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Optical Imaging in Microstructures**Final Report for DOE Grant DE-FG02-96ER14686**

Pamela M. Aker

Department of Chemistry, University of Pittsburgh
Pittsburgh, PA 15260

Phone: 412-624-8680 fax: 412-624-8552 e-mail: pamaker@vms.cis.pitt.edu

Program Scope

Our research was focused on developing morphology-dependent stimulated scattering (MDSRS) spectroscopy as an analytic optical imaging technique. MDSRS uses the cavity modes (called morphology dependent resonances, MDRs) associated with axisymmetric dielectric microstructures to generate nonlinear optical signals. Since different cavity modes span different regions inside the microstructure, it becomes possible to generate location-specific spectra. The information gotten from MDSRS imaging experiments is analogous with that generated from magnetic resonance imaging (MRI) studies in that spatial variations in chemical composition and molecular configuration within a structure can be mapped out.

We demonstrated that MDSRS imaging is feasible and is free from nonlinear artifact. We did this by measuring the molecular structure variations that are present in the interfaces of 180 μm dia. charged water droplets. The 4 publications that resulted from these studies are attached. From a chemical perspective a water droplet is, however, a simple thing. Will it be possible to use MDSRS imaging to study more complex systems such as combustng fuel droplets, layered polymer or glass fibers, or biological cells? The long-term goal of our research was to answer this question. The answer we have come up with is yes and no. Our results on nitrate aerosols show that it is possible to do imaging studies on optically non-absorbing, ion containing systems, but that the ultimate sensitivity is dictated by ion concentration. Hence systems containing large quantities of mobile ions will be difficult to look at, so this essentially eliminates being able to look at biological samples in situ. But on the positive side, organic systems, such as layered polymer and glass fibers, and combustng organic fuel droplets can looked at with MDSRS imaging.

Three graduate students, Cassandra Allen, Philip Moortgat, and Victoria Uvarova participated on this project along with one postdoctoral research associate, Merete Bilde. In addition, 3 undergraduate students participated during the course of this research, these were William Nichols, Amina Khan, and Omar Wooten. A sum total of 6 publication resulted. In addition, 18 invited talks, papers and posters were presented at various scientific society meetings and/or academic institutions.

Publications

1. *MDSRS Imaging I. Theoretical Aspects*, P. M. Aker, P. A. Moortgat and J.-X. Zhang, J. Chem. Phys. **105**, 7268 (1996).
2. *MDSRS Imaging II. Solvent Structure in the Diffuse Part of the Electric Double Layer*, P. M. Aker, J.-X. Zhang, and P. A. Moortgat, J. Chem. Phys. **105**, 7276 (1996).
3. *Response to "Further comments on the existence of a modified hydrogen bonding ratio*

DOE Patent Clearance Granted
4-11-01
Date
Mark P. Dvorscak
(603) 252-2393
e-mail mark.dvorscak@ch.doe.gov
Office of Intellectual Property Law
DOE Chicago Operations Office

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in laboratory generated water droplets by Campillo et al.", P. M. Aker, J. Geophys. Res. in press.

4. *Nitrate Ion Detection in Aerosols using Morphology-Dependent Stimulated Raman Scattering*, P. M. Aker, J.-X. Zhang and W. Nichols, submitted J. Chem. Phys. (1998).
5. *Charge-Enhanced Uptake of SO₂(g) at the Water/Air Interface*, J.-X. Zhang and P. M. Aker, Chem. Phys. Lett. 298, 183 – 188 (1998).
6. *Response to the commentary by Davidovits et al.*, P. M. Aker, Chem. Phys. Lett. 308, 444 (1999).

Presentations

Colleges, Universities, and National Laboratories

Carnegie Mellon University, Pittsburgh, PA, 2/96
University of Richmond, Richmond, VA, 10/96
Wesleyan University, Middletown, CT, 9/97
Columbia University, New York, NY, 9/97
Seton Hill College, Greensburg, PA, 9/97
University of California - Los Angeles, CA, 10/97
University of California - Irvine, CA, 10/97
University of California - Riverside, CA, 10/97
University of Southern California Los Angeles, CA, 10/97
University of Toronto, Toronto, Canada, 11/97
University of Colorado, Boulder, CO, 1/98
University of Chicago, IL, 2/98
Brookhaven National Laboratory, NY, 3/98
Georgetown University, DC, 4/98
Pennsylvania State University, State College, PA, 9/98

Conferences

70th International Meeting on Colloid and Surface Science, Postdam, NY, 7/96
MDSRS Imaging, an optical analog of MRI
XVIth FACS Meeting, Kansas City, MO, 10/96
MDSRS Imaging Studies of the Water/Air Interface
1997 Conference on the Dynamics of Molecular Collisions, Gull Lake, MN, 7/97
Structure Profiling Inside Microparticles – A new twist on vibrational spectroscopy
1998 Gordon Conference on Vibrational Spectroscopy, Plymouth State College, Plymouth, NH, 7/98.

Contributed Presentations

Structure of Charged Water/Air Interfaces

V. Uvarova, C. Allen, and P. M. Aker, poster presented at the 1997 Conference on the Dynamics of Molecular Collisions, Gull Lake, MN, 7/97.