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The Center For The Study Of Terrestrial And Extraterrestrial Atmospheres (CSTEA)

Dr. Arthur N. Thorpe, Director
Dr. Vernon R. Morris, Deputy Director

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Five-Year Report
April 1992-December 1996

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Five Year Report
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Center for the Study of Terrestrial and Extraterrestrial Atmospheres (CSTEA)
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CSTEA's EXISTENCE ... THEN AND NOW

The Center for the Study of Terrestrial and Extraterrestrial Atmospheres (CSTEA) was established in 1992 by a grant from the National Aeronautics and Space Administration (NASA) Minority University Research and Education Division (MURED). Since CSTEA was first proposed in October of 1991 by Dr. William Gates, then Chairman of the Department of Physics at Howard University, it has become a world-class, comprehensive, nationally competitive university center for atmospheric research ... with a major focus on student training.

The Center began in 1992 with fourteen (14) active Principal Investigators (PIs) from the Howard University Departments of Physics, Chemistry, and the School of Engineering. and one (1) subcontract. By the end of the initial funding cycle (December 31, 1996) there were **nineteen** (19) **PIs** and **one** (1) **subcontract**. Of the original CSTEA PIs named in 1992, nine (9) are still an integral part of the Center's research.

The research of the Center's PIs has, for the most part, continued in the same four (4) areas as presented in the original proposal -- **Remote Sensing**, **Atmospheric Chemistry**, **Sensors and Detectors**, and **Spacecraft Dynamics**. This research has produced many refereed publications and presentations by CSTEA faculty at national and international conferences. Their research reports and outcomes can be found in the section "The CSTEA PIs ... Their Research and Students." CSTEA PIs have written

approximately one hundred (100) **refereed articles and papers** and made over one hundred ten (110) **presentations at conferences** and NASA installations.

When CSTEA began its student training activities in April of 1992, the Center started with three (3) undergraduate students and sixteen (16) graduate students. For the Fall Semester 1996, CSTEA was supporting -- through stipends -- seventeen (17) undergraduate students and eighteen (18) graduate students. Twelve (12) of the eighteen (18) graduate students also receive tuition support from the Howard University Graduate School of Arts and Sciences (GSAS). All of the students -- throughout the entire five-year period -- performed research under a particular PI or the Director of the Center. As of the submission of this report, there have been **eleven** (11) **Ph.D. degrees** awarded, **ten** (10) **Master's degrees** awarded, and **twelve** (12) **Bachelor of Science degrees** awarded to CSTEA-supported[1] students.

In 1993, the Center's leadership changed. Dr. Gates was replaced by **Dr. Arthur N. Thorpe**, a long-time faculty member in the Howard University Department of Physics, as the **Center's Director**. Dr. Thorpe was appointed by Dr. Orlando L. Taylor, Dean, GSAS in September of 1993. Immediately upon Dr. Thorpe's appointment, he instituted several policies for the Center. Some of these policies included the following:

- Redoubled efforts to train and support underrepresented minority American students in the atmospheric sciences; from October 1993 to present, all of the CSTEA students are citizens of the United States and are

[1]CSTEA support to students came in the form of stipends and tuition. In some instances, CSTEA also supported graduate students through equipment and other purchases for a PI ... and thus the graduate student could complete his/her experiment for his/her thesis or dissertation. Some students began their studies and research with CSTEA, but did not complete the program for one reason or another. If these students were supported by CSTEA for more than one semester, they are counted in all statistics.

underrepresented minorities;

- A **seminar series**, featuring speakers from NASA installations, other government agencies, private industry, and faculty from universities from all over the country, was initiated for undergraduate and graduate students in January of 1994. These lectures -- an average of three (3) a month during the Fall and Spring semesters -- have continued to this date. Attendance is mandatory for students and they are encouraged to participate in this important aspect of the Center;
- Dr. Thorpe also began an active **recruitment** effort ... personally visiting many of the historically black colleges and universities (HBCUs). The result of these visits has benefitted not only the HBCU but Howard University and NASA as well. Since the Summer of 1994, Dr. Thorpe has recruited thirteen (13) students for graduate school from institutions of higher education such as Alcorn State, Fort Valley State, Grambling State, Jackson State, Stillman College, and Talladega; and
- In mid-March 1996, Dr. Vernon R. Morris was appointed as the **Deputy Director** of CSTEA. He has represented CSTEA at various conferences and presentations and assisted in the administrative duties of the Center.

Dr. Thorpe also concentrated his efforts on other aspects of the Center's program in order to fulfill the goals and objectives of CSTEA -- to establish at Howard University a world-class facility for the study of terrestrial and extraterrestrial atmospheres with special emphasis on the training of African Americans in space-based sciences and engineering.

In 1994, with the assistance of CSTEA, the Howard University Department of Chemistry hired an **Atmospheric Chemist**, Dr. Vernon R. Morris. Another Atmospheric Scientist, Dr. Gregory Jenkins, was hired by the Department of Physics beginning in the Fall of 1995. He began teaching in the Spring of 1996. Dr. Sonya Smith, a Ph.D. in Mechanical and Aerospace Engineering, was hired by the Department of **Mechanical Engineering** in the Fall of 1995. She brought to the Center an expertise in turbulence and wake vortex dynamics and contributed to the Stratospheric Wake Analysis Project (SWAP). Dr. Smith also worked with Dr. Morris on the course curriculum for the graduate program in Atmospheric Sciences.

During the Summers 1994-1996, CSTEA, in conjunction with the Washington, Baltimore and Hampton Roads Alliance for Minority Participation (**WBHR-AMP**), presented an eight-week Summer Institute and Research Traineeship in Atmospheric Sciences (**SIRTAS**) for minority undergraduate students. This lecture/research traineeship had an average of twenty-seven (27) students per Summer. The SIRTAS program was divided into two parts: (a) the first four (4) weeks were devoted to lectures, field trips and group discussions in the morning and research training in the afternoon; (b) the second four (4) weeks consisted solely of research, group meetings, and presentention of their research work. The students who participated in this program came from such institutions as the University of the District of Columbia, Morgan State University, Grambling State University, North Carolina A&T University, and Florida A&M University. Individual PIs conducted research during the Summers. Dr. Vernon Morris directed the SIRTAS program each Summer.

Another important student and research component for CSTEA was the develop-

ment and implementation of courses and a graduate course curriculum in Atmospheric Sciences entitled "**HUPAS**" (Howard University Program in Atmospheric Sciences). The first course in Atmospheric Sciences -- for graduates and undergraduates -- was offered during the Spring of 1995 by Dr. Vernon Morris. At present, HUPAS is composed of nine (9) faculty from Physics, Mechanical Engineering, Electrical Engineering, and Chemistry. Seven (7) new courses have been offered through HUPAS. HUPAS has been accepted by all parent Departments and graduate faculty, and endorsed by the President of Howard University. We now await the "formal" ruling of the Board of Trustees for its final inclusion as a degree-granting program. At present, there is a CSTEA-supported graduate student enrolled in HUPAS.

In 1995, CSTEA was connected to the **internet** and a website, including links to the home pages of several PIs, was established. Each PI and CSTEA student has an e-mail address -- either in their respective Departments or at the CSTEA administrative office. The CSTEA "home page" (http://www.cstea.howard.edu) is presently undergoing renovation. Students and faculty under the direction of a "webmaster" are performing this task.

Each year since 1992, CSTEA has undergone a thorough review by the Center's **Advisory Committee** and **Technical Review Committee**. The Advisory Committee consisted of a Chairman, Dr. William Jackson, and members George Carruthers, Joseph Francisco, Denise Hawk, and Keith Jackson. The Technical Review Committee was Chaired by Dr. Regina Cody of NASA/GSFC. Each year, the PIs gave presentations on their individual research and accomplishments to the panel members of the respective Committees; the Director also informed the members of each Committee of the other various accomplishments of the Center. In 1994, there were two visits by each

Committee. Each Committee gave their respective critiques and recommendations and the Center responded accordingly.

In the last year, several earnest attempts have been made to obtain **additional funding** for the Center's existence. Some of these proposals for student support and research have been submitted to the following government agencies: Department of Defense, including the Army and the Air Force, the Federal Aviation Administration, the Department of the Energy, and NASA. At least one has been approved for funding and monies will be received this year. The Director and Deputy Director will continue to actively seek funds -- as well as each PI in the Center.

CSTEA's Director, Deputy Director, PIs, and students have attended all of the **meetings** and **conferences** sponsored by NASA and other university research centers (URCs). CSTEA participated in the recent URC-TC in Albuquerque, New Mexico, February 15-19, 1997. CSTEA was represented by eight (8) faculty members and seven (7) students. Two of CSTEA's PIs gave tutorials -- Drs. Richardson and Smith -- and nine (9) papers were presented by students and PIs.

THE CSTEA PIs ... THEIR RESEARCH AND STUDENTS

What follows are the individual research reports of the PIs in the Center. These reports include: (a) the PIs accomplishments; (b) the students they have worked with; (c) publications in refereed journals; and (d) presentations at conferences and government and private institutions. Each report is written by the individual PI. They are arranged in alphabetical order -- according to the last name of the PI -- the date they became associated with CSTEA, and the name of their research project.

DR. PETER M. BAINUM (1992) ... Structural Dynamics And Flight Dynamics

Initial focus was on the development of mathematical models of upper atmospheric orbiting research platforms that could be used as a base for various sensors and instruments. This included the use of flexible manipulator links that could be used to position and re-position instruments at various locations on the platform. In order to consider the effects of parametric, noise, and other uncertainties in such platform systems a control robustness study was initiated based on LQG/Loop transfer recovery techniques.

Later emphasis was in providing support in the flight dynamics area to analyze the trajectories of various ER-2 test fights from Moffett Field, CA as well as the practice ER-2/Concorde test fight from Wallops Island to the Nova Scotia area.

Another recent task is the structural analysis and qualification of the QCM/SAW instrumentation unit attached to the pod of the ER-2 aircraft. The main objectives are to avoid potential resonances between the flexible vibrational modes of the instrumentation assembly with the natural and beat frequencies of the quartz oscillators within the QCM/SAW unit, and also to prevent undesirable stresses and strains to various structural loadings associated with the ER-2 flight paths.

Students:

Xu, Jianke, Ph.D. student ... "Dynamics and Control of Large Flexible Space-Robotic Systems" Ph.D in Mechanical Engineering/Aerospace Option *(Dec 1993) May 1994**

Ericsson-Jackson, Aprille, J., Ph.D. student ... "Dynamics and Robust Digital Control for Large Orbiting Space Structures" Ph.D. in Mechanical Engineering/ Aerospace Option, *(August 1995), May 1996**

* Date of Final Defense ** Date of Graduation

Jones, Phyllis, Master's Student ... "Structural Analysis of the QCM/SAW aboard the ER-2/Concorde Flight Experiment." Projected graduation date, May 1997.

Davis, Michelle, Master's Student, Fall 1996.

1994-96 SIRTAS Students

Mr. Omar Karim, Junior, Undergraduate AMP student form Howard University assisted Dr. Jianke Xu in graphical interpretation of robotics attached to platforms. 1994

Mr. Danny Suk Brown, Sophomore, Undergraduate AMP student at Howard University. Assisted Professor Xing Guang Qian in flight dynamics of ER-2, etc. 1994

Michael Brown, Junior, Undergraduate AMP Intern from University of the District of Columbia. Assisted with the ER-2/Concorde practice flight dynamics evaluation with

Prof. Xing. 1995

Anana Harris, Junior, Undergraduate AMP student from Howard University assisted with the ER-2/Concorde practice flight dynamics evaluation and the preliminary structural analysis of the QCM/SAW with Ms. Phyllis Jones. 1995

Sonia Gay, Sophomore, Undergraduate AMP Intern from Morgan State University. Assisted with the 3-D graphical computerized model of the QCM/SAW with Ms. Phyllis Jones. 1996

Steven Curry, Junior, Undergraduate AMP Intern from Howard University. Assisted with study focusing on the possibility of accurately intercepting the wake of a Concorde jet using improved GPS and ground based radar with Prof. Xing. 1996

Publications:

*Xu, J. and Bainum, P.M., "Dynamics of Flexible Multi-link Robot Arms with Mass Center Offset," Acta Astronautica, Vol. 36, No. 2, 1995, pp.99-111.

Li, F., Bainum, PM., Creamer, N.E., Fisher,S. and Teneza, N.C. "Three Axis Near Minimum Time Maneuvers of RESHAPE: Nominal and Experimental Results, " The Journal of the Astronautical Sciences, Vol. 43, No. 2, April-June 1995, pp.161-178.

*Xu, J., Bainum, P.M. and Li, F., "Non-linear Compensation Control of a Manipulator Tip on a Flexible Body," Acta Astronautica, Vol.35, No. 2/3, 1995, pp. 131-142.

Bainum, P.M. and *Xu, J., " Calibration of Tip Position During Maneuver of Space Robotic Systems," The Journal of the Astronautical Science, Vol. 42, No. 1, Jan-March 1995, pp.1-23.

Li, F. and Bainum, P.M. "Analytic Time-Optimal Control Synthesis of Fourth Order System and Maneuvers of Flexible Structures," Journal of Guidance, Control, and Dynamics, Vol. 17, No. 6, Nov-Dec. 1994, pp. 1171-1178.

Li, F., Bainum, P.M. and *Xu, J., "Centralized, Decentralized, and Independent Control of a Flexible Manipulator on a Flexible Base " Acta Astronautica, Vol. 29, N. 3, 1993, pp. 159-168.

*Ericsson, A. J., Bainum, P. M. and Xing, G. Q., "The Optimal LQR Digital Control of a Free-Free Orbiting Platform," Acta Astronautica, Vol. 29, No. 2, 1993, pp. 69-81.

*CSTEA student/former student

Presentations/Conferences:

*Jones, Phyllis D., Bainum, Peter M. and Xing, Guang qian, "Structural Analysis of the QCM aboard the ER-2," NASA University Research Centers Technical Conference

(URC-TC-97), Albuquerque, NM, Feb 16-19, 1997.

*Ericsson-Jackson, A.J., bainum, P.M., and Xing, G.Q., "Structural Modeling for Digitally Controlled Large Orbiting Platforms with Co-Located Actuators and Sensors," 3rd International Conference Dynamics and Control of Structures in Space, London, U.K., May 27-31, 1996, submitted for publication to Acta Astronautica.

Li, F., Bainum, P.M., Creamer, N.G., and Fisher, S. , "Near-Minimum Time Maneuvers of RESHAPE with Flexible Appendages," 20th International Symposium on Space Technology and Science, Gifu, Japan, May 19-25, 1996, Paper No. 96-c-07.

*Ericcson-Jackson, A. J., Bainum, P. M., and Xing, G. Q, "Development of Reduced Ordered Controller for Large Orbiting Platforms in Discrete Time Domain," AAS/AIAA Space Flight Mechanics Meeting, Austin, TX, Feb. 12-15, 1996, Paper No. AAS 96-162.

*Ericsson-Jackson, A. J., Bainum, P. M., and Xing, G. Q., AAS/AIAA Astrodynamics Specialist Conference, Halifax, N.S., Canada, August 14-17, 1995, Paper No. AAS 95-320, accepted for publication, The Journal of the Astronautical Sciences, 1997.

*Xu, J. and Bainum, P.M., "Variable Geometry Compensation Control for a Multilink Flexible Space Manipulator System," Proc. 5th Int'l Conference on Adaptive Structures, Sendai, Japan, Dec. 5-7, 1994, Paper No. B-3-2, Ed. Tani. J. et al, pp. 429-438.

Xing, G.Q., Bainum, P.M. , and Liu, G.R., "Design of a Reduced Order Robust LQG Digital Control System using Degree of Robustness and Degree of Sensitivity," 44th International Astronautical Congress, Graz, Austria, Oct. 16-22, 1993, Paper No. IAF93-A.4.32.

*Xu, J., Bainum, P.M., and Li, F., "Reaction Rejection Techniques for Control of Space Robotic Structures," Proc. of the IMACS/SICE International Symposium on Robotics, Mechatronics, and Manufacturing Systems, Kobe, Japan, Sept. 16-20, 1992, Vol II, pp. 1435-1440.

Xing, G.Q., and Bainum, P.M., "The LQG/LTR Methodology for Discrete-Time Systems," 43rd International Astronautical Congress, Washington, DC, August 28-September 5, 1992, paper No. IAF 92-0039.

Bainum, P.M., *Xu, J. and Li, F., "Modeling and Control Issues for Space Robotic Systems," Proc. of the 23rd Annual Pittsburgh Conference on Modeling and Simulation, Pittsburgh, PA., April 30-May 1, 1992, Ed. by Vogt, W.G. and Mickle, M.H., School of Engineering, Univ. of Pittsburgh, pp.2203-2210.

*CSTEA student/former student

DR. ANAND BATRA (1996) ... Solar Cycle Variations

Anand Batra, with Krishna Kumar, analyzed the data from the UARS/HALOE instrument to examine the solar cycle variation of atmospheric oxide. The time period covered is from October 1991 to February 1996. From HALOE data (version 17), the vertical column densities of nitric oxide and the associated uncertainties were derived. The column densities were separated into two altitude ranges, 30-50 km and 80-140km. The daily averages of the column densities in the equatorial zone 30°N to 30°S and the region poleward of 50° were obtained in the two altitude ranges.

Only for the equatorial belt at the high-altitude range, the column density seems to decrease over the time period by roughly a factor of three. This may be compared with the change in solar activity indicated by the F10.7 index which decreases from 200 in October, 1991 to 75 in February, 1996. Other features that emerged from the analysis are now being examined.

Students:

Jason Demory (Morgan State University) ... SIRTAS 1996

Presentations/Conferences:

C. K. Kumar, A. P. Batra, L. Klein. "Solar Cycle Variation of Atmospheric Nitric Oxide." NASA University Research Centers Technical Conference (URC-TC-97), Albuquerque, NM, Feb 16-19, 1997.

Meeting of the American Geophysical Union, San Francisco, December 15-19, 1996. "Solar Cycle Variation of Nitric Oxide," presented at he 1996 AGU Meeting, San Francisco (with C.K. Kumar, L. Klein, Arun Batra).

DR. ROBERT CATCHINGS (1994) ... Raman Microscopy Studies

The major research accomplishment has been the set-up of a Raman microscopy system in my laboratory. The system required the acquisition of an Olympus metallurgical microscope. The other components of the system, the laser and double spectrometer, were present in the laboratory. The system has been set-up and was operational, but the desired sensitivity has not yet been obtained. The system has the potential of obtaining the spectrum of materials as small as one micron in diameter or films as thin as one micron.

Students:

Summers 1994-1995

The following undergraduate students participated in CSTEA program as Summer research students:

David Burton ... Wendell Lucas ... They performed computer interfacing project involving the National Instruments Laboratory Windows data acquisition software. John Jordan ... Conducted resistance vs temperature measurements. Summer 1994

Michael Idun ... Performed Raman spectroscopy studies on a liquid polymer. Summer 1995

Messrs. Burton and Lucas graduated from the University of the District of Columbia. Currently, Mr. Lucas is attending graduate school in Physics at the University of California-San Diego.

The graduate student, Mr. Lamarr Brown, is currently conducting his Ph.D. thesis work on the project. He was initially supported by CSTEA -- both by tuition and stipend -- but currently his financial support is from a grant in the Graduate School. His project involves the investigation of various microbalance crystal oscillator systems. His support from CSTEA is in the form of equipment and supplies for the PI, Dr. Robert Catchings.

DR. L. Y. CHIU (1994) ... Photolysis And Structure Of *ClONO$_2$* And *ClO$_2$*

(1) Forbidden Photodissociation of Ozone:

To better understand the stratosphere ozone depletion, the spin-forbidden photo-dissociation process of ozone has been investigated theoretically. Through this forbidden process the ground state ozone($^1A_1$) is dissociated into (a) the excited O($^1\Delta$) radical plus the ground state $O_2(X^3\Sigma_g^-)$ molecule or (b) the ground state O(^3P_J) radical plus the excited $O_2(^1\Sigma_g^+$ or $^1\Delta_g)$ molecule. The spin-spin and the spin-orbit interactions in addition to the radiative interaction (which includes the spin-magnetic multipole interaction) have been considered to be the possible photodissociation mechanism. The correlation diagram (the Wigner-Witmer type) of ozone and its dissociated fragments has been constructed. To investigate the possible propensity in certain fine structure level J of the nascent O(^3P_J) radical produced, the relative cross sections of these processes will be computed. The integrals needed will be evaluated by the analytical methods developed in the project (2) below.

(2) Analytical Evaluation of multi-center Molecular Integrals over the spherical Gaussian wave functions:

Integrals over spherical Gaussian wavefunctions are needed when higher angular momentum wave functions are involved, i.e. when heavy elements are included in the molecular computations. Three different methods have been developed to evaluate analytically such molecular integrals, namely (1) rotational and translational expansion method (2) Fourier transformation method via Fourier convolution theorem. and (3) the generalized gradient operator method. The spherical Gaussian used in the first two methods consisted of solid spherical harmonics multiplied into an even powered radial function. In the case of the third method, the even powered radial function is replaced by a generalized Laguerre polynomial. Two-center integrals such as overlap, coulomb

repulsion, nuclear attraction, spin-spin and spin-orbit interactions have all been evaluated analytically. The results have been presented at the 49th International Symposium on Molecular Spectroscopy, Columbus, OH, June (1994), the American Chemical society Annual Meeting, Washington, D.C., August (1994), and the 50th International Symposium on Molecular Spectroscopy, Columbus, June (1995). They have also been published in J. Chem. Phys. **101**(1), 449-458, (1994). and J. Chem. Phys. **104**(2), 616-628 (1996). The results from the third method are more general and simpler. They include four-center two electron integrals in addition to the two center integrals. They have been presented at the 51th International Symposium on Molecular Spectroscopy, Columbus, June (1996), and will be submitted to the Journal of Chemical Physics for publication.

Students:

Graduate student:	Mohammad Moharerrzadeh (not funded), Ph.D. 1995
Undergraduates:	Bridgette McGhee (Summer 1994), B.S. 1995 ... Gerald Levert (Summer 1994), B.S. 1995

Publications:

Translational and Rotational Expansion of Spherical Gaussian Wavefunctions for Multicenter Molecular Integrals." L.-Y. Chow Chiu and M. Moharerrzadeh. J. Chem. Phys. **101**(1), 449-458, (1994).

"Multicenter molecular integrals of spherical Gaussian functions by Fourier transform convolution theorem." M. Moharerrzadeh and L.Y. Chow. Chiu. J. Chem. Phys. **104**(2), 616-628 (1996).

Lue-Yung Chow Chiu and Mohammad Moharerrzadeh "Analytical evaluation of spherical Gaussian Molecular Integrals by Generalized Gradient Operator method," to be submitted to The Journal of Chemical Physics for publication.

Lue-Yung Chow Chiu, M.H. Lin, and S.T. Lai "Ab initio Calculations on the photolysis of Chlorine Nitrate ($ClONO_2$)," to be submitted to Chemical Physics for publication.

Presentations/Conferences:

Lue-Yung Chow Chiu and Mohammad Moharerrzadeh "Molecular Integral of Spherical Gaussian and its Application in different Molecular State Geometries" Abstract, of 49th International Symposium on Molecular Spectroscopy, Columbus, OH, RCO2, P.194, June (1994).

M. Moharerrzadeh and Lue-Yung C. Chiu "Molecular Fine Structure Studies: Spherical Gaussian Integrals of Spin-Spin and Spin-Orbit interactions" Abstract of Physical Chemistry Division, American Chemical society Annual Meeting, Washington, D.C., 253, August (1994).

Lue-Yung C. Chiu and M. Moharerrzadeh "Multicenter spin-spin, spin-orbit and Coulomb repulsion integrals of spherical Gaussian functions by Fourier Transformation convolution theorem" Abstract, the 50th International Symposium on Molecular Spectroscopy, Columbus, OH, RC11, June (1995).

Lue-Yung Chow Chiu and Mohammad Moharerrzadeh "Molecular Multicenter Integrals of spherical Gaussian functions by Generalized Gradient Operator method" Abstract, the 51th International Symposium on Molecular Spectroscopy, Columbus, OH, RCO2, June (1996).

Lue-Yung Chow Chiu, M.H. Lin, and S.T. Lai "Ab initio Calculations on the photolysis of Chlorine Nitrate ($ClONO_2$)" Abstract, the 51th International Symposium on Molecular Spectroscopy, Columbus, OH, RCO2, June (1996).

Professional Meetings & Symposiums

Attended the International Symposium on Molecular Spectroscopy, Columbus, OH, June (1994), and presented: "Molecular Integral of Spherical Gaussian and its Application in different Molecular State Geometries," RCO2.

Attended the Physical Chemistry Division, American Chemical society Annual Meeting, Washington, DC, August (1994), & presented: "Molecular Fine Structure Studies: Spherical Gaussian Integrals of Spin-Spin and Spin-Orbit interactions."

Attended the 50th International Symposium on Molecular Spectroscopy, Columbus, OH, June (1995) & presented: "Multicenter spin-spin, spin-orbit and Coulomb repulsion integrals of spherical Gaussian functions by Fourier Transformation convolution theorem," RC11.

Attended the 51st International Symposium on Molecular Spectroscopy, Columbus, OH, June (1996) & presented two papers: (1) "Molecular Multicenter Integrals of spherical Gaussian functions by Generalized Gradient Operator method" RCO2, and (2) " Ab initio Calculations on the photolysis of Chlorine Nitrate ($ClONO_2$)" RCO2.

DR. BALARAM DEY (1992) ... Satellite Cloud Climatology/Aerosols, Clouds and Climate Interaction

The Principal Investigator conducted research and trained three undergraduate students in the field of satellite cloud climatology.

During January 1993 through December 1995, the research on atmospheric remote sensing was restricted to clouds using visible and thermal infrared wave lengths. NOAA/TIROS-AVHRR visible and thermal infrared cloud data were used in the analyses. The study was focussed on monthly and seasonal variations of cloud cover data over different geographical regions (USA, India, Senagal, Chile). Areas over southern California and southern Kerala indicated significant monthly and seasonal variations of

cloud cover. The most striking features are the seasons of high and low cloud covers in both areas. The southern coast of California had high cloud cover area during low sun period and low cloud cover area during high sun period. In contrary, the southern coast of Kerala had high cloud cover area during high sun period and low cloud cover area during low sun period. The high and low cloud cover areas relate to the seasons of high and low precipitation regimes. The California coast has peak precipitation during low sun period. The peak low sun period precipitation coincides with the southward retreat of subtropical high and advance toward lower latitudes of jet stream and storm belts. Contrary to California, the Kerala coast has peak precipitation during high sun period. The high sun period peak precipitation coincides with the summer (southwest) monsoon circulation in that region.

During January 1996 through December 1996, the research was restricted to aerosols, clouds and climate interactions. Greenhouse effect is a climatological fact of life. Atmospheric gases, particularly, CO_2 trap and hold heat resulting in warmer temperature at the earth's surface. Aerosols scatter, and also reflects sunlight back to outer space and, therefore, less solar radiation at earth's surface. The tropospheric aerosols cools climate in two ways: directly through the absorption of solar radiation, and indirectly, through modifying the optical properties and life time of clouds. The principal investigator is still examining the interactions between aerosols and climate forcing.

Students:

Undergraduates: Ramona Hilton (BS), Jeffery J. Hall (BS), and Christopher Hunter

Publications:

Dey, B., 1994: Monitoring the onset of summer monsoon over Kerala, India with satellite AVHRR visible and TIR cloud data, Abstract 1994 Western Geophysics Meeting, Hong Kong, July 1994, p.23.

Dey, B., 1995: Satellite cloud climatology for southwest California, USA and south-west Kerala, India, Indian Jn of Landscape Systems & Ecological Studies, 18(2), 73-78.

Dey, B., in press: Aerosols, clouds and climate interactions - a review, submitted for publication.

Presentations/Conferences:

1994: Western Geophysics Meeting, Hong Kong, July 1994.

DR. JOSHUA HALPERN (1992) ... Dynamics With Chemical Applications To Atmospheric Processes

The Halpern group's CSTEA research concentrates on free radicals and small

molecules, including kinetics, energy transfer and spectroscopic studies. We have worked in three areas: atom-radical reactions, energy transfer in small molecules and detection of molecules of atmospheric interest.

A. CN Energy Transfer

Our initial CSTEA project was a detailed study of CN energy transfer between involving roughly equi-energetic levels of the $A^2\Pi_i$ and $X^2\Sigma^+$ states[1-6]. The CN radical plays an important role in nitrogen-methane planetary atmospheres and comets, but it is also an important marker for spectroscopic observations of many different systems including red stars and diffuse interstellar clouds. Our research is needed to interpret such CN $A^2\Pi_i$ emission especially where there are collisions. Among the results were an improved value for the CN heat of formation[2], better measurements of CN $A^2\Pi_i$ v=2..7 radiative lifetimes[3,4] and electronic and vibrational state to state collisional rate constants involving many different partners. We demonstrated that the major collisional energy transfer mechanism was from a particular electronic state (X or A) vibrational level to the nearest energetically lower lying vibrational level of the other (A or X) electronic state[4,5]. Our new radiative lifetime measurements were particularly important to evaluation of the nitrogen content of cool stars, which is determined by observation of the strength of CN $A^2\Pi_i$ - $X^2\Sigma^+$ red system emissions. Our attempts to complete this study by observing the lowest two vibrational levels of the $A^2\Pi_i$ electronic state have failed because of the lack of a good detector at wavelength longer than 1000 nm. We hope that acquisition of a high sensitivity diode detector (InGaAs) (detectivity of 3 x 10^{-4} V/W and a 125 Mhz bandwidth) will enable us to detect fluorescence from the v=0 and 1 levels.

In addition, during the course of these studies on CN energy transfer, we collaborated with a group at the US Army Ballistic Research Laboratory in Aberdeen MD on the CN $B^2\Sigma^+$ - $X^2\Sigma^+$ (3,0) two photon absorption which is resonantly enhanced by the $A^2\Pi_i$ v'=4 level[7].

B. Spectroscopy and Photophysics of Cyanoacetylenes

Over the years our group has published many studies on the spectroscopy, chemistry and photophysics of cyanogen (ethanedinitirile), cyanoacetylene (propynenitrile) and dicyanoacetylene (butynedinitrile). These are among the most photochemically active molecules in nitrogen-methane atmospheres such as Titan, and, although minor species by concentration, an understanding of their behavior is needed. The long chain cyano-acetylenes are also prominent in observations of interstellar clouds. The mechanism for synthesis of these molecules is not well understood. To date, CSTEA supported work has concentrated on C_2N_2. It includes measurements of UV absorption cross-sections, and characterization of the excess energy distribution following UV dissociation by CN red system LIF. We studied the $A^1\Sigma_u^-$-$X^1\Sigma_g^+$ and $B^1\Delta_u$-$X\ ^1\Sigma_g^+$ transitions in detail with high resolution absorption spectra, LIF and dispersed fluorescence spectra in the $A^1\Sigma_u^-$-$X^1\Sigma_g^+$ transition (which we discovered[8]) and photofragment excitation spectra over the entire UV region. Lifetimes, dissociation and fluorescence quantum yields were determined for accessible vibrational levels in the $A^1\Sigma_u^-$ state and dissociation yields were measured for the $B^1\Delta_u$ state[1]. One paper has been submitted, another is finished and

two more are in preparation.

Last year we submitted a proposal to the NASA/Planetary Atmosphere program, which was not funded, but which will be resubmitted this May. We propose to study emission and photodissociation yield spectroscopes of HC_3N and NCC_3N. In addition we will attempt to find the C_3N free radical LIF spectrum. HC_3N, although less common than HCN[9], is photochemically more important, since their dissociative absorption spectra start at 240 nm and less than 190 nm respectively. For Titan's atmosphere, HC_3N is about ten times more common than C_2N_2 whose dissociation limit lies at 212 nm. We have shown that the primary photochemical process in the dissociation of HC_3N yields $H + C_3N$, it is likely that the carrier of nitrile chemistry in nitrogen-methane atmospheres and interstellar clouds will be C_3N[10].

C. Rotational Energy Transfer

A continuing collaboration on rotational energy transfer with Prof. Helmut Zacharias' group at the University of Essen has been very fruitful. Stimulated Raman pumping is used to excite a single rotational level of a Raman active vibrational mode. While our studies to date have used acetylene, we intend to broaden our work to include atmospherically important molecules such as nitrogen, methane and hydrogen. We have measured state-to-state collisional transfer cross-sections for acetylene with itself and several small atoms and molecules. These are particularly important, because *ab initio* potential energy surfaces are available for some of these systems, and the theoretical predictions can be evaluated against the measurements[11]. Moreover, simple parameterizations are available for such collisions[12]. Both *ab initio* theory and parameterizations are attractive for inclusion in atmospheric models to characterize energy transfer process, but must be validated against experiment. In particular our measurements of the elastic and inelastic collisions which alter the molecule's spatial orientation and alignment should be very sensitive tests of the theories[13-15]. We are also collaborating with a theoretical group at the University of Nijmegan in the Netherlands who are now calculating the probability of rotationally inelastic collisions of acetylene with helium to compare with our experimental data. In the coming summer, we will begin studying atom-molecule reactions of vibrationally excited and aligned molecules. Near IR combination bands will also be excited to measure energy transfer in states with about 1 eV of vibrational energy.

D. Radical Reaction Kinetics

Work on reaction kinetics of atoms and free radicals is being carried out at Howard by Dr. Tanya Titarchuk. We have published rate constant measurements for the reactions $CN + O$ and $CN + SO_2$[16]. To study the first reaction, CN was produced by excimer laser photolysis of BrCN and O atoms by excimer laser photolysis of N_2O or SO_2 We have tried and will continue to try detecting the CO products from the $CN + O$ reaction by laser induced fluorescence and multiphoton ionization.

E. Detection of Atmospheric Molecules

In 1995 we started use CW diode laser probes as a probe for atom-radical reactions and energy transfer experiments. The CW nature and narrow bandwidth of these lasers makes them ideal for kinetics and dynamics experiments. CN and NH_2 have low lying electronic levels which can be directly excited. A CSTEA graduate student has built a grazing incidence cavity external cavity for a NIR diode laser.

In order to gain more experience with diode lasers, we began to collaborate with several groups at NASA/GSFC who build and operate diode laser LIDAR systems. This has grown into a more formal collaboration on their project to This proposal is an extension of work at NASA/Goddard Space Flight Center to develop a miniature LIDAR for the Mars Lander. It involves scientists from the Laboratories for Atmospheres (Code 917) and Terrestrial Physics (Code 924) as well as the Engineering Directorate Optics Branch (Code 717). In addition there are collaborators at Bucknell University and NOAA. Since the fall of 1995 I have been doing research with the group, both on this project and on improving a LIDAR now operating at the South Pole. Our current emphasis is to build a 935 nm diode laser DIAL system for sensing water vapor on Mars. As opposed to the 811 nm LIDARs used on earth, the roughly 200 times stronger 935 nm absorption makes sense for Mars with its drier and less dense atmosphere. My contribution has been to provide spectroscopic information on the weak water overtone absorption at 935 nm as well as identifying sources of 935 nm lasers.

Over the past two years we have developed a new concept for detection of atmospheric trace gases - photodissociation excited fluorescence signature analysis. It is a development of a method which we had demonstrated in 1980, multiphoton laser photofragmentation fluorescence (MLPF)[17]. In that case, a focused ArF excimer laser beam was used to detect ammonia, by monitoring the multiphoton induced NH emission.

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Students:

Yuhui Huang - Chemistry, Ph.D. 1993. Thesis: Photophysics and Photochemistry of Ethanedinitrile and the CN Radical. After graduation, Dr. Huang took a post-doctoral position at Tulane University with Prof. Mark Sulkes, where he built a time of flight laser desorption mass spectrometer. He is now working in Prof. Alex. Wodtke's group at the University of California, Santa Barbara.

Timothy E. Betton - Undergraduate, Freshman, 1993-94, Nursing

James Smith - Undergraduate, Junior, 1996, Chemical Engineering

Bronjelyn Newman - Graduate, first year, 1996, Chemistry. Helped build an external cavity diode laser system.

Publications:

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National American Chemical Society Meeting, Boston, MA, April 1992 ... "The Radiative Lifetime and Quenching of CN ($A^2\Pi_i$)"

International Laser Science Meeting, Albuquerque, NM, September 1992 ... "Energy Transfer Between and Among the CN ($A^2\Pi_i$) and ($X^2\Sigma^+$) Electronic States"

Dalian Institute of Chemical Physics, Dalian, China, May 1993 ... "Energy Transfer in CN Free Radicals" and "The Spectroscopy of C_2N_2"

Chemical Physics Institute, Chinese Academy of Sciences, Beijing, China, May 1993, "Energy Transfer in CN Free Radicals"

Department of Physics II, Fudan University, Shanghai, China, May 1993, "Energy Transfer in CN Free Radicals"

International Conference on Chemical Kinetics, NIST, Gaithersburg, MD, July 1993 "Energy transfer in CN Free Radicals"

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Conference on High Resolution Spectroscopy, Riccione, Italy, September 1993, "The Spectroscopy of C_2N_2"

Department of Physics, Universitaet Kaiserslautern, Germany, November 1993, "Energy Transfer in CN Free Radicals"

Department of Physical Chemistry, Free University, Amsterdam, NL, April, 1994, "The Spectroscopy of C_2N_2"

American Chemical Society National Meeting, Washington, DC, August 1994, "Rotational Energy Transfer in Acetylene"

Chemistry Department Seminar, Howard University, Washington, DC, September 1994, "Rotational Energy Transfer in Acetylene"

Chemistry Department Seminar, Catholic University, Washington, DC, September 1994, "Rotational Energy Transfer in Acetylene"

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Gordon Conference on Molecular Energy Transfer, Ventura, CA, January 1997, "Rotational Orientation by Stimulated Raman Pumping"

NASA University Research Centers Technical Conference (URC-TC-97), Albuquerque, NM, Feb 16-19, 1997, The $C_3N_2C^1B_u <- X^1\Sigma_g^+$ Transition: Assignment of the Electronic State Origin and Vibrational Bands.

DR. PETER HAMBRIGHT (1994) ... The Nature Of Interstellar Dust And Gas Sensors

Although it has been over sixty years since their discovery, the species responsible for the more than 160 Diffuse Interstellar Bands (DIBs) from the absorption spectra of reddened stars which lie behind clouds of interstellar dust are unknown entities (W. H. Snow in *The Diffuse Interstellar Bands*, A. G. G. Tielens and T. P. Snow eds. Kluwer Press, Boston, 1995, Chap 1). The DIBs lie in the visible and near IR from 4000 to 13,000 Å, and are broader (0.8 - 30 Å) that atomic lines. Suggestions have been made

that the DIBs arise from polycyclic aromatic hydrocarbon cations (PAHs), polycarbon chains, the polyhedron form of carbon, C60 in its radical cation form. or unspecified organic fragments. The DIBs may come from small grains, or molecules on the surfaces or interior of grains. A recent review states that such proposals "....are either not supported by observations or await better data" (G. H. Herbig, Annu. Rev. Astrophys. 1995, 33, 19).

There have been several proposals that porphyrins and metalloporphyrins are constituents of interstellar dust. Miles and Sarre (J. Chem. Soc. Faraday Trans, 1993, 89, 1075) noted that the 6284.5 Å band from supersonic jet work of the simplest reduced porphyrin, the chlorine of porphin, matched in position and width the 6283.86 Å DIB peak. Johnson (*The Diffuse Interstellar Bands*, op cit. Chap 6) has claimed that the molecule bispyridine magnesium tetrabenzoporphyrin (MgTBPPy2) is responsible for more than 150 DIBs. We have studied the question of porphyrins as DIBs carriers. Johnson and others have attempted to match one of the strongest DIBs at 4428 Å band with laboratory species, and this was the starting point of our work. Johnson claims that only the porphyrin MgTBPPy2 has a 4428 Å peak, and pyridine is required to be present and coordinated to the central Mg atom. However, pyridine has not yet been identified as an interstellar molecule. We synthesized about fifty new porphyrins, not in the structural TBP class, and nine of them featured a near 4428 band, without the presence of pyridine. The new compounds either had protons at the center, or contained metals (P, Fe, W, Cr, Zn) in different oxidation states. The common feature was a metal in a high oxidation state, or a deformed porphyrin nucleus. Our absorption spectra were obtained in three types of frozen glasses at 77 K. Thus, MgTBPPy2 is not a unique porphyrin, and other porphyrins can be made with the 4428 feature. Most of Johnson's 150 bands were of fluorescence origin, but Donn and Khanna (App. Space Sci, 1980, 68, 19) are of the opinion that the DIBs cannot be in such electronically excited states. The five or six absorption bands of our porphyrins in the visible range are similar in wavelength to certain DIBs, but the overall relative intensities and bandwidths of all of the peaks are not in agreement with the DIBs. In addition, it is not obvious why one porphyrin, rather than a series of species should be present in space. A better technique will be to study such species using helium gas matrix isolation techniques, which better mimic the conditions of interstellar space. Such studies are planned later this year, when this apparatus is available at Howard. As it is, the question of matrix and intensity shifts are present in the current results, and our five or six wavelengths may in fact agree with some of the 160 DIBs peaks simply by chance. We synthesized the chlorine of porphyrin, and find that its strongest band at ~3900 is not a DIB peak, so this species might be eliminated from further consideration.

The tetrabenzoporphyrins mentioned by Johnson are a relatively under-studied class of porphyrin. However a recent method allows gram amounts to be prepared, and we then examined the solution coordination chemistry of this class of compounds, as the basis of a MS thesis for Ms. Cromer. She determined the stability constants of pyridine binding with Zn, Cd, Mg, VO(IV), Ni and Cu TBPs, and the entropy and enthalpy of pyridine ligation to the MgTBP. The latter values were negative, indicating that pyridine complexation was favored at low temperatures, in agreement with Johnson's dipyidinate hypothesis. The stability constants were compared to those of octaethylporphyrin, which

has saturated substituents around the beta-pyrrole positions, whereas those of TBP are conjugated benzene rings. She studied the rate laws for zinc and cadmium incorporation into both porphyrins, and certain acid solvolysis reactions. The general conclusion was that the TBPs are rigid molecules, and their observed coordination chemistry can be understood on this basis. These molecules are similar to phythalocyanines, which have been explored as NO2 sensors.

We attempted to purify the Cu(II) and Fe(II) tetrabenzoporphyrins by sublimation at high temperatures. Field and temperature dependent magnetic susceptibility studies done in Professor Thorpe's lab indicated that the Cu(II) TBP showed normal paramagnetic behavior. However, the Fe(II)-TMP gave evidence of superpara-magnetism, that is, magnetic susceptibilities substantially above paramagnetic values. The origin of this phenomena is the presence of very small iron particles, which arose during the decomposition of the iron porphyrin during the sublimation process. These small particles are of the order of magnitude of the size of interstellar dust particles. In addition, they are magnetic, also a necessary feature of interstellar dust. This work will be continued.

While we await construction of the matrix isolation apparatus, we are considering metalloporphyrins in the solid state as complexing agent for gas molecules, such as dioxygen, dinitrogen, CO, CO2, NO, N2O, N2O4 and O3. Different metals in the porphyrin will hopefully have selective affinities for certain species and not others, ie, Fe(III) for NO, Fe(II) for CO. This work will be done using surface acoustic wave (SAW) delay line oscillator devices, which we have at Howard.

Students:

Spring 1994	Quintence Mays, undergrad, Junior
Summer 1994	Quintence Mays, undergrad ... Cosmos George, undergrad ... Maressa Frederick, undergrad
Fall 1994	Quintence Mays, undergrad
Spring 1995	Quintence Mays, undergrad ... Sabrina Cromer, grad student
Summer 1995	Quintence Mays, undergrad ... Duyanne Jones, undergrad ... Sabrina Cromer, grad
Fall 1995	Quintence Mays, undergrad ... Sabrina Cromer, grad student
Spring 1996	Sabrina Cromer, grad student
Summer 1996	Dame Forbes, undergrad ... Sabrina Cromer, grad student
Fall 1996	Dame Forbes, undergrad ... Sabrina Cromer, grad student ... Yolanda Person, grad student
Spring 1997	Dame Forbes, undergrad ... Yolanda Person, grad student

Graduate: Ms. Sabrina Renee Cromer, M. S., Howard University December, December 1996. Thesis: "Solution Chemistry and Interstellar Implications of Tetrabenzoporphyrins." Ms. Cromer left Howard, and is seeking an industrial position.

Publications:

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Poster Session, P. Hambright and R. Pasternack, 207th American Chemical Society National Meeting, San Diego, CA, March 1994, "Resonance Light Scattering Studies of Porphyrin Diacid Aggregates."

Poster Session, P. Hambright and Kathy Parris, 2nd National Conference on Diversity in the Science and Technological Workforce, Washington, DC, October 1994, "The Synthesis and Properties of Water Soluble Sulfonated Porphyrins Containing both 2,6-dichlorophenyl and Phenyl Groups."

First National Student Conference of National Alliance of NASA Research Centers at Minority Institutions. Greensboro, NC March, 1996, S. Cromer, P. Hambright and Q. Mays "Do Porphyrins and Metalloporphyrins Occur in Interstellar Dust?"

Other:

Appointed to the Editorial Board of the new international Journal of Porphyrins and Phthalocyanines, Nov 1996.

DR. GARY HARRIS (1992) ... Silicon Carbide Crystal Microbalances

In this section, we propose to develop, calibrate and furnish the thrust areas with silicon carbide crystal microbalance (SiCCM) sensors for real time monitoring of atmospheric trace gas species, various pollants and other contaminates that are associated with NASA and CSTEA missions. The work also involved understanding the technology of SiC devices and applications.

Accomplishments

- Growth of $(AlN)_x(SiC)_{1-x}$ on 6H and 3C SiC for sensor applications
- Fabrication of high breakdown 3C SiC ion implanted diodes
- Design, fabrication, and characterization of SiC monolithic integrated op-amp circuit
- Development of SiC photoconductive UV devices
- Ion implantation and characterization of Be, N, and V in SiC
- SiC bulk delay lines
- Design of silicon carbide crystal microbalance (SiCCM)

Students:

1. Kalu K. Diogu, "Design Fabrication and Characterization of Beta Silicon Carbide MESFET Monolithic Operational Amplifier with an AlN Isolation Layer of (100) 6H-SiC," Ph.D. Thesis, May 1996
2. Granvill David Lee, Jr. "Ohmic Contacts Developed on 3D Silicon Carbide," Master Thesis, August 1995
3. Deven M. Collins, "The Characterization and Photoelctrochemical (PEC) Etching of Silicon Carbide and Other Semiconductor Materials for Micro-Machines and Device Applications," Master Thesis, August 1995
4. Juan White, "Ion Implantation into SiC," May 1996
5. Haldene S. Henry, "Design and Fabrication of SiC Crystal Microbalances," Ph.D., August 1997

Publications:

K. K. Diogu, G.L. Harris, H. S. Henry, K. Wongchotigul, M.G. Spencer, A, Mahajan, W. Wohlmuth, I. Adesida , F. Moeller, R. A. Bertram , "Implementation of a 85 MHZ High Temperature b-SiC MESFET Operational Amplifier, Third International High Temperature Electronics Conference (HiTEC), June 9-14, 1996, Transactions, Vol. 1 VIII-21,21-31

S. Sheng, X. Tang, M. G. Spencer, P. Zhou, K. Wongchotical and G. L. Harris, "The Performance of 3C-SiC Photoconductive Switch," Third International High Temperature Electronics Conference (HiTEC), June 9-14, 1996, Transactions, Vol. 2, P-257, 257-62

J. Coleman, G. L. Harris, and C. Taylor, "Fabrication of Beta Silicon Carbide Diodes Using Proton Isolation," Third International High Temperature Electronics

Conference (HiTEC), June 9-14, 1996, Transactions, Vol 2, p-83, 83-89

S. Sheng, M. G. Spencer, X. Tang, P. Zhou, and G. L. Harris, "An Investigation of 3C-SiC Photoconductive Power Switching Device," Materials Science and Engineering B, June 1996

D. Collins and G. L. Harris, "N-type SiC Electrochemical Etching Without Ultra-Violet Photoexcitation," Materials Research Society Conference Proceeding, Spring 1996

D. M. Collins and G. L. Harris, "Photocurrent Sensitivities, Surface Color and Auger Spectroscopy of SiC by Photoelectro-chemical Etching," Materials Research Society Conference Proceeding, Spring 1996

K. K. Diogu, G. L. Harris, K. Wongchotigul, H. S. Henry, C. Taylor and M. G. Spencer, "The Design and Computer Simulation of High Temperature B-SiC MESFET Operational Amplifier," Proceeding of the Workshop on High Temperature Power Electronics for Vehicles, 1995

G. L. Harris (ed.) "Properties of Silicon Carbide," INSPEC publication, July 1995

G. L. Harris, K. Wongchotigul, H. Henry, K. Diogu, C. Taylor and M. G. Spencer, "Beta SiC Schottky Diode FET Inverters Grown on Silicon," Chapter 7, 715-717, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materials Institute of Physics Conference Series Number **137** 1994

D. O. Arugu, G. L. Harris, and C. Taylor, "The Effects of Anneal Temperature on the Electrical Characteristics of nickel based Ohmic Contacts to º-SiC," accepted for publication Electronics Letters

Presentations/Conferences:

The Effect of Source Powder Height on the Growth Rate of 3C-SiC Grown by the Sublicmation Technique, H.N. Jayatirha and M.G. Spencer, Proceedings of the International Conference on Silicon Carbide and Related Materials, 1995, Kyoto, Japan.

A Variable Potential Porous Silicon Carbide Hydrocarbon Gas Sensor, V.B. Shields, M. A. Ryan, R. M. Williams and M. G. Spencer. Procedings of the International Conference on Silicon Carbide and Related Materials, 1995 Kyoto Japan.

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Kalu Diogu. Implementation of an 83 Mhz High Temperature b-SiC MESFET Operational Amplifier. Device Research Conference, June 21-24, 1996.

Haldane Henry. "Preliminary Studies on Silicon Carbide Bulk Acoustic Wave Devices." NASA URC/TC Conference in Albuquerque, NM, February 16-19, 1997.

DR. LEWIS KLEIN (1992) ... Line Mixing Studies

Dr. Klein completed the theory of the Hanle effect for the potential measurement of planetary magnetic fields. The results were presented at the 1994 fall meeting of Am Geophys. Union, San Francisco, CA Dec. 7-11. A very detailed presentation was made to David Glenar of NASA. This was followed by a discussion of the feasibility of using his acoustooptical spectrometer for the proposed test case measurements of the magnetic field in the earth's atmosphere. It was determined that Glenar;s instrument does not have the sensitivity to perform these measurements. A special purpose spectro-polarimeter is under consideration as a joint project.

Calculations of the depolarization due to the Hanle Effect on solar radiation scattered by the Gamma bands of NO and the first negative band system of N2 + were performed in 1994-95. The results of theses calculations permit one to relate the change in the plane of polarization of the scattered light to the strength and direction of the magnetic field present. These calculations have demonstrated that for magnetic fields in the militesla to microtesla range, the polarization of these lines is reduced from a range near 10% to about 1%. The remote observation of the depolarization of solar scattering by these bands can therefore be used to accurately measure the fields present at the altitude of the molecular layer involved in the scattering. Part of these calculations were

presented at the Am. Geophys. Union annual meeting in San Francisco, Dec. 5-9, 1995.

Professor Klein has also undertaken a theoretical investigation of the effect of line mixing collisions on the spectral line shape of molecular species of interest to climate models. Understanding the deviations from the usual Lorentzin line profile is important in the physics of modeling the temperature structure and the vertical height mixing ratio of atmospheric species. It is also possible that calculations of the effect of line mixing will be important for the determination of minor constituents in spectral regions where the stronger lines have windows created by the Line Mixing Effects in narrowing effect of mixing collisions. A frequency redistribution function that would be useful for line by line radiative transfer calculations is also under study. The works based on the published work on the plasma redistribution function, performed under the auspices of CSTEA. Results related to theses calculations were presented at the Am. Geophys. Union annual meeting in San Francisco, Dec. 13-19, 1996.

Students:

1995 Summer research project of graduate student in physics, Anthony Quash.
Dr. A. Asfaw, Ph.D. in Physics, Spring 1993.

Publications:

L. Godbert, A. Calisti, R. Stamm, B. Talin, J. Nash, R. Lee, L. Klein, S. Glenzer, and H-J. Kunze, "Plasma Spectroscopy of n=4 to 3 CIV and NV Lines in Hot and Dense Plasmas," Phys. Rev **E49**, 5889 (1994).

L. Godbert, A. Calisti, R, Stamm, B. Talin, R. Lee, and L. Klein "Plasma Diagnostics with Spectral Line Shapes," Phys. Rev. **E49**, 5644 (1994).

S. Glenzer, Th. Wrubel, S. Büscher, H.-J. Kunze, L. Godbert, A. Calisti, R. Stamm, B. Talin, J. Nash, R. Lee, and L. Klein. J. Phys. B: At. Mol. Opt. Phys. **27**, 5507, 1994.

B. Talin, A. Calisti, L. Godbert, R. Stamm, R.W. Lee and L. Klein, "Frequency Fluctuation Model for Line Shape Calculations in Plasma Spectroscopy," Phys. Rev. **A51**, 1918 (1995).

J. Koch, K. Estabrook, J. Bauer, C. Back, L. Klein, A. Rubenchick, E. Hsieh, R. Cook, B. MacGowan, J. Moreno, D. Kalantar, and R. Lee, "Time-Resolved X-Ray Imaging of High-Power Laser-Irradiated Under-Dense Silica Aerogels and Agar Foams," Phys. Plasmas **2**, 3820 (1995).

N. Woolsey, A. Asfaw, B. Hammel, C. Keane, R. Lee, A. Calisti, L. Godbert, C. Mossé, M. Koubiti, R. Stamm, B. Talin, J. Wark, R. and L. Klein, "Spectroscopic Study of Compressed High Energy Density Matter," Phys. Rev **E53**, 6396 (1995).

C. Mossé, A. Calisti, M. Koubiti, R. Stamm, B. Talin, J. Koch, R. Lee and L. Klein. "Redistribution of Resonance Radiation in Hot Dense Plasmas," (to be submitted to Phys.

Rev E.)

C. Mossé, A. Calisiti, M. Koubiti, R. Stamm, B. Talin, J. Koch, A. Asfaw, R. Lee, J. Seely, and L. Klein, "X-Ray Laser Photopumped Resonance Fluorescence," (To be submitted to Phys. Rev. E.)

Presentations/Conferences:

1992 Fall meeting of Am. Geophys. Union, San Francisco, CA, Dec. 7-11, 1992. C.K. Kumar and Lewis Klein, "Remote Sensing of Ionspheric Magnetic Field."

1993 Fall Meeting of Am. Geophys. Union, San francisco, CA, Dec. 7-9, 1993. C.K. Kumar and Lewis Klein, "Remote Sensing of Magnetic Fields in the Ionosphere."

1994 Fall Meeting of Am. Geophys. Union, San Francisco, Dec. 5-9, 1994. Kumar and Klein "Remote Sensing of Planetary Magnetic Fields."

American Geophysical Union in Baltimore, May 30-June 2, 1995.

1995 Fall Meeting of Am. Geophys. Union, San Francisco, Dec. 5-9, 1995, Kumar and Klein "Remote Sensing of Planetary Magnetic Fields."

1996 Fall meeting of Am. Geophys. Union, San Francisco, Dec. 14-19, 1996, Batra, Kumar and Klein "Solar Cycle Variation of NO."

DR. C. K. KUMAR (1992) ... Nitric Oxide Studies

In 1992 Kumar began changing his research field from astrophysics to atmospheric sciences. His first project, in collaboration with Lewis Klein was to develop the theory of Hanle effect with the goal of measuring the polarizations of resonance fluorescence lines in the spectra of planetary atmospheres to measure magnetic fields.

In 1993 Kumar started working on the study of nitric oxide in the terrestrial atmosphere with particular emphasis on the measurements of thermospheric and mesospheric concentrations of NO. This was done in collaboration with colleagues at JPL and JHU/APL. The research involved the analysis of data from the shuttle borne ATMOS spectrometer which measured solar occultation spectra in the IR. Following the publication of the results from this study of the ATLAS1/ATMOS data, Kumar has been supervising the M.S. thesis work of graduate students who have analyzed the data from the ATLAS2/ATMOS and ATLAS3/ATMOS experiments, all to derive nitric oxide mixing ratios in the thermosphere and mesosphere.

At this time Kumar is working with Batra and Klein to measure the solar cycle variation of nitric oxide in the earth's atmosphere. The work involves the analyses of data from the HALOE instrument on the UARS. The data was taken from 1991 to now (1/97) and covers the time from near the solar maximum to the current minimum.

Students:

Igwe Anya, MS in Physics, January 1997. Research on "Oscillator Strengths of Ar I Lines in the Vacuum Ultraviolet."

Anthony Patrick, BS in Physics, 1994. MS candidate; research on "Thermospheric Nitric Oxide from ATLAS/ATMOS." Research is completed and student is writing thesis.

Jerome Colvin, MS research on "Nitric Oxide from ATLAS/ATMOS." Thesis incomplete.

Publications:

"Thermospheric Nitric Oxide-Analyses of ATLAS1/ATMOS Data." C. Krishna Kumar, P.K. Swaminathan, D.E. Anderson, J.H. Yee, M.R. Gunson, M.C. Abrams, 1995, J. Geophysical Res. (Atmospheres), **100**, 16839.

"Nitric Oxide Abundance in the Mesosphere/Lower Thermosphere: Roles of Solar Soft X rays, Suprathermal N(^{4}S) Atoms, and Vertical Transport" P.K.

Presentations/Conferences:

"Measurement of Planetary Magnetic Fields by the Hanle Effect." C. Krishna Kumar and Lewis Klein, 1993 Fall AGU meeting.

"Nitric Oxide in the Thermosphere from ATLAS/ATMOS Measurements." C. Krishna Kumar P. K. Swaminathan, D. E. Anderson, M. R. Gunson, 1994 Fall AGU Meeting.

"Solar Cycle Variation of Nitric Oxide." C. Krishna Kumar, A. Batra, and Lewis Klein, 1996 Fall AGU Meeting.

DR. JAMES LINDESAY (1992) ... Computational Atmospheric Sciences

The Computational Physics Laboratory provides computational resources to students in the Department of Physics. The laboratory serves as the network hub for the entire Department and provides continuous resources for student research projects. In addition, the Laboratory provides a multi-disciplinary research environment with students involved in projects involving cosmology, biophysics, quantum field theory, condensed matter theory, and atmospheric physics and chemistry. This affords the students an opportunity to learn about several different disciplines and to develop broad based skills and exposures during the group meetings and presentations. Graduates of the group have excelled at institutions such as the University of Michigan (Beth Brown, BS in physics with honors suma cum laude, Phi Beta Kappa, "Black Holes, Do They Exist?"), Johns Hopkins University (Aaron Roane, MS Program, "Atmospheres Near Gravitationally Condensed Objects") and Georgia Tech (Gena Poe, BS in physics with honors, Summa cum laude, Phi Beta kappa, Stolonifier"). One of the present post-doctoral scholars

received his Ph.D from research within the group in 1990 (Devon McIntosh, Ph.D. "Microwave Gap Enhancement in Low Temperature Superconductors"). At present, the Laboratory supports about 15 students and post-docs, 6 of whom are associated with CSTEA, and has been the primary research group for 15 past and present CSTEA students.

Edward Colon, a graduate student, has already begun collaborations with NASA personnel on modeling Earth's atmosphere for a potential PhD project. Mr. Colon successfully defended his MS thesis on "Tidal effects on Titan's Atmosphere" during the summer of '95, and is continuing to progress admirably in his develop computational, networking, and programming skills as well as infrastructural support for graduate, post-doctoral, and faculty research efforts. Equipment support from CSTEA has been minimal in the past, and it is felt that the demonstrated utility of the computational facility for CSTEA's stated goals has justified that support. The Computational Physics Laboratory will continue to provide scholars with high end resources in the development of their academic talents, and NASA's support has enhanced these efforts, as well as provided those students in the group with expressed interests in atmospheric science with additional resources on their behalf.

Research Accomplishments

- Examined contribution of solar charging of fair weather earth electric field due to semiconducting components of water covered soils;
- Examined time dependent tidal effects on Titan's atmosphere due to Saturn's gravitational field;
- Examined behaviors of gaseous matter near dense gravitating objects.

Students:

Edward Colon:	Physics PhD candidate; Titan Tidal Effects; MS '95
Aaron Roane:	Physics MS candidate Grav dense objects until 1995; has passed Physics PhD qualifiers, Johns Hopkins University
Lamarr Brown:	Physics PhD candidate: Weighted oscillators - '95 works with new PI
Michelle Bell:	Physics - BS '95; Medical School
A. Patrick:	Systems operator - 1994
M. Figueroa:	Physics-Physical Therapy Systems operator continuing Under-graduate Director of Laboratory
Talibah James:	Physics - '95
Tanya Fulgham:	EE Senior Systems operator -'95
Marcus Alfred:	Physics PhD candidate Few particle physics -'95
Kecia Franklin:	Physics Junior Model flight experiment -'96 discontinued from program
S. McFarlane:	Physics Junior transferred to Atlanta
Lydia Kearney:	Physics Junior Research Networking continuing
T. Richard:	Chem. E. Junior Research networking continuing

C. Jackson: Physics MS candidate Cosmology first year grad

Summer Students

Have been directly involved with design and operation of Summer program since its inception.

Summer 1994: Mariesol Figueroa (systems operator) and Talibah James
Summer 1995: Stephanie McFarlane (Smith) (laboratory operations); Lydia Kearney (internet home page); Thefarro Richard (modeling of static plumes); Nikki-Nicole Miles (modeling of particle detectors).

Publications:

"Possible Solar Recharging of the Earth's Electric Field", D. McIntosh & J. Lindesay, accepted, Meteorology and Atmospheric Physics Journal; "Modelling Gravitationally Induced Semidiurnal Stationary Tidal Oscillation in Titan's Icarus (International Journal of Solar System Studies).

Presentations:

Edward Colon and Devon McIntosh Conference support
Where: NASA Earth Science Summer School, Cal Tech in Pasadena CA.
When: July 16-20, 1995
Topic: Earth Science Including Atmospheric Chemistry and Physics

Anthony Patrick conference support
Where: AT&T Learning Solutions Workshop, Los Angeles, CA
When: July 1994
Topic: TCP/IP Network Training

Edward Colon:
Where: NASA URC/TC Conference in A&T State University, Greensboro, North Carolina
When: March 31-April 2, 1996
Topic: Modelling Standing Title Oscillations in Titan's Lower Atmosphere

Edward Colon
Where: NASA URC/TC Conference in Albuquerque, NM
When: February 16-19, 1997
Topic: The Onset of the Madden-Julian Oscillation Within an Aquaplanet Model

DR. PRABHAKAR MISRA (1992) ... Laser Spectroscopy of Free Radicals of Atmospheric Significance

Laser-induced fluorescence (LIF) excitation and wavelength-resolved emission spectra of six atmospherically significant alkoxy (RO; R=CH_3, C_2H_5, i-C_3H_7) and alkylthio (RS) radicals have been obtained under moderate (0.2 cm^{-1}) and high (0.07 cm^{-1}) resolution. *For C_2H_5S and i-C_3H_7S, the rotationally-resolved and dispersed spectra have been reported by us for the very first time.* Peer-reviewed literature has often cited Misra's precise determination of spectroscopic parameters of hard-to-isolate transient molecular species that are critical for monitoring and elucidation of intricate and complex phenomena associated with atmospheric and combustion processes.

Accomplishments

Laser-induced fluorescence (LIF) excitation and wavelength-resolved emission spectra of six atmospherically significant alkoxy (RO; R=CH_3, C_2H_5, i-C_3H_7) and alkylthio (RS) radicals have been obtained under moderate (0.2 cm^{-1}) and high (0.07 cm^{-1}) resolution. *For C_2H_5S and i-C_3H_7S, the rotationally-resolved and dispersed spectra have been reported by us for the very first time.* Peer-reviewed literature has often cited Misra's precise determination of spectroscopic parameters of hard-to-isolate transient molecular species that are critical for monitoring and elucidation of intricate and complex phenomena associated with atmospheric and combustion processes.

Students

Undergraduate (5): Michael A. Holt, Kristi C. White, Rafiu A. Abina, Carron Sandifor & John Jordan

Graduate (6): Abdullahi H. Nur, Hosie L. Bryant, Jr., Mohammed M. Kamal, Michael E. King, Abdullahi Aw-Musse & Edward H. Dowdye, Jr.

Research Associates (2): Xinming Zhu & Abdullahi H. Nur

Number of Students Graduated with the Assistance of CSTEA - 4

M.S. (2): Abdullahi H. Nur & Mohammed M. Kamal
Ph.D. (2): Abdullahi H. Nur & Michael E. King

Publications:

Laser-induced excitation and dispersed fluorescence spectra of the ethoxy radical, X. Zhu, M.M. Kamal and P. Misra, *Pure and Applied Optics* (in press, 1996).

Laser-induced fluorescence spectroscopy of the jet-cooled methylthio radical, P. Misra, X. Zhu and H.L. Bryant, *Pure and Applied Optics* **4,** 587-598 (1995).

Polarity of laser excited optogalvanic transitions in neon, A.H. Nur, X. Zhu and P.

Misra, *Spectrosc. Lett.* **28,** 367-377 (1995).

Laser optogalvanic wavelength calibration with a commercial hollow cathode iron-neon discharge lamp, X. Zhu, A.H. Nur and P. Misra, *J. Quant. Spectrosc. Rad. Transf.* ***52,*** 167-177 (1994).

Laser excitation and emission spectroscopy of the methoxy radical in a supersonic jet, P. Misra, X. Zhu, C.-Y. Hsueh and J.B. Halpern, *Chemical Physics* **178,** 377-385 (1993).

Laser excitation spectroscopy of the jet-cooled methoxy radical amidst hydroxyl transitions, P. Misra and X. Zhu, *Spectrosc. Lett.* **26,** 389-402 (1993).

Rotationally-resolved excitation spectroscopy of the methoxy radical in a supersonic jet, P. Misra, X. Zhu and A.H. Nur, *Spectrosc. Lett.* **25,** 639-649 (1992).

Laser-induced fluorescence spectroscopy of the hydroxyl radical, P. Misra, X. Zhu and A.H. Nur, *Spectrosc. Lett.* ***25,*** *547-557* (1992).

Presentations/Conferences:

P. Misra, X. Zhu, H. Bryant, A. Nur, and M. Kamal. Vibronic and rotational analyses of LIF spectra of CH_3O and CH_3S radicals. Joint Meeting of the American Physical Society and the American Association of Physics Teachers, Washington, DC, April 1993. Bull. Am. Phys. Soc. **38 (2)**, E11 7, 970 (1993).

P. Misra, S. Misra, D. L. VanderMeulen, and K. G. Spears. Multiphoton cycling in controlled laser-induced release of organic dyes from liposomes. Joint Meeting of the American Physical Society and the American Association of Physics Teachers, Washington, DC, April 1993. Bull. Am. Phys. Soc. **38 (2)**, E11 10, 971 (1993).

Laser-induced fluorescence spectroscopy of jet-cooled free radicals. Invited Talk, Paper TG2, LASERS '93 International Conference, Lake Tahoe, NV, December 1993.

Mohammed M. Kamal, Xinming Zhu, and Prabhakar Misra. Laser spectroscopy of alkoxy & alkylthio radicals. Paper 93, Graduate Research Symposium, Howard University, Washington, DC, April 1994.

Abdullahi H. Nur, Xinming Zhu, and Prabhakar Misra. Laser optogalvanic spectroscopy. Paper 92, Graduate Research Symposium, Howard University, Washington, DC, April 1994.

P. Misra, X. Zhu, M. M. Kamal, and A. H. Nur. Molecular Spectroscopy of Supersonically Cooled Transient Species. Joint Meeting of American Physical Society and the American Association of Physics Teachers, Crystal City, VA, April 1994. Bull. Am. Phys. Soc. **39 (2),** G7 13, 1119 (1994).

P. Misra, X. Zhu, and A. H. Nur. The Nature and Utility of Laser Optogalvanic Transitions in Spectroscopy. Joint Meeting of American Physical Society and the American Association of Physics Teachers, Crystal City, VA, April 1994. Bull. Am. Phys. Soc. **39 (2),** G7 13, 1119 (1994).

P. Misra, X. Zhu, and A. H. Nur. Laser Optogalvanic Transitions of Neon in the Near Ultraviolet and Visible. Paper TA09, 49th International Molecular Spectroscopy Symposium Abstracts, Columbus, OH, June 1994.

P. Misra, X. Zhu, M.M. Kamal, A.H. Nur, and H.L. Bryant, Jr. Vibrational and Rotational Laser Spectroscopy of Supersonically Cooled Alkoxy and Alkylthio Radicals. Paper MG04, 49th International Molecular Spectroscopy Symposium Abstracts, Columbus, OH, June 1994.

Rovibronic Spectroscopy of the Ethoxy Radical in a Supersonic Jet Environment. Joint Meeting of the American Physical Society and the American Association of Physics Teachers, Washington, DC, April 1995. Bull. Am. Phys. Soc. **40 (2)**, I11 1, 998 (1995).

Time-Resolved Emission Spectroscopy of the Alkoxy Radicals. Joint Meeting of the American Physical Society and the American Association of Physics Teachers, Washington, DC, April 1995. Bull. Am. Phys. Soc. **40 (2)**, I11 15, 1000 (1995).

P. Misra, X. Zhu, and M. M. Kamal. Determination of Several New Vibrational Frequencies for the Ethoxy Radical. Paper TJ10, 50th International Molecular Spectroscopy Symposium Abstracts, Columbus, Ohio, June 1995, p. 215.

P. Misra, C. Sandifor, and X. Zhu. Fluorescence Lifetimes of Laser-Excited Alkoxy Radicals. Paper TJ11. 50th International Molecular Spectroscopy Symposium Abstracts, Columbus, OH, June 1995, p. 216.

P. Misra, A.H. Nur, and X. Zhu. Chemical Kinetics of the Reaction of Methoxy with Molecular Oxygen for Various Temperatures, Pressures and Buffer Gases. Paper TJ04, 50th International Molecular Spectroscopy Symposium Abstracts, Columbus, Ohio, June 1995.

Michael King and Prabhakar Misra. Measurement of the Rate Constant of the Reaction of Methoxy (CH_3O) with Nitrogen Dioxide (NO_2). American Physical Society March Meeting, St. Louis, MO, March 18-22, 1996.

Michael King and Prabhakar Misra. Experimental Error in the Measurement of the Rate Constant of the Reaction of Methoxy (CH_3O) with Nitrogen Dioxide (NO_2). American Physical Society March Meeting, St. Louis, MO, March 18-22, 1996.

R. A. Abina, P. Misra, and H. Okabe. FTIR Spectroscopy of HNO_3 and NO_2 Relevant to Stratospheric Wake Analysis. First National Student Conference, The National Alliance of NASA University Research Centers at Minority Institutions, North Carolina A & T University, March 31-April 2, 1996.

J. Jordan, H. Lauziere, M. Kamal, C. Haridass, P. Misra. Fourier Transform Infrared (FT-IR) Spectroscopy of NO_2, HCl, and CH_3NO_2 Pertaining to Atmospheric Phenomena. NASA University Research Centers Technical Conference (URC-TC-97), Albuquerque, NM, Feb 16-19, 1997

DR. VERNON R. MORRIS (1994) ... Photochemical Processes in Gas-Aerosol Systems In Planetary Atmospheres

My research projects 1994-1996 are comprised of laboratory, theoretical, and field experimental studies of atmospheric chemistry. A primary focus of these projects has been to address the Mission to Planet Earth (MTPE) objective of expanding scientific knowledge of the Earth system using space, aircraft, and in-situ platforms. Another focus of my work has centered on using physical methods in laboratory experimental and theoretical tools to investigate the atmospheric chemistry of the Earth's troposphere and that of interstellar atmospheres. Specific projects and accomplishments are detailed below.

I. Development of QCM/SAW Cascade Impactor and Chemical Sensors

Support for the laboratory calibration and field operations of the Stratospheric Wakes Analysis Project (SWAP). Determination and characterization of suitable chemical sensors for the QCM/SAW instrument and other candidates for the suite of instruments in the flight campaign has been carried out in my laboratory. I have actively participated in the flight experiments carried out at Moffet Field, CA and at Wallops Island, VA. Under my direction, two graduate students (Janel Cobb and Cassandra Williams) have obtained masters degrees through this work and another (Kapres Meadows) is on track to finish with his masters degree in chemistry in 1997. There have been two other graduate students (Shondalette Sims and Jerome Colvin) and several undergraduates who have worked on this project as well. Collaborators: Arthur Thorpe, Sonya Smith, Hideo Okabe, P. Misra, F. Sentfle

Summary of Calibration Results to Date. 1) Completed calibration of ozone on the 10 MHz Quartz and 200 MHz SAW crystal in the flight and laboratory instruments; 2) Completed calibration of O_3, SO_2, HNO_3, and HCl on each of the coatings PBD, P4VCS, nitron, and PEA; 3) Performed semi-quantitative tests for ozone loss through series configuration of the instrument; 4) Redesigned the gas sampling component of the instrument; 5) Calibrated the temperature response of the aerosol QCM stages; 6) Students have prepared and submitted six different abstracts of their research to five different national conferences; 7) Three proceedings papers have been published as a result of 6). The citations are: K. Meadows, C. K. Wright, S. C. Sims, V.R. Morris "Preparation of Nitron for Use as a Chemical Sensor for Nitric Acid," ***Proceedings of the 24th Annual Meeting of the NOBCChE 1996.*** J. B. Cobb, V. R. Morris, and A. N. Thorpe, "Mass Loading Character-istics of Crystal Clock Oscillators," ***Proceedings of the AIAA, (1996).*** S. C. Sims, C. K. Wright, and V. R. Morris, "The Impact of Aircraft on the Chemistry of the Upper Atmosphere," ***Proceedings of the 23nd Annual Meeting of the NOBCChE (1995).***; 8) Developed a "Laboratory Procedures" manual for the calibration experiments; 9) Begun initial testing of chemical sensors for CO and CO_2; 10) Begun

testing of polymeric candidates for HCl detection; 11) Set up a state-of-the art aerosol test and calibration laboratory; 12) Set up NIST calibrated calibration system for the gas sensors; 13) Performed all of the primary interferences for new co-polymer candidates for nitric acid. Currently testing NO and NO_2.

II. Laboratory Experimental Studies of Atmospheric Chemistry

A. Time-resolved IR Spectroscopy. Time-resolved IR spectroscopy has been used to study fundamental atom-molecule reactions of relevance to extraterrestrial atmospheres. One paper has been published. The citation is: V. R. Morris Ke-Li Han, and William M. Jackson, "Time-Resolved Chemiluminescence from Reactive Collisions Between Translationally Hot H-Atoms and SO_2." ***J. Phys. Chem. 99, 10086 (1995).***

B. Heterogeneous Reactions on Atmospheric Aerosols. I have begun setting up the laboratory equipment for the studies of matrix isolated and gas-phase systems. Time-resolved IR spectroscopy and UV-visible absorption techniques will be employed to investigate the photochemistry of the SO_x/ClO_y cycles. There are also immediate applications to two other proposals submitted (1 to NASA, 1 to NSF) concerning the photochemistry of organic and pure carbonaceous aerosols and gases, which has implications to exobiology and the effects of biomass burning.

III. Theoretical Investigations

A. ClOO Molecule. This work was comprised of a theoretical study of the geometrical structures and harmonic frequencies of the chloroperoxy radical and an intercomparison of theoretical methods, density functional theory (DFT) vs configuration interaction (CI) for challenging free radicals. A paper was published with citation: V. R. Morris, S. C. Bhatia, T. S. Dibble, J. S. Francisco, "Evaluating the Accuracy of Density Functional Methods for ClOO." ***J. Chem. Phys. 104, 5345, (1996).***

B. Intersystem Crossing on the lowest potential energy surfaces of butatriene. Collaborator: Steven Pollack. This work has been presented at the National meeting of the ACS and a manuscript is in preparation for submission to the Journal of Computational Chemistry. This work has clarified the mechanism for a reaction which has relevance for both the Jovian atmosphere and some fundamental aspects of polymer chemistry.

C. Venus Aerosol Precursors. Theoretical studies of acid gas clusters and aerosol precursors will be performed. Particular applications will be the SO_x/ClO_y photochemistry in the Venusian atmosphere and low energy pathways for gas phase nitric acid aerosol formation. Geometry optimizations and energy calculations have been performed for all reactants, collision adducts and products of the SO + ClO reaction. This work will be presented at the national meeting of NOBCChE in 1997. IN addition a proposal based on this work and its relevance in the lower atmosphere of Venus has been prepared for submission to a Planetary Atmospheres NRA.

D. C_2H + H Reaction. Ab initio calculations have been performed to computed

reaction profiles for C_2 product channel of the C_2H + H reaction. This reaction is known to be important in cometary coma as a key initiating photochemical reaction. However, very few studies have been performed on the direct formation of C2 and the implications of the ensuing chemistry that might result. This work is yet ongoing. Thus far, I have determined that vinylidene intermediate is not necessary for H_2 formation and calculated the potential surface in the vicinity of potential transition states for this reaction. These studies are being pursued at the configuration interaction level of theory but the use of density functional methods will also be investigated. I am in the process now of generating a high quality PES for QCT 3-Body and 4-Body scattering calculation for C_2 product channel.

IV. Modeling Lightning Production of NO_x and O_x in the Troposphere

Two presentations at the AMS national meeting have been made and a manuscript has been accepted in the Journal of Geophysical Research. The title is: G. S. Jenkins, A, Mohr, V. R. Morris "The Role of Convective Processes Over the Zaire and Congo Basin in the Southern Hemisphere Ozone Maximum and the EXPRESSO Field Campaign" ***(J. Geophys. Res. 1996)***. There are follow up studies being performed which involve (i) the modeling of the chemistry of lightning and (ii) the analysis of satellite imaging of lightning, NO_x, NO_y, and ozone to give a more quantitative picture of the influence of lightning discharges on tropospheric chemistry. An undergraduate student is scheduled to present the former portion at a national conference in early 1997. Collaborator: Gregory Jenkins (PSU).

Other Activities in the Center Include:

1. Deputy Director March 1996-present;
2. Director and chief architect of the Summer Institute and Research Traineeship in Atmospheric Sciences (SIRTAS) 1994-1996;
3. Organized and drafted the Howard University Program in Atmospheric Sciences (HUPAS), a new graduate program to be implemented at Howard University. (see attachment 1);
4. Designed and taught 4 new courses in atmospheric sciences -- Current Topics in Atmospheric Sciences, Introduction to Atmospheric Chemistry, Introduction to Atmospheric Sciences, Air Pollution Meteorology;
5. Recruited students to CSTEA and into the HUPAS;
6. Represented CSTEA at several research conferences and planning meetings in order to arrange for additional leveraged funding;
7. Reviewed NASA and NSF proposals;
8. Published a refereed paper on the Center and its research. The citation is: V. R. Morris and A. N. Thorpe The Center for the Study of Terrestrial and Extraterrestrial Atmospheres: Cutting Edge Research and Training at Howard University ***The Journal of the NTA 70, 27 (1996)***.
9. Assisted in the development of new brochures, recruitment materials, and webpage.

Students:

Overseen and mentored five (5) graduate students and eleven (11) undergraduate students funded under CSTEA. I have also sponsored several students during the Summer program.

Graduate Students: Janel Cobb (MS, August 1996), Cassandra Williams (MS, January 1997), Shondalette Sims, Kapres Meadows, Preston Heard

Undergraduate Students: Silas Anamelechi, Elim Betton, Jeremy Bright, Lauren Denkins, Reyna Lewis, Bridgette McGhee, Breanne Peterson

Summer (SIRTAS) Program: Prisca Anamelechi, Silas Anamelechi, Michael Fleming, Stephanie McFarlane, Bridgette McGhee, Kimberly Pete, Ama Tyus, Tanyifor Tohnya

Publications:

G. S. Jenkins, A, Mohr, V.R. Morris, "The Role of Convective Processes Over the Zaire and Congo Basin in the Southern Hemisphere Ozone maximum and the EXPRESSO Field Campaign" (Accepted for Publication. 1997).

V. R. Morris, S. C. Bhatia, T. S. Dibble, J. S. Francisco "Evaluating the Accuracy of Density Functional Methods for ClOO." *(J. Phys. Chem. Phys. 104, 5354, 5345, (1996).*

V.R. Morris and A.N. Thorpe, "The Center for the Study of Terrestrial and Extraterrestrial Atmospheres: Cutting Edge Research and Training at Howard University" **The Journal of the NTA 70, 27 (1996).**

V. R. Morris and William Jackson "Time Resolved Chemiluminescence from Reactive Collisions Between Translationally Hot H-Atoms and SO_2." J. Phys. Chem. 99, 10086 (1995).

Selected Presentations/Conferences:

Conference Proceedings

K. Meadows, C. K. Wright, S. C. Sims, V. R. Morris. Preparation of Nitron for Use as a Chemical Sensor for Nitric Acid. Proceedings of the 24th Annual Meeting of the NOBCChE 1996.

J. B. Cobb, V. R. Morris and A. N. Thorpe. Mass Loading Characteristics of Crystal Clock Oscillators. Proceedings of the AIAA, (1996).

S. C. Sims, C. K. Wright, and V. R. Morris. The Impact of Aircraft on the Chemistry of the Upper Atmosphere. Proceedings of the 23rd Annul Meeting of the

NOBCChE (1995).

Poster Presentations

V. R. Morris and S. K. Pollack Moller-Plesset Studies of the Singles-Triplet Gap in Butatriene. Poster presented at the 211th ACS National meeting, New orleans, LA, march 24-28, 1996.

S. C. Sims, C. Wright, J. Cobb, T. McCalla, R. Revelle, V. R. Morris, and S. K. Pollack. New Polymer Coatings for Chemically Selective Mass Sensors. Poster presented at the 211th ACS National Meeting, New Orleans, LA, March 24-28, 1996.

C. K. Wright, S. C. Simms, C. B. Peterson, and V. R. Morris. Calibration of the QCM/SAW Cascade Impactor for Measurement of Ozone in the Stratosphere. Poster presented at the 211th ACS National Meeting, New Orleans, LA, March 28, 1996.

Oral Presentations

C. Wright-Williams, C. B. Peterson, V. R. Morris. Calibration of the QCM/SAW Cascade Impactor for Measurement of Ozone. URC-TC Conference in Albuquer-que, NM, February 15-19, 1997.

K. Meadows, C. Wright, S. C., Sims, V. R. Morris. Preparation of Nitron for Use as a Chemical Sensor for Nitric Acid. Presented at the 23rd Annual NOBCChE National Conference, Detroit.

Invited Talks

V. R. Morris. Atmospheric Chemistry and development of Instrumentation for Stratospheric Flight Experiments. Department of Chemistry, **Morehouse College, Atlanta, GA Feb 2, 1996.**

V. R. Morris. Chemistry and Dynamics Behind Supersonic Aircraft in the Stratosphere. Presented at the Saturday Workshop in Aerospace Science and Technology, ***The National Air and Space Museum, Washington D.C. July 8, 1995.***

V. R. Morris. Development of a Model Atmospheric Chemistry Laboratory Presented at the Preparing Future Scientists Workshop ***Spelman College, Atlanta, GA March 3, 1995.***

DR. HIDEO OKABE (1992) ... Studies Of Earth And Planetary Atmospheres

To understand the evolution of Titan atmosphere by solar radiation from the original methane, nitrogen, and hydrogen mixtures, we have measured the quantum yield of photochemical products by mass spectroscopy and Fourier Transform Infrared (FT-IR) spectrometer, and have measured the UV absorption cross section of acetylenes.

1. Photochemistry of methylacetylene at 193.3 nm (1992). 2. Photochemistry of acetylene at 193.3 nm (1993). 3. Photochemistry of cyanoacetylene at 193.3 nm (1996). 4. Reaction rates of the CN radical with diacetylene and dicyano-acetylene (1996). Recently we have studied photochemistry of dicyanoacetylene.

Students:

Rafiu A. Abina	FT-IR spectroscopy of atmospheric trace gases
Alexine Martin	Summer 1996
Tamara Carrington	Chemiluminescence measurement of trace gases

Publications:

Photodissociation of methylacetylene at 193 nm. K. Seki and H. Okabe J. Phys. Chem., **96**, 3345 (1992).

Photochemistry of acetylene at 193.3 nm. K. Seki, and H. Okabe, J. Phys. Chem., **97**, 5284 (1993).

Photochemistry of cyanoacetylene at 193.3. K. Seki, M.Q. He, Renzhang Liu, and H. Okabe, J. Phys. Chem., **100**, 5349 (1996).

Reaction rates of the CN radical with diacetylene and dicyanoacetylene. K. Seki, M. Yagi, M.Q. He, J. B. Halpern, and H. Okabe, Chem. Phys. Lett, **258**, 657 (1996).

Photochemistry of dicyanoacetylene at 193.3 nm. K. Seki, H. Okabe, (in preparation)

Preparation of oxygen free AlN thin films by pulsed laser deposition. M. Q. He, N.Q. Chen, P. Z. Zhou, H. Okabe, and J. B. Halpern, submitted to J. Vac. Sci. and Tech. **A**.

Presentations/Conferences:

XXI informal conference on photochemistry, May 15 1994, Toronto, Ontario, Canada Photochemistry of acetylenes.

Photochemistry of Cyanoacetylene at 193.3 nm. Twenty-third International Symposium on Free Radicals, August 13-18, 1995, University of Victoria, Victoria, B.C. Canada.

CN Reactions with C_4N_2 and C_4H_2. With K. Seki, Japan Chemical Society, April 95, Kyoto, Japan.

Photochemistry of dicyanoacetylene at 193 nm. Japan Chemical Society, April 1996, Hawaii with K. Seki.

DR. STEVEN POLLACK (1995) ... Development Of Polymeric Coatings To Increase The Specificity Of Piezoelectric Mass Sensors

This project, underway since June of 1995, has focused on developing new and novel coatings to create specificity for Quartz Crystal Microbalances. Our focus has been on sensors for nitric acid vapor. It was shown that the poly (sty-rene-co-pyridine) in addition to giving a signal for hydrochloric acid, which was reversible, also showed sensitivity to nitric acid. This latter response was shown to be non-reversible. It was assumed that this was due to nitration of the aromatic rings of the styrene and pyridine rather than a simple acid-base reaction. We undertook to develop a polymer more reactive than this system to nitration but unreactive to acid-base chemistry. To this end, we synthesized a range of copolymers of styrene and dimethoxystyrene, an electron rich variant. Initial studies indicated that this system also gave a response to nitric acid, but was unresponsive to hydrochloric acid, ozone and air. When control studies with pure polystyrene were conducted, we saw a similar response, including a response to nitric acid. We take this to indicate that the simple polystyrene is sufficiently reactive to produce a response to nitric acid. This has added benefit as this is a truly low cost coating.

In addition to the chemical studies, we have developed a PC based data acquisition system consisting of a HP Frequency Counter, a Visual Basic Control program and a single IC oscillator driver. This circuit is compact and stable and can be incorporated directly onto the test apparatus to minimize noise.

Students:

During the initial summer of 1995, I supervised the activities of Ms. Tiffany McCalla in synthesizing poly(glycidyl methacrylate), a potential hydrogen chloride sensor material and Mr. Ron Revelle in the synthesis of poly(3,4-dimethoxystyrene) and poly (styrene-co-3,4-dimethoxystyrene), two potential nitric acid sensor materials. I also presented a lecture on the principals of piezoelectric mass sensors and their specificity to the CSTEA summer program students. Ms. McCalla continued her research work during the Fall of '95 and Spring of '96. The culmi-nation of this study, a polystyrene based nitric acid sensor was a presentation given in collaboration with Professor Morris's Students at the National ACS meeting in New Orleans in the Spring of 1996. In May of 1996, Mr. Kahsay Habte, a graduate student in chemistry and Ms. Sarda Mittipali, a undergraduate student in chemistry joined my group as CSTEA sponsored students. Ms. Mittipali worked on developing conducting polymer coatings, but due to family illness did not perform much actual work. Mr. Habte developed a Visual Basic program to control data acquisition from a quartz crystal microbalance oscillator developed in our laboratories. He is currently analyzing the nature of the interaction of nitric acid with polystyrene coated oscillators.

Additionally I supervised the activity of 8 graduate students, a visiting scientist and a postdoctoral fellow involved in other sponsored programs.

Ms. Tiffany McCalla, Junior, Chemistry, Project: (see above)

Mr. Ron Revelle, B.S. awarded, June 1995, Project (see above)
Ms. Sarda Mittipali, Junior, Chemistry, May 1996-July 1996.(see above)
Mr. Kahsay Habte, Graduate Student, Chemistry May 1996-present.

Presentations/Conferences:

"Development of Chemically Specific Polymer Coatings for Piezoelectric Mass Sensors. A Nitric Acid Specific Sensor Based on Simple Materials." URC/TC Conference, February 16-19, 1997, Albuquerque, NM.

DR. STEVEN RICHARDSON (1993) ... Computational Chemistry Of Neutral And Radical Molecules In Terrestrial And Extraterrestrial Atmospheres

Our research program in CSTEA, 1993 to 1996, in collaboration with Dr. Joseph S. Francisco, Professor of Chemistry and Earth and Atmospheric Sciences at Purdue University and Dr. Keiji Morokuma, Professor of Chemistry and Director of the Cherry L. Emerson Center for Scientific Computation at Emory University, has involved state-of-the-art first-principles quantum chemical methods to study the energetics, structure, and vibrational properties of molecular and radical intermediates that play a significant role in atmospheric chemistry, both in terrestrial as well as extraterrestrial atmospheres.

Summary of Research Projects For 1993-96

I. A Computational Study of the Reaction of C_2 with CH_4
II. Determination of the Heats of Formation of CCCN and HCCCN
III. Determination of the CC Bond Dissociation Energy in Cyanogen
IV. Towards an Understanding of the Chemical Evolution of Titan's Atmosphere: A Theoretical Examination of Decomposition Pathways of Methylacetylene
V. Theoretical Studies of Ion-Molecule Complexes and Their Role in the Formation of Molecular Chlorine in the Earth's Stratosphere

Students:

Mr. Radhay K. Shiamsundhar, an undergraduate electrical engineering major at Howard, worked in our group during the 1994 CSTEA summer program and throughout the 1994-1995 and 1995-1996 academic years. He graduated from Howard in the Spring of 1996 with two years of CSTEA support as an undergraduate research assistant.

Mr. Jeremy D. Bright, a sophomore electrical engineering major at Howard, worked with our research group during the 1995 CSTEA program. In particular, Mr. Bright assisted in developing new graphics packages for visualizing some of the chemical reactions we have been studying in our research program.

Publications:

Joseph Francisco and Steven L. Richardson, Determination of the Heats of Formation of CCCN and HCCCN, J. Chem. Phys. 101, 7707 (1994).

Steven L. Richardson and Joseph S. Francisco, A Computational Study of the Reaction of C2 with CH4 mol. Phys. 83, 1041, (1994).

Joseph S. Francisco and Steven L. Richardson, Determination the CC Bond Dissociation Energy in Cyanogen, J. Chem. Phys. 102, 1100 (1995).

Steven L. Richardson, Joseph S. Francisco, Alexander Meibel, and Keiji Morokuma, Can Chlorine Anion Catalyze the Reaction of HOCl with HCl? submitted to the Journal of American Chemical Society.

Steven L. Richardson and Joseph S. Francisco, Towards an Understanding of the Chemical Evolution of Titan's Atmosphere: A Theoretical Examination of Decomposition Pathways of Methylacetylene, in preparation for submission to The Astrophysical Journal.

Presentations/Conferences:

20th Army Science Conference, Norfolk, Virginia, June 24-27, 1996

NASA 1997 URC Technical Conference on Education, Aeronautics, Space, Auto-nomy, Earth, and Environment. Tutorial presented on "Physical & Chemical Modeling for Atmospheric Sciences." Albuquerque, NM, February 16-19, 1997.

"Can Chlorine Anion Catalyze the Reaction of HOCl and HCl?" NASA 1997 URC Technical Conference on Education, Aeronautics, Space, Auto-nomy, Earth, and Environment. Albuquerque, NM, February 16-19, 1997.

DR. YEHUDA SALU (1993) ... Applications of Neural Networks to Remote Sensing

A new neural network, the Binary Diamond, was developed and tested on real life data. The network can learn how to classify satellite pixels from examples provided to it and then use this learned information to classify pixels from other scenes. The network was trained on classified LANDSAT pixels, that included four spectral bands for each pixel and the land cover class to which it belonged. Based on this information, the network determined its architecture and weight. It then classified about 80,000 pixels that it has never seen before. The land cover of these pixels were also known from land and aerial surveys. The results of the classifications of the Binary Diamond were compared against the real classifications. Other classification methods were tried also on the same data. It was found that the Binary Diamond performed comparable or better than the other traditional classification methods.

General Algorithm Development for Remote Sensing

AVIRIS is an air borne imaging spectrometer that collects more than two hundred bands of spectra from 20X20 m pixels. The recorded data combines the reflective properties of the pixel and the interaction of the atmosphere with the light rays. For some applications it is important to filter out the atmospheric effects from the recorded spectra. If the reflective properties of some pixels in the scene are known, the effects of the atmosphere could be estimated from the recorded spectra of these pixels. These estimations could be used for filtering the effects of the atmosphere from the rest of the scene. Many land scenes have highways and roads, the reflective properties of which can be found once and for all. By analyzing the total recorded refection from these pixels, the estimate of the atmospheric contribution can be computed. The problem is that roads cover only parts of pixels. An algorithm was developed for determining what portion of a pixel is being covered by a tranversing road. The algorithm was tested on an AVIRIS scene. It was found that the algorithm localizes the road within the pixels with an accuracy of+- 2 m.

Students:

Lashawn Prudhomme, summer project 1994
Olu Bamiduro, summer project 1995.
George Ellis, summer project 1995.
Damali Ankoanda-King, summer project 1996.

Lectures on remote sensing and computer courses in CSTEA Summer Institutes, 1994, 1995, 1996.

Publications:

Y. Salu and J. Tilton "Classification of multi-spectral image data by the Binary Diamond neural network and by non-parametric, pixel-by-pixel methods" IEEE Transactions on Geoscience and Remote Sensing, 31, 606-617, may 1993.

*Y. Salu "The use of the binary diamond neural network in learning in letter-phoneme associations" International joint Conference on Neural Network, July 1993.

*Y. Salu, "Classification of satellite multi-spectral image data by the binary diamond neural network". Advances in Neural Information Processing Systems 6, 1143-1150, 1994.

*Y. Salu "A neural network for analogical reasoning" World Congress on Neural network, IV pp 418-423, 1994, and Proceedings of IEEE International Conference on Neural Networks, VII pp 4772-4777, 1994.

Y. Salu "sub-pixel localization of highways in AVIRIS images. " in Summaries of the fifth JPL annual airborne earth science workshop. JPL Publication 95-1, Vol 1, 137-141, 1995.

*Y. Salu "detection of contradictions in a semantic neural network" Proceedings of the IEEE 1996 International Conference on Neural Networks, Washington, DC. Vol 2, 762-767, 1996.

(An asterisk (*) indicates a full length reviewed paper, which has also been presented in a meeting)

Presentations/Conferences:

Advances in Neural Information Processing Systems (NIPS) Denver 1992
CESDIS Seminar at NASA/Goddard 1992
World Congress on Neural Network. San Diego 1994
IEEE International Conference on Neural Networks. Orlando 1994.
IEEE 1996 International Conference on Neural Networks, Washington, DC 1996.

DR. SONYA SMITH (1995) ... In Support Of The Stratospheric Wake Analysis Project (SWAP) Of Wing-Tip Trailing Vortices Plume/Wake Dynamics And Stability/ Breakdown

Characterization of flowfield through the QCM/SAW cascade impactor as currently designed was found to have a limit on the allowable flowrate. This work described the flowrate using a computational model and the results also showed the same limit on flowrate. The results of this work will be used in calibrating the experiment for flight.

The objective of the wing-tip vortex breakdown work was to numerically calculate the wake location dynamics (e.g. drift, decent, dissipation, vortex formation, vortex breakdown) Dominant factors affecting the description of the motion include the atmospheric stability, the initial properties of the wake and the turbulence in the atmosphere and in the wake, which govern the rate at which the entrained fluid is mixed into the wake. It is here that the dynamics of a vortex breakdown can have the most significant impact. Although significant progress was made in the area during the past year we are testing the code.

Students:

Undergraduate student: Matthew Berg, Mechanical Engineering Department ... Initial computation of the flowfield through California Measurements instrument. This instrument is an older design of cascade impactor. This instrument has been tested to detect flowrate limits like those found in the QCM/SAW.

Undergraduate student: Kim Pete, Mechanical Engineering Department ...

Wing tip vortex breakdown. The objective os this work was to numerically calculate the wake location dynamics (e.g. drift, decent, dissipation, vortex formation, vortex breakdown) Dominant factors affecting the description of the motion include the atmospheric stability, the initial properties of the wake and the turbulence in the atmosphere and in the wake, which govern the rate at which the entrained fluid is mixed into the wake. It is here that the dynamics of a vortex breakdown can have the most

significant impact. Although significant progress was made in the area during the past year we are testing the code. Students Involved: One undergraduate student: Eric Phillips; M.E. Dept.

Presentations/Conferences:

Tutorial presented on "Physical & Chemical Modeling for Atmospheric Sciences at the NASA URC Technical Conference in Albuquerque, New Mexico, February 16-19, 1997.

DR. MICHAEL SPENCER (1992) ... Fabrication of GaN/AlN and $(SiC)_2(AlN)_{1-x}$ UV Sensors

Objective

To fabricate and characterize UV detectors of AlN/GaN and solid solutions of SiC/GaN and alloys of AlN for applications in the 3 - 6ev spectral region.

Accomplishments

- Growth of $(AlN)_x(SiC)_{1-x}$ on 6H-SiC and Si
- First demonstration of growth of solid solutions by MOCVD
- Determination of the dependence of compositions of solid solution on growth parameters
- First demonstration of AlN/SiC heterojunctions by MOCVD
- Demonstration of SiC/AlN/SiC heterojunctions
- Determination of polytype of solid solution as a function of AlN% (currently known for 20%)
- Fabrication of Schotky diodes on solid solutions
- Measurements of electron concentration a function of AlN%
- Measured optical absorption for 20% solid solution
- Fabrication photoconductive device from 20% solid solution deposited on sapphire

Students:

Ronald Green - Graduate Student in Electrical Engineering (left Fall 1996)

Publications:

X. Tang, K. G. Irvine, Z. Ping, and M. G. Spencer. Measurement of Electro-Optical Properties of b-SiC on Sapphire Substrates and Free Standing Films. Mat. Sci. and Eng. B, 11 (1992), 39.

V. B. Shields, K. Fekade, M. G. Spencer. Near Equilibrium Growth of Thick, High Quality Beta-SiC by Sublimation. Appl. Phys. Lett., **62**, p. 1919-1921, April 19, 1993.

R. Magno and M. G. Spencer. Defect Asssisted Tunneling in GaAs/AlAs/GaAs Heterostructures. J. Appl. Phys. **75** (1), January 1994.

V. A. Dmitriev, K. C. Irvine, M. G. Spencer, G. Kelner. Low Resistivity (10^{-5} Ohm-CM^2) Ohmic Contacts to 6H-SiC Fabricated Using Heteropolytype Junctions. J. Appl. Lett. **64**, p. 318, January 17, 1994.

K. Wongchotigul, M. G. Spencer, N. Chen and D.P. Prasad. Crystal Structure of $(SiC)_x(AlN)_{1-x}$ Grown on 6H-SiC by MOCVD. Materials Letters, **21** 381, 1994.

K. F. Dombrowski, U. Kaufmann, M. Kunzer, K. Maier J. Schneider, V. B. Shields and M. G. Spencer. Identification of the Neutral V^{4+} Impurity in Cubic 3C-SiC by Electron-Spin Resonance and Optically Detected Magnetic Resonance. Physical Review B, 1994.

K. F. Dombrowski, U. Kaufmann, M. Kunzer, K. Maier J. Schneider, V. B. Shields and M. G. Spencer. The Deep Donor State of Vanadium in Cubic Silicon Carbide (3C-SiC). Appl. Phys. Letters, 1994.

C. M. Su A. Fekade M Spencer and M. Wuttig. Stress in CVD Grown Epitaxial 3C-SiC Membranes. JAP Letters, 1994.

K. Wongchotigul, M. G. Spencer, N. Chen D. Zhang, K. Fekade, A. Gomez, C. Thomas, V. Dimitriev and K. Irvine. Growth of Solid Solutions of Aluminum Nitride and SiC in Low Pressure Vertical Reactor MOCVD. p 397, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materails Institute of Physics Conference, Series Number **137**, 1994.

K. Fekade, M. G. Spencer K. Irvin A. K. Ballal D. P. Besabathina and L. G. Salamanca-Riba. TEM Study of Low-temperature CVD Silicon Carbide Films Grown on-axis 6H-SiC Substrates. p 287, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materails Institute of Physics Conference, Series Number **137**, 1994.

V. A. Dmitriev, K. C. Irvine, M. G. Spencer and M. Wuttig. Dynamic Characterization of Mechanical Properties of 3C Epitaxial SiC. p. 189, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materials Institute of Physics Conference, Series Number **137**, 1994.

K. Fekade, Q. M. Su, M. G. Spencer and M. Wuttig. Dynamic Characterization of Mechanical Properties of 3C Epitaxial SiC. p 189, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materials Institute of Physics Conference, Series Number **137**, 1994.

V. Sheilds, K. Fekade and M. G. Spencer. A Process for the Growth on Monocrystalline Beta-SiC Substrates. p 21, Silicon Carbide and Related Materials Proceedings of the 5th International Conference on SiC and Related Materials Institute of Physics Conference, Series Number **137**, 1994.

A. Moki, P. Sheng, D. Alok, B. J. Baliga, M. G. Spencer. Low Resistivity As-Deposited OHMIC Contacts to 3C-SiC. J. Electronic Materials, V24 N4: 315-318, April 1995.

K. Wongchotigul, N. Chen, D. P. Zhang, X. Tang, and M. G. Spencer. Low Resitivity of Aluminum Nitride: Carbon (AIN-C) Films Grown by Metal Organic Chemical Vapor Deposition. Mat. Lett., Vol. **26**, No. 435, pp. 223-226. March 1996.

S. Sheng, M. G. Spencer, X. Tang, P. Zhou and et al. An Investigation of 3C-SiC Photoconductive Power Switching Device. Materials Science and Engineering, B, June 1996.

X. Tang, Y. Yuan, K. Wongchotigul, and M. G. Spencer, Dispersion Properties of Aluminum Nitride as Measured by and Optical Waveguide Technique. Submitted to Appl. Phys. Lett.

Presentations/Conferences:

6th Brazilian Workshop on Semiconductor Electronics

DR. GEORGE MORGENTHALER (1992) ... University of Colorado at Boulder Subcontract

Since mid-1992, the University of Colorado at Boulder has actively contributed to the development of a central unifying research theme for CSTEA. CU has provided system engineering, extensive research, and experimental support for the following CSTEA research areas:

Tethered Satellites (1992-1993). The region between 90 km and 150 km in the atmosphere is known as the "ignoro-sphere" due to the relatively scarce in situ measurements available. The primary mechanisms for in situ measurements of the atmosphere are aircraft, balloons, and satellites. However, the service ceiling of the highest flying scientific aircraft is approximately 20 km. Balloons or blimps can provide measurements to much higher altitudes but cannot climb to the height of the "ignoro-sphere." While the density of the atmosphere is too low for aircraft and balloons, it is too high for satellites. In the "ignorosphere," the drag on the satellite will prevent the satellite from maintaining its orbit. These are the basic reasons why the "ignorosphere" atmosphere data have been scarce. CSTEA's research objective was to utilize NASA's emerging tethered satellite program to study the ignorosphere by reeling a satellite down into the altitude of interest from a much higher orbiting spacecraft such as the Space Shuttle. Once in the "ignorosphere," the tethered satellite with its suite of instruments could take a wide variety of in situ measurement which were previously non-existent. CU provided many of the initial feasibility studies and made many contacts with the participating U.S. industries, specifically, the Martin Marietta Astronautics Group in Denver. Global Positioning System (GPS) studies were performed and directed towards applications useful to CSTEA's interests in the tethered satellite program. A number of

papers were written and presented at the Space '94 Conference in Albuquerque, NM.

Concorde/ER-2 Plume Intercept (1994-1996). In support of CSTEA, CU has developed optimal search models constrained to the limitations of the ER-2, QCM, and Federal air safety regulations. While giving the best flight path for intercept, the model also identified that the probability of a successful altitude intercept was low. The model showed that:

a) if the QCM required a flight time in the plume of 3-10 seconds, the angle between the plume axis and the ER-2 flight direction would pose a great burden on the ER-2's ability to intercept the Concorde's wake;

b) if there was relatively instantaneous identification of the plume when in fact it was intercepted, a figure "S" interception path could be followed by the ER-2 and the intercept probability was then high. Without such instantaneous recognition, lidar or other terminal guidance to find the plume was needed by the ER-2.

Flights off the coast of New Zealand in late 1994 proved the validity of the model. The plume of the Air France Concorde was intercepted with the greatest uncertainty being from the altitude of the plume, which at times was above the flight path of the Concorde. Later attempts at intercepting the Concorde plume off of New Brunswick were physically successful, but turbulent winds scattered the plume.

ER-2/QCM flight tests were made in November 1994, May 1995, and January 1996. CU has provided flight support for all three ER-2 test flights. CU has extensively researched the ability of the ER-2 to retrace its flight path and determined that a tear drop flight pattern gave the ER-2 the highest probability of retracing its flight pattern and intercepting its own wake while serving as a useful diagnostic to test the QCM. Post flight data analysis has also been performed. Plume displacement algorithms have been developed by CU as well as a FORTRAN program which calculates the closest distance in three dimensions of each t on the return ass to every point on the initial pass.

Prior to the Wallops Island ER-2/Concorde intercept mission of May 1995, lines of communication were established with British Airways in London and Moncton Air Traffic Control in New Brunswick. Personnel at both sites provided critical information and assistance needed to complete the ER2/Concorde plume interception mission. On the day of the flight, communications between the Wallops Island ER-2 take-off point, British Airways, and Moncton Air Traffic Control were coordinated by Prof Morgenthaler through a telephone Conference call set in Boulder, CO. Wind compensation nomographs and basic plume search instructions were provided to the ER-2 pilots. The ER-2 successfully rendezvoused with the expected plume location in space, but highly turbulent stratospheric winds seemed to have dispersed the plume and made measurement difficult.

Students:

Bjorn Johns, Graduate Student, Aerospace Engineering Sciences, May 1992 - January 1994 ... Todd Mosher, Ph.D. Graduate Student, Aerospace Engineering Sciences, January 1994 - July 1994 ... Russ Riecken, Graduate Student, Aerospace

Engineering Sciences, May 1994 - May 1995 ... Paul Leuthaeuser, Graduate Student, Aerospace Engineering Sciences, July 1994 - December 1995 ... Nader Khatib, Graduate Student, Aerospace Engineering Sciences, January 1996 - December 1996

Summer Minority Access to Research Training (SMART)

Every year since the inception of CSTEA, the University of Colorado at Boulder has hosted number of minority students during the summer to work on CSTEA's unifying project. Past Howard University students who have performed valuable research for CSTEA are listed as follows:

1993: Michael Holt, Physics Undergraduate and Radhay Shiamsundar, Electrical Engineering Undergraduate. These SMART students, under the guidance of Dr. Morgenthaler and CU graduate student Bjorn Johns, produced a Report, *Opportunities For Upper Atmosphere Spaceflight Experiments,* which outlines potential spaceflight opportunities for CSTEA and provides a detailed description of the following three areas: 1) Communications Architecture of the TSS-2 Atmospheric Mission - Radhay Shiamsundar performed extensive research on the existing Space Shuttle communication system and how it will be utilized for a tethered satellite atmospheric research mission; 2) Selection of Sensors for Tethered Satellite Atmospheric Mission - Michael Holt surveyed Howard University faculty for experiment ideas and incorporated input from LASP scientists to outline potential tethered satellite instrumentation. Some additional sensors were also studied, and a Binary Integer Programming method to experiment selection was suggested by Dr. Morgenthaler.

1994: Phyllis Jones, Masters Graduate Student, Mechanical Engineering, and Christopher Rivera, Undergraduate Student, Electrical Engineering. During the Summer of 1994, CU teamed four SMART students with two additional CIMD (Coalition to Increase Minority Degrees) students, mentored by Prof. Morgenthaler, Todd Mosher, Russ Riecken, and Paul Leuthaeuser, to produce the report *Study of SST (Concorde) Wake Plume Sampling by the NASA ER-2 High Altitude Scientific Research Aircraft.* This report addressed CSTEA's new direction of interception and sampling of the wake of the Concorde by the ER-2 and provided the following: 1. Quartz Crystal Microbalance (QCM) - Phyllis Jones described the theory and capabilities of QCM and its applicability in the ER-2/Concorde intercept program; 2. Plume and Wake Characteristics of the Concorde - Christopher Rivera studied the dispersion and movement of the Concorde's wake as it flew supersonically through the stratosphere.

1995: Kecia Franklin, Undergraduate Student, Physics. With CSTEA's first attempt at an interception of the wake of the Concorde occurring in May 1995, Kecia Franklin was given a unique opportunity to analyze these data during the following summer under the tutelage of Dr. Morgenthaler and Paul Leuthaeuser. Ms. Franklin developed an algorithm to predict the lateral location of the plume which has been displaced by the winds aloft. This algorithm was applied to the data recorded by the Concorde, Air Traffic Control, and ER-2 during the intercept attempt. The report, *Analysis of Previous ER-2 Flight Data to Locate the Plume of the Concorde,* covers the development of the plume displacement algorithm and its application to the flight data.

1996: Matthew Berg, Undergraduate Student, Mechanical Engineering. During the Summer of 1996 and under the supervision of Prof. Morgenthaler and Nader Khatib, Matthew Berg performed research towards CSTEA's new unifying research direction of surface flux measurements. A variety of mass transport models were surveyed for applicability for land surface flux measurements, for the ability to modify the model, for ease of data analysis, and for accessibility to CU and Howard. The Community Climate Model 3 (CCM3), developed by the National Center Atmospheric Research (NCAR), was found to meet the needs of the above criteria. A CCM3 model modified for sulfur compounds was used to estimate the transport of sulfur compounds emitted from the surface, such as SOx and DMS, throughout the atmosphere. These estimates were compared with in situ airborne measurements and were found to have good correlation. This research provides a trial run of the much large research effort CSTEA is going to perform in the near future. This research is described in the report, *Estimating Particle Composition in the Upper Troposphere and Lower Stratosphere using the NCAR CCM3 Transport Model,* by Matthew Berg, Prof. George Morgenthaler, and Nader Khatib.

Student Progress and Successes

The University of Colorado at Boulder, under a sub-contract from CSTEA, has supported five graduate students over the past five years. Bjorn Johns graduated from the Aerospace Engineering Science Department with a M.S. degree and is currently working for UNAVCO doing GPS consulting. Todd Mosher is finishing his Ph.D. on optimization of spacecraft design and construction. He is resident in Southern California at the Aerospace Corporation where he is utilizing their data on spacecraft design and construction. Russ Riecken has graduated with a M.S. degree in Operation Research at the Colorado School of Mines. Paul Leuthaeuser is working for Ball Aerospace in Boulder, Colorado and will be receiving his M.S. degree on December 21, 1996. Nader Khatib received his M.S. degree on December 21, 1996 as well, and he will be entering the Ph.D. program at the University of Colorado at Boulder.

Papers:

Berg, Matthew, Estimating Particle Composition in the Upper Troposphere and Lower Stratosphere Using the NCAR CCM3 Transport Model, SMART 1996, Aug. 7 1996.

Franklin, Kecia, Analysis of Previous ER-2 Flight Data to Locate the Plume of the Concorde, SMART, 1995, August 9, 1995.

Johns, Bjorn, "Use of GPS for Tethered Satellite Position Determination," Engineering Construction and Operations in Space IV, Proceedings of Space '94, Vol. 1.

Leuthaeuser, Paul, Search Model for a High Altitude Aircraft Plume Interception, August 10, 1995.

Morgenthaler, George, B. Johns, M. Holt, R. Shiamsundar, J. V. Sivico, Opportunities For Upper Atmosphere Spaceflight Experiments, SMART 1993.

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