croscopy and Ellipsometry", Y.S.Tung, R. Mu, A. Ueda, D.O. Henderson, W. Curby, A. Mercado.

❑ Papers published:

"Adsorption Kinetics of EGDN on ZnO by Diffuse Reflectance Fourier Transform Infrared Spectroscopy", D. O. Henderson, E. Silberman, N. Chen, and F. W. Snyder, Appl. Spectroscopy 47, 528 (1993).

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"Optical and Atomic Force Microscopy Imaging of 2,4,6-Trinitrotoluene Droplets on Mica", D. O. Henderson, M. A. George, A. Burger, R. Mu, Z. Hu and G. C. Huston, Scanning Microscopy 9, 387 (1995).

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"Decomposition Kinetics of EGDN on Zinc Oxide", D. O. Henderson, R. Mu,Y. S. Tung, Appl. Spectros. 49, 444 (1995).

"Vibrational Spectroscopy and Trace Detection of Explosive Materials", An invited review paper to be published in *Research Trends In Vibrational Spectroscopy*, 1998.

"Diffusion Kinetics of TNT in Nitrile Rubber via FTIR-ATR Spectroscopy", Y. S. Tung, R. Mu, D. O. Henderson, W. A. Curby, and A. Mercado. Invited paper to the *Internet Journal of Vibrational Spectroscopy* (1998).

"Fourier Transform Spectroscopy Applied to Explosive Vapor Detection", D. O. Henderson, E. Silberman and F. W. Synder, Proceeding of the First International Symposium on Explosives Detection Technology, 1991.

❑ Six Master of Science (M.S.) students trained in explosives related research.

❑ Four undergraduate students supported by grant

❑ Invited talk at the Optical Society of America Conference, "Fourier Transform Infrared Spectroscopy of Solid, Liquid and Nanometer Particles" OSA, October, 1997.

From a broad perspective, the CPL team's contribution to explosive detection technology has been fundamental and applied, but always linked to one another. The nature of the interaction of molecules with a surface is a fundamental question pursued by physicists, chemists, and biologists. Knowledge of how explosives interact with different surfaces has allowed the team to understand the nature of the forces that retain an explosive on a surface. While such information is fundamental within the realm of pure science, it is also the basis for optimizing the design and efficacy of explosive detection systems. That is, for example, for a collector, one must have a material that is efficient for concentrating explosives and for transport lines that deliver an explosive to a detector, it would require surfaces that resist explosive molecule adsorption. These fundamental studies of the CPL team permit the development of first principles models that predict which class of materials are best for incorporation in explosives detection systems. Naturally, this approach wins over an empirical one whereby finding the appropriate material and design is a problem of trial and error. Further studies of FAA sponsored research on explosives detection and characterization are certain to advance the progress in this difficult field.

Author: Trudy Gray, Office of Research and Technology Applications, AAR-201

The driving force behind this highly productive and successful team, with all of its diversity, is a common value: an opportunity to contribute to meaningful state-of-the art research; and in this particular case, with the potential to save lives.

Aviation Research Grants Program

Grants Success Story

"People Behind the Partnership"

Fisk University

Prior to the establishment of the Aviation Research Grants Program, in 1990, most of the procured research for the Federal Aviation Administration (FAA) was acquired through the contracting process. Although research contracts produced some very successful and beneficial research, the process eluded the benefits of a partnership. The grants process promotes partnerships between the FAA and researchers. These partnerships foster open forums to discuss technical issues, promote cost sharing opportunities, and provide the necessary tools to produce the best results while containing costs. Fisk University was performing research for the FAA under a contract. Although considered successful in their research, the FAA and Fisk University acknowledged the benefit of the "partnership" element of an aviation research grant. In 1993, Fisk University applied for and was awarded an aviation research grant creating a partnership with the FAA Aviation Security Division and its technical experts in explosive detection, continuing with and expanding on their research previously carried out under contract.

Background:

Fisk University, located in Nashville, Tennessee, is a small, Historically Black University (HBCU), primarily known as a liberal arts school. However, Fisk has established itself as a leader in science, taking great pride in its contribution to education in the area of Physics and the sciences. The 1997 publication *Peterson's Top Colleges for Sciences* lists Fisk among the top 200 universities in sciences. In 1871, just six years after Fisk was established, the new school was in such serious financial trouble that many feared it would have to close. A music professor assembled nine of his best students, and all but a few dollars of the school's treasury and started on a fund-raising concert tour. Fisk's *Jubilee Singers*, began an ambitious and historic journey to raise money to save their fledgling school. That tradition continues today, however support from the FAA, NASA, and many other federal agencies allow this to be a "valued" tradition, not a necessity.

Fisk University President, Dr. Rutherford H. Adkins, commencement exercises.

About the Research

Purpose:

To obtain fundamental physical and chemical properties of explosives that can serve as a basis for designing and improving the efficiency of explosives detection systems (EDS) . The detection of explosive materials is important to global security. Aviation security and unexploded ordnance are just two areas where explosive detection has played a central role in ensuring the safety of lives of citizens in many countries.

Objective:

To further the development of explosive vapor detection through explosive vapor preconcentration and explosive characterization studies to establish protocols for quantitative evaluation of explosive detection systems, assisting in the prevention of terroristic bombing of airplanes and other public transportation vehicles.

Key objectives:

❑ Measure the emission rates of explosives from various surfaces in the solid and liquid states

❑ Determine the diffusion rates of explosives in polymer films

❑ Characterize the thermodynamic properties of explosives from the bulk to the mesoscopic scale

❑ Characterize explosive interactions with surfaces and adhesion forces

❑ Develop a particle standard for calibrating explosive detection systems.

Approach:

Several approaches have been taken to detect explosives that include x-ray imaging, neutron activation and spectroscopic methods.

A high resolution Fourier transform ifrared spectrometer. This instrument is used for measuring the infrared signatures of explosives in the solid, liquid and vapor phases and for explosives adsorbed on various surfaces used as collectors in explosive detection systems (Dr. Henderson).

Among these techniques, vibrational spectroscopy has shown great potential for detecting and characterizing explosives in the gas, supercooled liquid, and solid phases for explosives adsorbed on a variety of surfaces and for determining the transport properties of explosives in polymers.

Major Project Areas:

Emission Rates of Explosives:

For many explosives, there is little data on their emission rates. For the data that does exist, there is considerable spread in the values reported in the literature. The lack of emission rate data is even more striking for explosive ultrafine particles. The explosive emission rate is useful for EDS design and is an indication of the collection time (sniffing) necessary for detecting the explosive materials in the suspected area. Quite possibly this data may be applied for developing a source for vapor calibration of EDS. Two different methods are applied in this research, ellipsometry and atomic force microscopy (AFM) to determine the emission rate of explosives. The results of these experiments fill the missing gap on the emission rate of explosives and can be applied to the aforementioned concerns.

An atomic force microscope, purchased through an FAA grant, used for imaging nanoparticles of explosives deposited on various substrates.

The CPL team with its long track record in the physics and chemistry of mesoscopic or nanophase materials, is currently recieving support from the Department of Energy (DOE) and NASA, sponsoring research on nanophase materials. While the projects supported by other agencies and materials of interest from the FAA, such as quantum dots and metal nanocrystals, the projects share in common the basic physics and chemistry of nanophase materials. Much that the team has learned about the physics and chemistry of quantum dots and metal colloids has been applied to explosive ultrafine particles and is conversely true for explosive particulates. Thus, because the projects feed off one another, they result in a synergy that advances the research at an accelerated pace.

Left to right, Drs. Akira Ueda, Rixiang (Richard) Mu, Yie-Shin (David) Tung, Don Henderson, and Marvin Wu with the femtosecond Ti: Sapphire laser pumped with an Argon laser.

Significant Results/ Accomplishments/ Measurable Successes:

❑ The demonstration that the nucleation of a supercooled fluid confined in porous media occurs by homogeneous nucleation and that the nucleation through the pores occurs via percolation.

❑ The Chemical Physics Laboratory (CPL) together with Oak Ridge National Labo- ratories were the first to demonstrate the synthesis of III-V and II-VI quantum dots isolated in optical grade fused silica by ion implantation.

❑ The identification of surface phonon polaritions of the III-V and II-VI quantum dots which have been successfully predicted by Fuch's theory of polaritons.

❑ A technique using atomic force microscopy for determining the interfacial interaction potential for explosives adsorbed on various substrates was developed. This development establishes a means to calibrate explosive detection systems and to screen materials that may serve as collectors for explosive vapors or particles. Accepted for publication in *Scanning 1997 Proceedings Volume, Plenum Press*: "A New Approach to Examine Interfacial Interaction Potential Between a Thin Solid Film or Droplet on a Smooth Surface", R. Mu, Y.S. Tung, D.O. Henderson, W. Curby, A. Mercado and "The Sublimation Rates and Nucleation and Growth of TNT and PETN on Silica and Graphite Surfaces by Atomic Force Miwith explosives may lead to the collection of not only molecules, but also ultrafine particles. Consequently, the particulate detection as well as vapor detection may be important for evaluating EDS. From this perspective, a particle standard is necessary for evaluating the performance of EDS for mesoscopic particles. The research project and its results offer a means to develop such a standard that can be used for evaluating EDS performance of explosive ultrafine particles.

About the People

Professor Henderson holds a discussion with Jilin University students after a lecture on the optical properties of quantum dots.

Dr. Don Henderson, the Principal Investigator, is well known in the field of Materials Science, particularly in the area of nanophase materials. He was invited recently, to lecture at Jilin University in Changchun Province, Peoples Republic of China, assisted by Dr. Rixiang Mu, a Fisk Research Associate Professor in Physics on nanophase materials. This was a two week series of lectures.Dr. Henderson has responsibility for the overall conduct of this research. However, all members of the research team contribute to the program, integrating all aspects of the research. Each member focuses on specific tasks for which they have developed expertise over the years from FAA sponsored research.

The Chemical Physics Laboratory (CPL) has a tradition of involving undergraduates in ongoing research in the laboratory. The undergraduate student works side-by-side with the research associates in the CPL in various aspects of the research tuned to the level of the student's background. The undergraduates work on atomic force microscopy and study spectroscopy which has lead to research that is presented at international meetings and is published in peer reviewed journals.

Graduate student Dennis Denmark, Graduate student Taravia Taylor and Dr. Marvin Wu with a picosecond Nd: YAG laser and an optical parametric generator.

Partnerships:

This partnership with FAA technical personnel has also been particularly fruitful in the investigations of explosive ultrafine particles. This stems from the fact that in many cases the facilities and expertise in the CPL compliment those at the FAA William J. Hughes Technical Center.

The area of spectroscopy in the CPL has a long tradition. Over the years, the CPL has gathered basic data on the vibrational resonance of explosive molecules and ultrafine particles which are required for designing new methods of detection such as nonlinear spectroscopy of explosives. This data is shared with FAA technical personnel for application development. The close collaboration of FAA technical personnel with members of the CPL and research on other nanophase systems, supported by other agencies, has led to a robust research program in explosive materials detection.

Diffusion of Explosive in Polymers:

The diffusion rates of explosives in polymer films used to conceal them is required to establish the time required for explosive molecules to transport across the polymer film and reach the surface. The time required to transport explosive molecules across a film is clearly linked to the feasibility of their vapor detection, and therefore, these measurements will assess the likelihood of detecting concealed explosives. This effort will establish the time interval necessary for detecting a concealed explosive from the time it was prepared, to the time it was placed in an area intended for terrorist acts.

Thermodynamic Properties of Bulk and Ultrafine Explosive Particles:

The thermodynamic properties of matter reduced to the nanometer size differ from the bulk. Melting, freezing and other first and second order transitions are typically depressed from the bulk material. Clearly then, the bulk thermodynamic properties cannot be used for modeling conditions under which an EDS may operate for detecting ultrafine particles. Consequently, this project 's experiments results will allow for determining the thermodynamic properties of bulk and mesoscopic explosives.

Dr. David Tung imaging particles with an atomic force microscope.

Explosive Molecule Interactions with Surfaces:

An EDS is composed of components that have surfaces that at one point or another may be in contact with explosive vapors or particles. One obvious component in the EDS is the preconcentrator where the explosive molecules, or particles are first adsorbed and later released for detection. Therefore, the interactions at the explosive molecule-preconcentrator surface are central to optimizing operating conditions of this component. Also, it is essential to know if any chemistry has occurred between the preconcentrator and the explosive molecules. This project's studies are aimed at characterizing preconcentrator-explosive molecule interactions as a means to screen materials for their use as preconcentrators. The efforts will certainly lead to a better understanding of explosive molecule preconcentrator interactions and thereby provide input for preconcentrator design and development. Transport lines in EDS are another concern; they may be surfaces where explosives molecules are adsorbed or decomposed and thereby degrade signal at the detector. These effortsaimed at characterizing surfaces and how they interact with explosives is one of the keys for improving the design of the EDS.

Ultrafine Particle Standards:

There is a need to consider not only vapor detection of explosive molecules, but also ultrafine particles that may be collected by a sniffer. It is clear that sampling from the garment of a human subject contaminated

Graduate Student Taravia Taylor, analyzes the UV-Vis spectra of nanophase materials that show promise for explosive collector technology.