiments with spherical water droplets of 0.5 to 5 µm. As measured from the data sets it is found to be ± 0.194 in arbitrary units. The instrumental errors are plotted as error bars in the experimental plots of all the comparative analyses.

A number of shape models (different geometries) were designed with different roughness and porosity by varying surface deformation and number of dipoles respectively. Finally a near perfect combination of surface roughness, porosity and size distributions representing the target geometries (or scattering particles) was arrived in the computations, which gave the best possible fit and match to the experimental data obtained in the laboratory measurements. The developed models were proved to be efficient in computations of size shape averaged values of $F_{11}(\theta)$ and $-F_{12}(\theta)/F_{11}(\theta)$ at the respective wavelengths. However, discrepancies were observed at the higher scattering angles with an exception of the negative polarization values observed in experimental results. A particle size range of 0.3 µm to about 5 µm are considered to keep the $|m|kd$ values within DDA permissible limit for majority of the cases. This modeling approach can explain light scattering properties of single or mixtures of dust analogue samples with a higher degree of accuracy. But small scale errors are still present owing to the limitations in computational resources and also the restrictions applied by the computational technique involved.

In the first simulation work, light scattering properties of shape and size distributed interstellar dust analogue graphite particles are studied and the effects of particle shape and surface roughness on scattering parameters are demonstrated. It is observed from the comparative analyses that the experimental plots are almost identical with the computational plots for both phase function and degree of linear polarization at two wavelengths 543.5 nm and 632.8 nm.

In the next phase laboratory dust analogue samples of interstellar and circumstellar fayalite (or iron silicate), the end member of the most important olivine group, was synthesized and studied in the visible wavelength region. The developed theoretical models can explain the experimental light scattering properties using size and shape averaged scattering parameters to higher degrees of accuracy.

In the next simulation work the light scattering properties of silica microparticles are studied, due to its importance as an atmospheric aerosol and drug delivery agent in medications. These studies provided important clues about the modeling techniques to detect and characterize the properties of highly irregular unknown scatterers with complex optical properties. A comparative analysis of the computational and experimentally acquired results are done and a good agreement is found in the forward scattering lobes in all the cases and for each of the measured scattering parameters. This study also provides an efficient way of detection and particle size distribution measurements for irregular micro and nanoparticles that is highly applicable in remote sensing, atmospheric studies, astrophysical studies, medical applications and also for finding potential health hazards in the form of inhalable and respirable small particulate matter.

Finally a mixture of graphite and fayalite as interstellar dust aggregate samples are used to develop a dust model. The comparative analysis of the theoretical and experimental results of shape and size averaged scattering parameters shows the effects of variables used in the modeling approach, the percentage composition, number of dipoles, and number of directions considered for orientational averaging on modeling accuracy. This study demonstrates a well-defined model to calculate the light scattering parameters of dust aggregates with two or three constituent elements.

Future directions

The future directions include extending the studies to infrared wavelengths with a view to include particles with higher size parameters upto about 30 μm for direct application in interpretation of observed astrophysical scattering and absorption peaks.

Also it is important to study more complex mixtures of three or more dust species for e.g. graphite, amorphous carbons, fayalite, forsterite, enstatite, pyroxene and olivine along with the newly discovered PAHs to simulate more realistic dust cloud environments in interstellar medium and circumstellar systems.

Incorporating more powerful computational tools to carry out complex computations, including higher number of model shapes or target geometries and further enhance the time required for calculations is another necessity of the study. Particularly the number of orientation directions must be chosen as near to realistic values as possible for higher accuracy of DDA calculations.

Development of more sophisticated instrumentation to further minimize the experimental errors, using optical laser traps with a possibility to directly levitate the scattering particles at the scattering center is another future requirement. Photodetectors of higher sensitivity and more efficient polarizers can also be incorporated in the setup for more reliable experimental results.