The Center for Laser Applications

“An accomplished Center of Excellence”

University of Tennessee Space Institute

Annual Report
FY 2009-2010
September 22, 2010
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Ultrasensitive Spectroscopy

Ultrasensitive Fluorescence Spectroscopy / Nanophotonics
  Maximum-likelihood multichannel fluorescence microscopy
Single-molecule Delivery and Trapping in a Nanochannel
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CLA Budget
Executive Summary

The Center for Laser Applications continues to move forward despite very difficult economic times. We have benefited American Reinvestment and Recovery Act funds through a grant supplement to Professor Chen, as well funds for the repair of equipment, upgrade of the Jade x-ray analysis software and some modest equipment purchases. We have added a Photon Technology International Modular Fluorometer/Phosphorimeter to the laboratory for fluorescence studies of new materials and a JOEL 6320FE field emission scanning electron microscope for analysis of laser modified structures. These tools have increased our capabilities and are being used extensively in research projects. Our research expenditures are steadily growing as shown in Figure 1. This growth will continue as awarded grants and contracts have increased.

Last year CLA supported 20 graduate students through research, university and THEC funds. We welcomed six new students, one of which is entering our growing Materials Science and Engineering program. Five students were awarded degrees last year. During the summer we mentored undergraduate and high school interns by involving them in research in the laboratories. Our faculty and students continue to be engaged in outreach, conducting experiments and working with local student groups. The students worked with the Tullahoma Hands-On Science Center to teach day long science programs to alternative school students.

The seven faculty and seventeen students at CLA published 21 journal papers in fiscal 2009-2010, published four book chapters and contributed 19 other papers. We have been active on the university seminar circuit with nine lectures in an attempt to improve recruiting and generate a higher profile among local colleges and universities. CLA associates made 29 conference presentations in the past year.

We hope you enjoy the research summaries that follow in this year’s Annual Report.

Sincerely,

William Hofmeister
Research Professor of Materials Science and Engineering
Director Center for Laser Applications
Center for Laser Applications - Strategic Plan

Mission Statement

The CLA mission is to advance laser applications in spectroscopy and materials synthesis. CLA is an accomplished Tennessee Higher Education Commission Center of Excellence in Laser Applications. We pursue our mission in three areas:

♦ Education
  • Provide a quality graduate education to UTSI students with emphasis on apprenticeship
  • Generate opportunities for undergraduate and high school student research

♦ Innovation
  • Develop a world class reputation for research and innovation

♦ Service
  • Assist businesses in development and implementation of technology
  • Increase interest in STEM areas, i.e. support science education for local students and teachers

Research Plan

The over-arching research theme of CLA is photonics.

Our specific research thrusts are applications of lasers in ultrasensitive and ultrafast spectroscopy, and materials synthesis and modification far from equilibrium. There is tremendous potential for growth of this research, particularly in nanotechnology and biomedical applications. We have a concerted effort in carbon based materials from diamond like carbon films to diamond microelectronics. The addition of George Murray has opened up research in molecularly imprinted polymers and polymer synthesis. We have an excellent funding history in laser material processing, single-molecule spectroscopy, propulsion and magnetohydrodynamics. The National Institutes of Health is our largest external funding source.

Our strengths include a well equipped research facility and baseline funding from the Tennessee Higher Education Commission that allows us to maintain the facilities and fund internal research. Our association with AEDC represents a unique opportunity, and CLA faculty have several projects with collaborators at AEDC. The University of Tennessee and Oak Ridge National Laboratory are also powerful research partners. CLA faculty collaborations include NASA Langley, Johns Hopkins Applied Research Laboratory, Sandia National Laboratory, Argonne National Laboratory, Wang Vision Institute, Vanderbilt University, LSU, and many private companies. In a highly interdisciplinary environment we must find the internal synergies and research thrusts that allow us to collaborate and move ahead as a team. This has to be done considering the available faculty, the mission of CLA, and the availability of research support. Research opportunities are increasingly application-based and require large multidisciplinary teams. Consequently, strategic partnerships are necessary to compete for these grants.
Research training, management and evaluation

From the outset, the Center of Laser Application focuses on research including training at the postgraduate level. Also efforts were underway to introduce K-12 students to the research experience by either visiting select schools in the local area or inviting school field-days. During this reporting period several management and evaluation components were reviewed leading to the following goals for the near future.

The primary objectives for management and evaluation are:

- Implement a previously successful model for management of a multi-disciplinary (M-D) research environment;
- Cooperate with university administration to create faculty accountability methods that both encourage faculty to venture into the proposed M-D environment and provide university administration with measures of productivity;
- Refine, expand, and use methods of evaluation that were previously developed for CLA to measure performance and efficiencies;
- Develop a methodology to educate university administration to learn and understand frequently changing needs of faculty to perform efficiently in the proposed M-D environment;
- Continue and expand current and perhaps new electronic methods of recruiting outstanding students who are interested in participation in graduate research in the Materials Science/Applied Physics areas that require the M-D approach;
- Continue to visit primarily regional universities for student recruitment and present research opportunities;
- Continue to increase women participation in Science and Technology. Noteworthy is that more than 20% major faculty participants for this proposal are women;
- Continue to make use of electronic means to communicate to prospective U.S. and international students details of the academic and research programs within the participating cross-institution departments;
- Continue with international collaborations, including plans of establishing new international activities, e.g., collaborative efforts with so-called Boltzmann Institutes in Austria, or establish new exchange programs of students/researchers with Materials Science Research Centers in Germany, viz. Berlin.

Accomplishment of research training will also include the gradual introduction of doctoral to postdoctoral researchers to state-of-the art research. Active collaborations with researchers in the U.S. and overseas will allow us to expose our students and PostDocs to research activities of interest, both within and outside the U.S. Examples here include researchers exchange programs in a way similar to so-called sabbatical programs for faculty: Postdoctoral researchers will be exposed to international research opportunities. A significant aspect of postdoctoral activities will be participation in publication activities. These activities span from novel research activities to review of manuscripts. Conference participations will include a selection of conferences, for example OSA Annual Meeting, FACSS Annual Meeting, LACSEA and/or LIBS or NASLBS/EMSLIBS or MMISLIBS or APS/SES-APS meetings. Past success of doctoral students and post-doctoral employees shows that weekly or bi-weekly meetings are preferred. These meetings usually include doctoral students as well to address aspects of research.

A specific example of doctoral and post-doctoral mentoring includes planned face-to-face time with visiting scholars during a 600-level PhD-type class, namely “Physics643: Computational Physics,” offered by the PI/PD Dr. Christian Parigger. This class also allows us to enhance our multi-disciplinary research and education efforts. Topics include but are not limited to: Fourier Series/transforms, Autocorrelation, An-harmonic oscillator, Classical Chaotic Scattering, Bifurcations and Chaotic Pendulum, Digital Wavelet Transform, Logistic Map, High-Throughput
Computing: Condor, High-Performance Computing: Mpich2, Metropolis algorithm, Feynman Path Integration, Radiation Transfer Equation and Diffusion for Photon Transport in Biological Tissue, Diffusion Limited Aggregation, Molecular Dynamics Simulations, Finite Element Method via Galerkin Spectral Decomposition, Crank-Nicolson Method, Wave Equation for a String, Time-Dependent Schrödinger Equation: Quantum Wave Packet Implementation and Animation, Diffraction of a 2D Wave Packet, Circularly polarized Electromagnetic Waves, Burgers Shock Equation, Korteweg and deVries Equation (solitons), Navier Stokes Equation, Gaussian Integration for Integral Equations, Delta-Shell Potential Scattering. Invited U.S. speakers will present seminars along the lines of above topics, but will also be available for research communication.

For career development, several elements mentioned in professional development will also be important here. Over and above, doctoral and postdoctoral researchers will be exposed to variety of opportunities within The University of Tennessee, and to opportunities at national and international levels. Participation in seminars and/or other university activities will also be important, as well as communication with colleagues and activities in professional societies. Noteworthy is that efforts are underway to possibly host an important International Conference on Spectral Line Shapes at UTSI in 2014, 22-nd ICSLS conference. This conference usually is held bi-annually, alternating between Europe and North America. Dr. Christian Parigger has been invited to host this ICSLS XXII conference with strong encouragement and indication of support by the current Executive Director at UTSI, Dr. Robert Moore.

Principal Investigator: Dr. C. Parigger
Focus Area: Materials for Medical Imaging

**ZBLAN glass ceramics**

Research to understand the requirements for production of large, optical quality glass plates is ongoing. This activity progressed significantly during the third year of the NIH R01 support. The glass materials are made using a two-step melting process in which the fluoride reagents are weighed and mixed in a new glove box facility (see Figure 1). These compounds are melted together at a temperature of $\sim$800 °C. The resulting liquid is then cooled to form a crystalline mixture. The barium and europium chlorides are added to the mixture and it is re-melted at a temperature of $\sim$750 °C, then cooled to 725 °C and held for a short period to remove dissolved gases. The liquid is then cast into a preheated brass mold. The two-step melting procedure was shown to substantially decrease the loss of chlorides during the processing step. The two-step process results in a high quality glass sheet – see Figure 2.

![New glove box facility. Inset is a platinum crucible with a glass melt in progress.](image1)

Figure 1: New glove box facility. Inset is a platinum crucible with a glass melt in progress.

![High quality glass sheet after heat treatment. Work is continuing to fabricate and finish large plates that will be used to investigate the x-ray behavior of the glasses and glass ceramics.](image2)

Figure 2: High quality glass sheet after heat treatment. Work is continuing to fabricate and finish large plates that will be used to investigate the x-ray behavior of the glasses and glass ceramics.
It is essential to introduce divalent europium into the glass in order to achieve the PSL storage behavior. Recent work has focused on understanding and controlling processes that affect the oxidation state of europium species in the glass. It was shown that heating pure EuCl$_3$ produces a mixture of approximately 50% each of EuCl$_2$ and EuCl$_3$. The ratio of Eu$^{2+}$/Eu$^{3+}$ added to melts made using the two-step process was modified. The samples were prepared according to the compositions shown in the following table.

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Molar % EuCl$_2$</th>
<th>Molar % EuCl$_3$</th>
<th>Process Temp. ($^\circ$C)</th>
<th>Process Time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Z01</td>
<td>-0-</td>
<td>100</td>
<td>710</td>
<td>10</td>
</tr>
<tr>
<td>Z02</td>
<td>-0-</td>
<td>2.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z03</td>
<td>0.4</td>
<td>1.6</td>
<td>Zr, La, Al, Na and In fluorides melted at 800 °C, then Ba and Eu chlorides added and the mixture re-melted at 750 °C</td>
<td>2 hours total heating time</td>
</tr>
<tr>
<td>Z04</td>
<td>0.8</td>
<td>1.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z05</td>
<td>1.2</td>
<td>0.8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z06</td>
<td>1.6</td>
<td>0.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z07</td>
<td>2.0</td>
<td>-0-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z08</td>
<td>-0-</td>
<td>-0-</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A combination of Mössbauer and fluorescence spectroscopy was used to measure the Eu$^{2+}$ and Eu$^{3+}$ contents – Figures 3 and 4 show representative Mössbauer and photoluminescence spectra, respectively. The fluorescence measurements showed that the Eu$^{2+}$/Eu$^{3+}$ ratio is essentially the same in the glass as it is in the starting materials. These results show that while pure EuCl$_3$ is easily reduced by heating, when it is dissolved in the fluoride-based melt, its oxidation state does not change significantly during processing. Even though the exchange reaction {1} between ZrF$_4$ and EuCl$_2$ is thermodynamically favored, the kinetics of this reaction is slow enough to prevent a significant reaction.

$$\text{ZrF}_4 + \text{EuF(or Cl)}_2 = \text{ZrF}_3 + \text{EuF}_3 \quad \{1\}$$

Figure 3 (left): Representative Mössbauer spectrum showing Eu$^{2+}$ (-12 mm/s) and Eu$^{3+}$ (0 mm/s) components. Figure 4 (right): Photoluminescence result for ZBLAN sample JJ096 annealed at 280 °C and 290 °C for 5 minutes, blue line and dark line, respectively. The peak around 400 nm is growing as the annealing temperature increases. The peak represents the orthorhombic phase of BaCl$_2$ forming in the sample.
Secondary Ion Mass Spectroscopy (SIMS)
Secondary ion mass spectrometry has been used to analyze the composition of the ZBLAN glass surfaces. The technique provides information on the oxygen to fluorine ratio on the surface and inside the ZBLAN glasses. Oxygen content must be low to obtain the high light output, which is required for image plates. Figure 5 shows a typical result for SIMS in these materials.

![SIMS result for a representative glass sample inside and on the surface for as-made glass. The peak centered at 16 amu gives the oxygen content, at the peak at 19 amu gives the fluoride content.](image)

In situ High resolution TEM
Work has been initiated due to funding from the Ceramics Program at the National Science Foundation on observing the heat treatment of ZBLAN glasses in situ. Initial results have been obtained and Figure 6 below shows a crystalline nanoparticle of Barium Chloride at time t and sometime later (t + Δt) during which the nanoparticle has grown significantly. The interface kinetics between the nanoparticle and the amorphous glass matrix is being investigated.

![HRTEM image of BaCl₂ nanoparticle at time t (left) and time t + Δt (right).](image)
**Hardware progress**

Components for the large-format telecentric optical scanner to act as a readout system for the ZBLAN x-ray image plate were obtained; mounting hardware was designed and built, and the apparatus was assembled, aligned and optically tested.

![Figure 7: Photograph of large format telecentric optical scanner.](image)

Pulse height spectrum measurements have been used to study the possible effects of light trapping on conversion gain of the glass-ceramic plates, by varying the coupling efficiency between the plate and the photodetector using coupling fluids. Surprisingly and encouragingly, little evidence of light trapping at the glass/air interface was found.

![Figure 8: Measured PHS using prompt light from a glass-ceramic storage phosphor sample, varying optical coupling between the plate and photodetector.](image)

Principal Investigators: Professor Jacqueline Johnson, Manh Vu, Dr. Charles Johnson and Mr. Rick Weber

Sponsor: National Institutes of Health
Focus Area: Diamond-like Carbon: Synthesis and Characterization

During the past year, UTSI personnel, Lee Leonard, Alexander Terekhov, and Jacqueline Johnson have continued their research synthesizing and characterizing diamond-like carbon (DLC) thin films. They are working to develop biocompatible DLC for applications such as heart stents, hip prostheses and bronchoscopes. Both doped and undoped films have been produced by pulsed laser deposition (PLD). The films have been characterized by Raman spectroscopy, contact angle measurements, atomic force microscopy (AFM), ball-on-flat tribometry, and spectrophotometry. Film adhesion has been checked by soaking the films in simulated body fluid (SBF) and monitoring the quality of the film surface at varying time intervals using an optical microscope.

Synthesis of DLC Films

DLC films are produced at UTSI using a pulsed laser deposition system as shown in Figure 1. In this system a laser ablates a target, creating a plume which coats the substrate material.

In addition to traditional non-doped DLC films made from ablating a pure graphite target, UTSI has begun making DLC films doped with additional elements. This is made possible by the development of a system for creating multi-component targets, composed of both graphite and the desired dopant material. Interchangeable wedges of dopant material and graphite allow for the percentage of doping material to be adjusted from deposition to deposition as shown in Figures 2 and 3. Multi-component targets have been made combining carbon with silicon, titanium dioxide, silicon monoxide, and silicon nitride. By doping the DLC films, the properties of the films may be tuned to be more desirable.
Raman Spectroscopy
After a new series of films is produced, it is characterized by Raman Spectroscopy to determine how the structure of the film changes with varying process parameters. Spectra have been made for DLC films produced with varying laser fluence and deposition temperatures.

Contact Angle Experiments
It is important to understand the effect that a biomaterial will have with its environment at the surface interface. To this end, contact angles have been established for the DLC films produced to determine their suitability for various biomedical applications.
Atomic Force Microscopy
The roughness of a biomaterial can have a great effect upon its usefulness. For example, rougher contact surfaces in prosthetic joints will cause greater friction that can lead to premature failure; increased surface roughness may lead to platelet adhesion in stents causing thrombosis and clogging of the repaired artery. To understand the roughness of the DLC films produced, they were viewed under an atomic force microscope (AFM).

Ball-on-flat Tribometry
Some of the DLC films produced were evaluated using ball-on-flat tribometry to determine their potential for use as a coating for wear surfaces on prosthetic joints. UTSI has produced films with a lubricated coefficient of friction of less than 0.08 as shown in Figure 8.
Spectrophotometry

For DLC films to serve as coatings for optical lenses such as those found on bronchoscopes, the films must be transparent. UTSI has produced DLC with varying degrees of transparency. Films produced have been quantitatively evaluated using a spectrophotometer for characterization.
Soaking Experiments
For a material to be biocompatible, one requirement is that it must be stable within the human body. In vitro testing in simulated body fluid provides an inexpensive way to determine the stability of the DLC films. DLC sample PLD#36, DLC deposited on fused silica, is shown in Figure 11 after seventeen weeks of soaking in SBF. It is significant that no change can be seen in the film, even at the interface created by a scribe mark that was made before soaking began.

Future Research
Future research will include synthesis of new films using additional doping materials to improve film properties. Surface modification techniques will also be explored. Properties that will be tuned include the following: transparency, roughness, contact angle, hardness and wear resistance, adhesion, biocompatibility/inertness, and thrombogenicity.

Principal Investigators: Lee Leonard, Alexander Terekhov, and Professor Jackie Johnson
Sponsor: The Center for Laser Applications
Focus Area: Nonequilibrium Fluid Physics

Nonequilibrium Fluid Physics

In prior years, the nonequilibrium fluid physics focus area included research in electromagnetic railguns and plasma space propulsion devices such as arc jet thrusters, ion engines, Hall thrusters, pulse plasma thrusters, and laser-sustained plasma thrusters. Advanced plasmas diagnostics were utilized in these programs to characterize plasma and fluid conditions to gain a better understanding of the detailed physical processes occurring within them. Laboratory work was often accompanied by meticulous computer simulations.

Current programs in the nonequilibrium fluid physics area built largely on plasma propulsion expertise gained in the activities mentioned above. A program to develop highly sensitive electric propulsion thrust stand for the Arnold Engineering Development Center (AEDC) was completed this year, and a program to help develop a thermal management system for the US Air Force was also completed. Additionally, modeling of a laser ablation thruster for micro satellites was performed. These efforts are detailed below using excerpts from Ref. 1.

Vertical EP Thrust Stand for 12V Vacuum Chamber, AEDC TASK 06-03

The primary objective of this research and development effort was to develop a vertical thrust stand for use in the AEDC 12V chamber. This thrust stand will provide AEDC customers the ability to make thrust measurements on various electric propulsion thrusters ranging in size from about 1 kW to about 50 kW.

A variation of a hanging pendulum thrust stand capable of measuring the performance of an electric thruster operating in the vertical orientation was developed. The vertical orientation of the thruster dictates that the thruster must be horizontally offset from the pendulum pivot arm, necessitating the use of a counterweight system to provide a neutrally-stable system. Motion of the pendulum arm is transferred through a balance mechanism to a secondary arm on which deflection is measured. A non-contact light-based transducer is used to measure displacement of the secondary beam. The members experience very little friction, rotating on twisting torsional pivots with oscillatory motion attenuated by a passive, eddy current damper. Displacement is calibrated using an in situ thrust calibration system.

The Vertical Thrust Stand (VTS) has been specifically designed for use in the Arnold Engineering Development Center (AEDC) 12V test facility. Like all other displacement-based thrust measurement techniques, the VTS is susceptible to errors introduced by ‘zero drift’, which means that the displaced member does not return to the initial position when the thruster is turned off. Minor distortions in a vacuum chamber, caused either through mechanical loading during chamber evacuation or thermally-induced expansion and contraction, can cause the thrust stand to deviate from an initially-level position. The VTS incorporates several subsystems to counteract these effects, including active thermal management of the thrust stand platform, in situ leveling capabilities, and real-time monitoring of the level to ensure it remains aligned with Earth’s gravity vector. In addition, the thrust stand possesses in situ calibration capabilities, has a passive oscillation damping system, employs nonmetallic thrust stand members near the thruster to eliminate induced currents, and uses liquid metal pots to transfer power from the stationary portion of the thrust stand to the thruster. A photograph of the VTS mounted on its support structure is shown if Figure 1.
The thrust stand assembly was calibrated in the open air while mounted on the support structure as shown in Figure 1. Two simulated thruster masses of 26.8 lbm (12.1 kg) and 200 lbm (90.7 kg) were used in the collection of calibration data. The in situ thrust calibration system was used to apply a series of six weights to the balance. The masses of these weights are known to within 0.1 g, with a calibration mass of 41.3 g used for the lighter simulated thruster and a mass of 172.2 g used for the heavier simulated thruster. Before a calibration sequence was performed, the thrust stand leveling sequence was initiated to ensure that the thrust stand was within +/- 0.001 degrees of a set reference position. The output of the LGDT is plotted as a function of time in Fig. 2a for the lighter simulated thruster and in Fig. 2b for the heavier thruster. As each calibration mass is applied to the thrust stand balance, the stand rotates, yielding a stair-step shift in the output of the LGDT. The reverse situation occurs as the calibration masses are removed. The mechanism exhibits very little drift during the course of a calibration trial, effectively returning to zero displacement at the end of the calibration sequence. The repeatability of the calibration process was tested by performing three separate calibration trials for the 200 lbm simulated thruster (Fig. 2b). The first and second calibration trials were conducted eight hours apart on one day, while the third calibration trial was conducted on the ensuing day, approximately 24 hours after the first calibration. The LGDT data from these tests exhibit excellent repeatability (less than 1% deviation between trials, with much less deviation as more weights are applied to the stand).
Figure 2: Time history of VTS calibration data showing LGDT measurements as calibration weights were added and removed for a simulated thruster of (a) 26.8 lbm and (b) 200 lbm. Three trials over a span of 24 hours were performed for the latter case. Applied calibration forces and curve fits to the data plotted as a function of average LGDT response for a simulated thruster of (c) 26.8 lbm and (d) 200 lbm (all three trials worth of data).

The applied calibration forces plotted as a function of the average LGDT response, and a resulting fit to the data set for simulated thrusters of 26.8 lbm and 200 lbm, are plotted in Figures 2c and d. Note that all three trials shown in Figure 2b were lumped together in one single curve fit in Figure 2d. Given the still relatively large uncertainties in these data owing to the fact that the stand is not mounted in a vacuum chamber and is, consequently, exposed to air currents and other external disturbances, only a quick calibration analysis was performed without expending significant effort on quantifying all the errors that could propagate through the calibration routine. The error on the slope of each calibration curve represents only the error on the curve fit of the data, which has in past experience with the VAHPER thrust stand typically been the dominant source of error on the calibration data. The VTS thrust measurement error arising from the calibration was approximately 1% for the lighter thruster and 0.6% for the heavier thruster. The maximum force values given for each calibration run (Figures 2c and 2) compare favorably with the theoretical maximum measurable thrust.

Reference


Principal Investigator: Professor Trevor Moeller
Sponsor: Arnold Engineering Development Center
Mega Electric Power Systems MEPS

The University of Tennessee Space Institute partnered with General Atomics on a thermal management program for the U.S. Air Force. This export controlled program started in November of 2006 and completed in 2009. Additional information on this program has not been cleared for public release at the writing of this report.

Principal Investigator: Professor Trevor Moeller
Sponsor: US Air Force through a General Atomics sub-contract

Cryo Deposition Research, Experimentation, and Development of Early Warning and Mitigation Techniques, AEDC TASK 08-03

Arnold Engineering Development Center (AEDC) is home to the 7V and 10V Sensor Chambers, space environment test facilities used to test satellites, space propulsion systems and infrared target sensors. These facilities simulate the cryogenic rarefied gas environment of space, while providing ground-based laboratory diagnostic equipment for the test and evaluation of critical test components. However, during operation of the AEDC cryogenically-cooled 7V and 10V Sensor Chambers, the condensation and buildup of frost on optics and mechanical systems have proven to be problematic. Condensation on optics inside the chamber can affect radioactive transfer and thus compromise the efficacy of diagnostic systems. The accumulation of frost on mechanical systems, such as linear actuators, will eventually impede the motion of these devices and possibly force the premature conclusion of an experiment.

The University of Tennessee Space Institute (UTSI) has extensive experience in optical diagnostic techniques, as well as long-established expertise in rarefied gas flows and plasma physics. This multi-disciplinary experience can thus be applied to this issue to model and experimentally investigate the contamination of optical and mechanical components in cryogenic vacuum facilities with the ultimate goal of providing a means to detect and/or mitigate the detrimental effects. A unified study consisting of analytical and computational modeling of these so-called cryo-deposits, along with an extensive program of experimental testing and verification is proposed to understand the physical processes involved and to develop methods for alleviating their adverse effects.

Therefore, the purpose of this proposed Task Order contract is to conduct research into the causes, physics, and effects of cryo-deposition on mechanisms and optics and the development of methods to avoid or mitigate the effects of cryo-deposition. This information will be used in the AEDC 7V and 10V Sensor Chambers located on Arnold Air Force Base in Tullahoma, Tennessee. The information produced under this Task Order will be made available via peer reviewed publication in scientific journals to other cryogenic test facilities.

Principal Investigator: Professor Trevor Moeller
Sponsor: Arnold Engineering Development Center
Combined Recovery Factor for a High-Temperature Probe, AEDC TASK 09-02

The following description of this work is taken entirely the public release document:


Intrusive probes for temperature measurements in high-temperature flows, such as the flow downstream of a jet engine augmenter, scramjet, or rocket, must be maintained at a temperature significantly below that of the flow. The temperature difference between the probe and the flow results from heat transfer between the flow and the probe through radiation and convection. In addition, the mechanical probe support provides a conduction path to carry heat away from the probe. Heat transfer between various parts of the temperature probe itself further complicates the situation. The heat transfer associated with the probe will lead to a direct temperature measurement that is different from the true temperature of the flow. The ratio of the actual temperature to the measured temperature is called the temperature recovery factor. The recovery factor always varies from unity, regardless of whether a thermocouple or a different scheme for converting temperature to a recordable quantity is used. Therefore, knowledge of the recovery factor for a probe is essential for direct measurements of the temperature in a high-speed flow. The objective of this work is to develop a numerical model of the probe to calculate a combined recovery factor.

A schematic of a typical single-shielded total temperature probe is shown in Figure 3. The high-speed, high-temperature flow crosses a bow shock in front of the probe (for the case of supersonic flow) and enters the probe, which is comprised of a sheathed thermocouple centered in a shield. The shield has multiple vent, or aspiration, holes that are sized to control the flow of the gas into the probe cavity. These characteristics are included in the model described herein.

In 1956 George Glawe and his associates at what was then NACA Lewis Laboratory, experimentally measured the combined recovery factors of a number of different temperature probe designs [1]. In the paragraphs below, the data for one of those designs is compared with calculations made with the computer model developed at UTSI. The probe being considered
consists of an exposed junction chromel-alumel thermocouple shielded with a vented inconel shield. The test conditions reported for this probe [1] were Mach 0.3 vitiated air at 1 atmosphere.

The gas thermodynamic and transport properties for vitiated air were obtained from calculations made with the NASA CEA chemical equilibrium computer program [2] using air heated to the desired temperature with the combustion of JP5.

The results of the UTSI model calculations for three free-stream gas temperatures are shown in Figure 4. The gas temperature in the cavity decreases slightly with axial distance as heat is transferred to the thermocouple and shield. The thermocouple is cooler than the gas and hotter than the shield. There is essentially no radial temperature gradient aft of the vent holes where the properties of the gas are replaced by those of the spacer, which is a composite of inconel tube and ceramic insulator. The points on the plot signify the center of the computational cells, and the value at the first cell of the thermocouple is taken to be the measured temperature.

![Figure 4: Calculated Temperature Distribution for Glawe Probe at Three Free-stream Gas Temperatures](image)

The comparison of calculated and experimental results for this probe design using an adiabatic downstream boundary condition (negligible axial conduction to the sting) shows a consistent over prediction of the difference between the probe and the gas temperature (comparison of adiabatic case with data in Figure 5). The reported [1] experimental correction at a gas temperature of 2500 R is about 4.5 % and the computation is 2% larger than that.
There are several design and environmental factors in the experiments whose effects are probably real but are difficult to quantify. If the conductivity of the insulating ceramic is assumed to be 1.0 W/mK, as opposed to about 35 W/mK in the baseline case, the computed thermocouple temperature increases to 2343 R (Figure 6). A conductivity of 1.0 W/mK would imply a porous insulator, as this is about 10 times the conductivity of the vitiated air at 2500 R and an order of magnitude less than most solid insulating ceramics.
The test cell is water-cooled [3], however, the 4-inch diameter nozzle does not appear to be cooled, and a radiation shield in the plenum is in the line of sight through the nozzle. If this hot-parts radiation source is modeled as a 4-inch disk at the nozzle exit plane at the gas total temperature and with the emissivity of inconel (0.7), additional irradiance terms are added to the energy balance of the probe.

In the model an adiabatic boundary condition on the rear surface of the computational domain is normally assumed. When irradiance from the nozzle is added, the temperature of the thermocouple increases from 2323 R with an adiabatic boundary and no hot-parts radiation to 2377 R (Figure 7), comparing favorably to the 2384 R indicated from the Glawe data [1].

![Figure 7: The Effect of Nozzle Radiation and a Specified Temperature Boundary Condition on the Simulation of the Glawe Probe](image)

If the same emissivity and view factors are used for the 2000 R and 1500 R cases, the model matches the data very closely (Figure 5 specified temperature + radiation). This shows that modeling the ambient radiation and the heat transfer to the probe support in a consistent way is necessary for the accurate prediction of the experimental results. These results indicate that the most likely source of error in the ability to calculate a probe temperature, or conversely to use a measured probe temperature to estimate the gas temperature, are factors that may be poorly known such as the ambient radiation, the optical and physical properties of the probe materials, and the boundary conditions appropriate to the probe installation. The results of this effort strongly suggest that the UTSI model provides good predictive results given adequate knowledge of the conditions of the measurement and that the model can be utilized as a tool for predicting combined recovery factors of high-temperature probes with vented radiation shields.

References
Recent interest in the reduction of satellite size has motivated several new investigations to accommodate the mass restrictions such a satellite introduces. Micro- and nanosatellites present an abundance of design challenges, but arguably one of the most important design considerations is a suitable propulsion system. This has led to the development of the micro-laser plasma thruster (µLPT), a relatively simple and effective form of propulsion in which the propellant is ablated by a laser. [1, 2] Extensive experimental investigations have already been performed that demonstrate the feasibility of such a propulsion system. [1-7]

Although a large body of experimental work has been collected over the last several years, computational modeling of the micro-thruster has remained relatively unexplored. Computational simulations of the micro-thruster were constructed as early as 2003 [8] that modeled the end-to-end transmission-mode operation and plume expansion of the micro-thruster using combined DSMC/particle-in-cell simulation techniques. Previous work has also introduced a two-dimensional axisymmetric model of the micro-thruster operation by use of the magnetohydrodynamic code, MACH2. [9]

The work presented in the subsection below is an extension of the previous MACH2 computational model, which has been applied to a modified microthruster design incorporating a conical nozzle and used to demonstrate improved performance over the previous solid-propellant model. The subsequent subsection details the modeling of the microthruster with an energetic propellant.

Nozzle Simulations

While previous experimental work on the µLPT has largely focused on investigating the advantages gained by increasing the laser power or by ablating a more suitable propellant, [1-6] other studies have already demonstrated the feasibility of applying nozzles to improve the performance of larger thrusters that operate by the laser ablation of its propellant. [11] In fact, the MACH2 code has already been used to demonstrate nozzle performance improvements for pulsed plasma thrusters, and the results were in good agreement with experimental measurements. [10] Our work investigates operation performance enhancement when nozzles are added to the microthruster by use of the MACH2 computational model.

A demonstration of a nozzle enhancement to the µLPT device has not been found in the literature, either experimentally or computationally, although there has been experimental investigation into the demonstration of nozzle performance trends for some similar laser propulsion devices. [11] The results of these investigations suggest that nozzle performance enhancement is likely for the µLPT device as well, since in general, the thrusters have very similar operation. [11] These prior investigations have also provided us with some general trends of nozzle performance for laser propulsion devices that may be compared to the simulations presented here.
The previous MACH2 microthruster model was modified into a new micro-thruster design with the addition of a nozzle (Figure 1). Some differences exist between this model and the experimental data available in literature. [1, 2, 4, 9] Experiments had applied laser pulse durations as long as 2ms [1, 2, 4] but the availability of computational resources precluded a simulation of a 2ms duration. Therefore, the simulations were run within a two to four microsecond time, and the laser power was much higher than in the experimental case. This qualitatively still simulated the ablation of the micro-thruster propellant but in a much shorter time than experimental cases (corresponding to a much higher laser power). Furthermore, experimental data had suggested polyvinylchloride (PVC) was a suitable solid propellant due to the low thermal conductivity and high coupling coefficient. Because of limitations of available equation-of-state data, the solid propellants in these simulations and in the previous MACH2 model [9] were modeled as polytetrauoroethylene (Teflon®).

The new micro-thruster design was run for several divergent nozzle half-angles ranging from 2 degrees to 43 degrees and a nozzle length of 120µm, corresponding to area expansion ratios between 1:17 to 10:5. The baseline micro-thruster case with no nozzle addition was run and presented at an area expansion ratio of 1:00. This was done to develop evidence that typical nozzle trends are present if a nozzle were added to the micro-thruster. In Figure 8, we have included contour plots of the density within the computational domain for a nozzle expansion ratio of 3.0 to provide a qualitative picture of what is happening in the micro-thruster operation as time progresses. The subfigures present different times between 0.48µs and 0.55µs.

The nozzle results demonstrate up to a 36% improvement in the coupling coefficient and 50% improvement to the specific impulse by means of a nozzle addition to the µLPT device design, with the same mass ejection. This indicates that nozzle performance enhancement is very likely for the micro-thruster with the presence of a nozzle. Furthermore, the general trends with the area expansion ratio show that there is an optimal expansion ratio to improve the micro-thruster performance. This result agrees with other investigations into laser propulsion nozzle performance and chemical systems. [17] The model is exceptional at investigating the time dependence of the performance quantities.

Figure 8: Density contour plots (in [kg/m3]) within a subsection of the computational domain for an area expansion ratio of 3.0 at times between 0.48µs to 0.55µs.
Energetic Propellant

Original work on the µLPT focused on ablation of passive solid propellants to achieve thrust [1, 2]; most of this work advocated the use of polyvinylchloride as a suitable solid propellant due to its low thermal conductivity and measured laser momentum coupling coefficient [1, 2]. More recent work [2-7] on the µLPT operation has explored the use of exothermic (or energetic) propellant targets, which allow for a large amount of additional chemical energy to be released during the ablation process. This significantly improves the thrust achievement of the µLPT design, since the release of additional chemical energy contributes to the energy of the resulting plume. In such cases, the ablation efficiency may be much higher than unity, while the solid passive propellant case is always limited to ablation efficiencies less than unity. Recent investigations [7] of the µLPT thruster operation have considered higher-thrust modes of operation wherein exothermic compounds such as glycidylazide polymer (GAP) have been ablated. Experimental work has already led to the successful demonstration of the use of such compounds and significant micro-thruster performance enhancement.

The results of the sub-detonation ablation of glycidyl azide reflects the results of the experimental investigations using exothermic fuels to improve the micro-thruster operation [2-7]. The use of an exothermic fuel without achieving laser-supported detonation demonstrates an improvement of 70% and 20% of the coupling coefficient and specific impulse, respectively, over the baseline solid-propellant simulation. This agrees well with the experimental performance of the glycidyl azide exothermic fuel, which provided an increase by up to an order of magnitude in the coupling coefficient over the solid-propellant PVC case [1-7]. In both the experimental cases and presented simulations, the use of an exothermic propellant generally increases the coupling coefficient by an order of magnitude and slightly increases the specific impulse. Note that the coupling coefficients are higher in the simulations than in experimental cases.

Laser-supported detonation simulations were also performed; the detonations always destroyed all of the propellant present, indicating that the fuel supply could easily be damaged. Shock waves were observed to form and propagate through the fuel supply, initiating strong detonations that ejected very large amounts of mass. However, very large coupling coefficients and large increases in specific impulse were realized during this process. This is due to the extra chemical energy released during detonation. As a means of exploring the possibility of using controlled detonations in the fuel tape for achieving large improvements in coupling coefficients, the thruster was simulated with the glycidyl azide fuel and constrained by rigid walls along the edge of the fuel tape. The simulation achieved laser-supported detonation, but the detonation was noticeably weaker than in the previous uncontrolled detonations; propagation of shocks was also suppressed, even though large amounts of propellant were still ejected. This suggests the feasibility of a new mode of operation for the µLPT device that achieves ultra-high thrusts without destroying the fuel supply. However, this would necessarily require a different fuel tape construction that incorporates inhibitors that would stop the propagation of the detonation. Note that additional simulations not presented were run for other fuels ablated with 20µJ of energy; several of these fuels visibly achieved laser-supported detonation, and usually at the end of the simulation no propellant fuel was left.

Figure 9 shows a comparison of the final state of the sub-detonation simulation, the laser-supported detonation, and the laser-supported detonation in the rigid-wall geometry as density contour plots. Sub-figure 9(a) reflects the resulting difference in the behavior of glycidyl azide with different laser energies; Sub-figure 9(b) shows the effect of using a rigid wall to control the detonations and still achieve large coupling coefficients.
The onset of laser-supported detonation in the fuel tape was also investigated. The ablation pressure during the sub-detonation simulation reached an average of 14MPa; in the case of the detonation simulation, the ablation pressure averaged 136MPa, an order of magnitude larger. This suggests that the threshold ablation pressure is on the order of 108 Pa, which is within one order of magnitude of previous predictions. [2]

![Figure 9](image)

(a) A comparison of the previous simulation results and the glycidyl azide simulation. Both graphs shown are at 2.1ps and at the same scale.

(b) The final state of the detonation of glycidyl azide in Geometry #2 at 4.0us.

Figure 9: A comparison of results from the baseline previous solid-propellant work [9] the glycidyl azide sub-detonation simulation and the detonation in a rigid-wall geometry.

References

Future Use of the UTSI High Enthalpy Test Facility
Developed during an MHD generator test program, the high enthalpy combustion driven test facility is available for use in other programs. This facility burns jet fuel in gaseous oxygen to provide a Mach 2 flow with static temperatures exceeding 2700 K at the nozzle exit. This facility could be utilized in the study of new test materials for hypersonic thermal protection and propulsion systems, including thermal barrier materials, catalytic materials, and non-catalytic materials. The facility can also provide data for the evaluation of new thermal probe analysis techniques, such as those developed by Jay Frankel at UT in Knoxville [1, 2]. Frankel’s techniques allow for the determination of surface temperature and heat flux using temporal data from a single embedded thermocouple. Additional embedded thermocouples allow for the assessment of material thermal properties. Frankel’s analysis techniques have been utilized to determine preliminary estimates for the surface temperature and heat flux at two locations in the UTSI combustion-driven test facility nozzle. Multiple US government agencies have voiced interest in this proposed program.

References:


Principal Investigator: Professor Trevor Moeller
Sponsor: Arnold Engineering Development Center
Focus Area: Molecular Recognition

IMPACT (Imprinted Polymer Array for Counterterrorism): A Simple, Low-power Approach to Explosives Detection

This project involves the production of sensors for explosives vapors or explosive residues based on the electronic properties of charge transfer complexes combined with the selective binding of molecularly imprinted polymers (MIPs). Explosive materials are chemicals dominated by organic compounds with nitro (NO₂) substituents, such as trinitrotoluene (TNT). This class of compounds is notorious for having little affinity for other chemicals. However, the electronic energy levels of these compounds make them good acceptors in the formation of charge transfer complexes. This complex formation yields an electronic avenue for the detection of the explosives. By using the method of molecular imprinting to form a polymeric material with a propensity to rebinding a template molecule, a binding affinity can be established based on relatively weak binding forces. This imprinting process gives selectivity and prevents false positive detections. The combination of the two effects will result in a sensing strategy that is rugged and compatible with a high degree of miniaturization.

Principal Investigator: Professor George Murray
Sponsor: John Hopkins APL

Preparation and Characterization of Molecularly Imprinted Ion Selective Electrodes for Uranyl Ion

This is a continuation of a project began last year that received follow on funding. The purpose of this research is to develop improved molecularly imprinted ion selective electrodes for uranyl ion monitoring in aqueous solutions. The sensors are being prepared by using glassy carbon electrodes coated with an electroactive polymer doped with a polymeric ionophore. This all solid-state design results in electrodes that are more stable and long lasting and require no internal fill solutions.

![Figure 1: The potentiometric response of the composite electrode described above to uranyl ion and to two interferents.](image)

Principal Investigator: Professor George Murray
Sponsor: Babcock and Wilcox Technical Services Y-12, L.L.C.
Development of Electro-active Polymers for Explosive Detection

This is a new project to prepare electroactive polymer films for the detection of explosives residues. In this approach polymer films are prepared by electro-polymerization using an imprint ion as the supporting electrolyte. The oxidative polymerization of electro-active mers creates films that incorporate anions from the solution used to form the polymers. Electro-polymerization creates branched and crosslinked polymer films. The crosslinking makes cavities around the anionic analyte template. In this manner ion imprinted polymers are made. The polymer films can be evaluated for selectivity and sensitivity by employing them in an electrochemical cell and using them as potentiometric sensor. This simplifies preparation and provides an electrode-supported film for ease of characterization. Optimized polymers will be prepared on interdigitated gold electrode substrates and evaluated by conductivity measurements as direct electrical transducers for explosives residues. Explosive molecules that cannot be converted to ionic conductors will be imprinted into composite polymer films using polystyrene sulfonate as supporting electrolyte.

![Figure 2: Interdigitated gold electrode prior to coating with electroactive polymer imprinted with an explosive molecule using 5 X objective.](image)

![Figure 3: Polymer coated interdigitated electrode using a 10 X objective.](image)

Principal Investigator: Professor George Murray
Sponsor: Raptor Detection, Inc.
Focus Area: Laser Materials Processing

Introduction
During the past year we have continued to develop various laser materials processing techniques that are of current interest as rapid fabrication tools in a number of fields. Laser Induced Surface Improvement (LISITM) has been successfully used to protect six and eight-foot long sections of railway track with sliding wear resistant coatings. Femtosecond laser machining of fused silica has been successfully used to fabricate a new generation of microfluidic lab-on-a-chip devices for chemotaxis imaging. And single-shot femtosecond laser machining of transparent dielectric materials is being used to form high-aspect ratio nano-pores on the surface of fused silica substrates. These nano-pore filled substrates are used as templates to fabricate arrays of 10-20 µm long polymer nano-wires, via the nano-imprint lithography (NIL) route, for various applications. The results of our research efforts, our collaborations, and our vision of where we want to take this research in the future are outlined in the sections that follow.

Exploratory LISI Coating of Transportation Rails
The recent work done on surface protection of mild steel substrates with corrosion and sliding wear resistant Cr-CrB2 and Mo-MoB LISITM coatings, described in detail in the CLA 2008 Annual Report and published in Surface & Coatings Technology1,2, has attracted the attention of the Transportation Technology Center, Inc. (TTCI), located in Pueblo, Colorado. TTCI, a subsidiary of the Association of American Railroads (AAR), is interested in assessing the suitability of these coatings as a real-world rail protection solution. To be successful, the LISITM coatings have to meet the following basic requirements:

- The coatings must be fully dense, crack-free and present a good metallurgical bond to the substrate;
- The coatings must have a hardness of approximately 400 HB and a dry sliding wear resistance significantly higher than the base rail steel;
- The heat affected zone (HAZ) formed within the rail steel during laser processing must be minimized.

CLA is currently working with TTCI to develop a suitable LISITM based rail protection solution. Our joint research and development effort is focused on producing coatings that are approximately 200 µm thick and meet the outlined basic requirements. In Phase I, LISITM processing of chromium and dual molybdenum-on-chromium coatings on rail steel was investigated, the dependence of coating characteristics on the processing conditions and on the proportion of boride phase present in the LISITM precursors was examined, and suitable material compositions and processing conditions were identified. The candidate material compositions and processing conditions were validated in Phase II, when two 136 RE six-foot long rail sections, coated with numerous individual Cr – 2.5 wt. % CrB2 and Cr – 5.0 wt. % CrB2 LISITM patches laser processed using different hatch orientations, successfully passed extensive indoor rolling load machine and outdoor fast track wheel-on-rail wear tests performed on-site at TTCI. In Phase III, currently underway, two 141 RE eight-foot long rail sections, each coated with a Cr – 2.5 wt. % CrB2 LISITM layer using a single hatch orientation, will be tested extensively on a curved section of the outdoor TTCI fast track facility.

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1 Surface & Coatings Technology 203, 1984-1990 (2009)
2 Surface & Coatings Technology 203, 1281-1287 (2009)
Phase I – Selection of candidate material compositions and laser processing conditions
LISITM processing of chromium and dual-layer molybdenum-on-chromium coatings was performed on ¼” thick 0.85 % C, 1.10 % Mn, 0.59 % Si rail steel plates provided by TTCI. The coatings are based on the Cr-CrB₂ and Mo-MoB systems and the alloying compound powders were mixed with the i8 water soluble thixotropic binder and reducer (by Warren Paint and Color Company, Nashville, TN), according to the proportions listed in Table 1.

Table 1: Precursor mixes prepared for LISITM processing of rail steel plates.
For screening purposes, several different compositions were considered.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Powders</th>
<th>i8 Binder and reducer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr</td>
<td>CERAC C-2015 -325 mesh Cr</td>
<td>30 wt. % binder 0.25 wt. % reducer</td>
</tr>
<tr>
<td>Cr – 2.5 wt. % CrB₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cr – 5.0 wt. % CrB₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cr – 7.5 wt. % CrB₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cr – 10.5 wt. % CrB₂</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mo</td>
<td>Climax EM-MM2 Mo</td>
<td>40 wt. % binder 10 wt. % reducer</td>
</tr>
<tr>
<td>Mo – 15.0 wt. % MoB</td>
<td>Climax EM-MM2 Mo</td>
<td>CERAC M-1090 -325 mesh MoB</td>
</tr>
</tbody>
</table>

In each case, the resulting liquid precursor was applied to a steel plate using a DeVillbiss JGHV-531 high volume low pressure spray gun and an approximately 180-220 µm thick deposit of bonded powders was obtained. After drying under a heat lamp, the Cr-CrB₂/steel and Mo-MoB/steel plates were laser processed in open air using a 1.06 µm 1 kW YLR-1000-WC diode-pumped ytterbium fiber laser (IPG Photonics) and a hurrySCAN® 30 (Scanlab, Germany) galvomirror scan head. During laser processing, the powders melt into the surface of the rail plates to form the corresponding LISITM layers. Representative samples are shown in Figure 1.

All samples were laser processed using a 0.4 mm diameter laser beam spot size. For screening purposes, a series of LISITM laser processing trials were performed for different combinations of laser beam power, scan speed and beam hatch spacing, as listed in Table 2. To satisfy screening test requirements, 25×38 mm² individual coupons were produced for each of the conditions listed in Table 2.

Table 2: Range of laser processing conditions explored for screening purposes.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Laser beam power (W)</th>
<th>Beam scan speed (mm/s)</th>
<th>Beam hatch spacing (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr – CrB₂</td>
<td>170-230</td>
<td>21-27</td>
<td>0.15</td>
</tr>
<tr>
<td>Mo</td>
<td>175-185</td>
<td>21-27</td>
<td>0.1</td>
</tr>
<tr>
<td>Mo – 15.0 wt. % MoB</td>
<td>170-200</td>
<td>22-25</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Chromium coatings
Within the various formulations investigated, the Cr – 2.5 wt. % CrB₂ and Cr – 5.0 wt. % CrB₂ LISITM coatings were found to be the most promising candidates for developing a LISITM based real-world rail protection solution. These coatings, formed in just one single LISITM processing step, are approximately 200 µm thick and are fully dense, crack-free and metallurgically bonded to the substrate. Microstructural analysis of these coatings revealed adequate melt and mixing of the Cr and CrB₂ precursor compound during laser processing, as shown in Figure 2. Metallographic analysis also revealed the existence of a 120-140 µm deep heat affected zone (HAZ) within the base material just adjacent to the LISITM layer.

These Cr – 2.5 wt. % CrB₂ and Cr – 5.0 wt. % CrB₂ LISITM coatings present an average hardness of 42 HRC, which closely matches the 400 HB hardness requirements, while the HAZ has a hardness of 60-65 HRC. The hardness profile of a Cr – 2.5 wt. % CrB₂ LISITM coated sample, obtained using a LECO AMH-3000 automatic microhardness tester, is shown in Figure 3.

During dry sliding wear testing, performed in accordance to the ASTM G77 – 93 standard using a block-on-ring wear testing apparatus running at 1000 rpm and using a 4 lb load and a hardened steel counterbody, the Cr – 2.5 wt. % CrB₂ and Cr – 5.0 wt. % CrB₂ LISITM coatings wore at a rate that was 1/2 and 1/3 of that of the rail steel, respectively. The experimental wear data obtained for Cr – 5.0 wt. % CrB₂ layers produced under different laser processing conditions is displayed in Figure 4.
The dry sliding wear data of 2.5 and 5.0 wt. % CrB₂ layers are compared in Figure 5.

It was found that the higher the CrB₂ hard phase content, the lower the wear rate. However, the Cr – CrB₂ LISITM coatings formed with higher proportions of CrB₂ were found to be significantly harder and brittle, and not suitable for rail protection purposes.

**Dual-layer molybdenum-on-chromium coatings**

Given their general characteristics, Cr – 5.0 wt. % CrB₂ layers were selected as first LISITM layer of the molybdenum-on-chromium coatings. Initial LISITM processing trials of molybdenum layers on Cr – 5.0 wt. % CrB₂ layers were performed for two proportions of MoB, namely 0 and 15.0 wt. %. For both these compositions, the Mo-MoB layers produced were found to be extremely hard and brittle, and not suitable for rail protection purposes.
In an attempt to reduce the hardness and increase the toughness of the Molybdenum layers, laser processing of the second LISITM Mo layer was also performed under an Argon cover gas flow in an effort to protect the molybdenum from oxidation and thus prevent the possible hardening effects caused by the formation of MoO2 which is known to act as a dispersion strengthener. These Argon cover gas experiments were performed using a TZM-like precursor layer containing 1 wt. % of Titanium and 1 wt. % Zirconium, elements known to have beneficial effects on the mechanical properties of Molybdenum. This Argon cover gas and alloying strategy failed, however, to improve the mechanical properties of the LISITM Molybdenum layers. Here again, one can identify a hard heat affected zone (HAZ) within the base material. In general, the deposition of the second LISITM layer did not either soften or crack the HAZ formed during the deposition of the first LISITM layer.

The molybdenum-on-chromium LISITM coatings produced during phase I failed to meet the basic requirements.

**Phase II – Validation of candidate compositions and laser processing conditions on rail sections**

In phase I, we concluded that both Cr – 2.5 wt. % CrB2 and Cr – 5.0 wt. % CrB2 LISITM coating formulations are suitable candidates for developing a LISITM based rail protection solution, given that both formulations meet the basic requirements. It was also concluded that for successful application, these Cr-CrB2 formulations should be laser processed using a laser beam power of 200 to 220 W and laser beam scan speed of 25 mm/s.

To validate the results of phase I, two six-foot long 136 RE rail sections, one brand-new and one used, were LISITM coated with these formulations for extensive wheel-on-track testing to be performed at the TTCI facility. Each half of the rail sections was coated with one of the formulations, and for each formulation several individual LISITM coated patches, formed using a particular hatch orientation and a particular wheel-entry angle, were created (Figure 8).
Figure 8: A close-up of a six-foot long 136 RE rail section, coated with several individual LISITM patches, being laser processed on the Techno Isel Gantry table.

This coating strategy was designed to allow the effect that several different factors, namely:
- the initial state of the base material;
- the LISITM material formulation;
- hatch orientation;
- coating wheel-entry angle,
have on the performance of the coatings to be evaluated during wheel-on-rail testing.

These LISITM coated rails were tested at the TTCI facility in Pueblo, Colorado. One of the rails was inserted into the fast track railway line (Figure 9) and subject to an equivalent of 21 MGT of traffic (Figure 10).

Figure 9: LISITM coated 136 RE rail inserted in the fast track railway line, at TTCI.

Figure 10: LISITM coated 136 RE rail inserted in the fast track railway line, at TTCI, after being subject to an equivalent of 21 MGT of traffic. The individual LISITM patches are still visible.
The other rail was mounted on a rolling load machine setup (Figure 11) and subject to an equivalent of 22 MGT of traffic (Figure 12).

After extensive testing, the applied coatings continue to protect the rails. The results obtained so far are very promising and we expect this collaboration to continue in the near future.

Currently, analysis of the collected data is still being performed. In a first analysis, the wear of the coatings appears to be minimal, and the overall performance appears to suggest that these coatings are in fact promising candidates for a real-world rail protection solution. The Cr – 2.5 wt. % CrB₂ formulation, with the lower wear resistance, appears to be the most favorable, given the apparent superior toughness and fatigue resistance when compared to the Cr – 5.0 wt. % CrB₂ formulation.

We plan to publish the results of this research in a peer reviewed journal, in the near future.

**Phase III – LISI™ coating of eight-foot long rail sections for additional in-track testing**

Phase III is currently underway. Two 141 RE eight-foot long rail sections, each coated with a Cr – 2.5 wt. % CrB₂ LISI™ layer using a single hatch orientation, will be tested extensively on a curved section of the TTCI fast track facility. One section has just been inserted in the inside track and the other section was inserted on the outer track of the railway line. Testing will commence this month.

Principal Investigators: Dr. Lino Costa, Kate Lansford and Professor Hofmeister
Sponsor: Transportation Technology Center, Inc. (TTCI)

**Femtosecond Laser Machining of Microfluidic Devices for Chemotaxis Imaging**

Chemotaxis, the directed movement of cells along extracellular chemical concentration gradients, is a vital cellular response that plays a critical role during the life cycle of many organisms. Chemotactic behavior of cells is routinely analyzed using a micropipette generated gradient, based on the method originally developed by Gundersen and Barrett. Here, a radially diffusive concentration gradient forms in the extracellular environment as the biomolecule solution emanates from the 1 µm ID tip of a micropipette, positioned in the vicinity of the cells using a mechanical manipulator. Although micropipette generated gradients readily enable quantitative
characterization of the chemotactic response of cells, this method does not generate highly reproducible or controllable gradients and allows only for a restricted number of micropipette tips to be placed around the cells, thus limiting the number of gradient forming devices that can be integrated into a single experiment. Microfluidic gradient forming devices can readily circumvent these shortcomings, given the micrometer precision and the small physical footprint with which each individual device can be fabricated. Considering that cells are sensitive to changes in their environment that occur at the micrometer scale, there is definitely a need for biomolecule concentration gradient forming devices for chemotaxis analysis containing biomolecule solution delivery channels with micrometer and sub-micrometer ID. Femtosecond laser machining of transparent dielectrics, demonstrated in the recent past as a viable, fast and flexible direct-write method of fabricating microfluidic devices, offers unprecedented capability when it comes to machining sub-micron features that cannot be attained using conventional lithography techniques. In particular, single-shot femtosecond laser machining using high numerical aperture micro-objectives has been successfully used to open multi-micrometer long sub-micrometer wide pores in fused silica substrates, a technique that can be possibly used to open nanovias in microfluidic devices, be they in fused silica or in soft lithography PDMS.

In the last year, CLA has been working with Dr. C. Janetopoulos of the Vanderbilt University Department of Biological Sciences to develop a new generation of biomolecule concentration gradient forming devices, containing both micro and nano fluidic biomolecule solution delivery channels, specifically designed for lab-on-a-chip chemotaxis analysis. So far, several of these devices have been fabricated in fused silica (SiO$_2$) substrates, using femtosecond laser machining, and analysis of the chemotactic behavior of the social amoeba Dictyostelium discoideum, exposed to a 10 µM chemoattractant folic acid solution, has been performed using some of these devices. Initial results of our common research effort will be presented at the 2010 ICALEO conference and published in the conference proceedings$^3$.

The general layout of the microfluidic devices fabricated so far is shown in Figure 10 and Figure 11.

![Figure 10: Side view schematic of a microfluidic device for chemotaxis analysis.](image)

![Figure 11: Top view schematic of a microfluidic device for chemotaxis analysis.](image)

The biomolecule solution delivery channels are patterned on the bottom surface of a 500 µm thick fused silica substrate where two chemoattractant delivery ports and one cell delivery port have been opened from side to side. The chemoattractant delivery manifold is connected to the top surface of the fused silica substrate via an acrylic interconnect. The bottom of the fused silica substrate is sealed with a Polydimethylsiloxane (PDMS) coated coverslip. Cells suspended in a buffer solution are loaded into the cell delivery port and allowed to settle and attach to the PDMS.

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coated floor, from where they migrate towards the chemoattractant source. This design ensures reliable, direct and clear observation and imaging of the individual cell responses.

Device fabrication and assembly is done in the CLA class 1000 clean room, where the femtosecond laser machining facility is located. Femtosecond laser machining of UV grade fused silica is performed using the system described in detail in the paper by Zalloum et al. Amplified femtosecond pulses are generated by a system consisting of Tsunami oscillator (Spectra Physics – model 3941) seeding a Ti-Sapphire RegA 9000 (Coherent, Inc) regenerative amplifier, both of which are pumped with a cw green solid-state Verdi-18 laser (Coherent, Inc.). This system is operated at a center wavelength of 800 nm, with a repetition rate of up to 250 kHz, with a measured pulse width of 160 fs (FWHM), and average power of 1.4 W. The laser beam is focused on the surface of the fused silica substrate using a H32x/0.60 dry microscope objective (LEITZ WETZLAR). The beam is expanded using a pair of lenses so as to fill the entrance pupil of the objective. The fused silica substrate, affixed to an aluminum sample holder that is attached to an Aerotech ANT95 -50 -XY nMT stage (controlled by Aerotech A3200 Npaq MR controller), moves under the microscope objective in a pre-programmed {X, Y} pattern, with nanometer resolution, under LabView control. Surface patterning of the fused silica is performed using a travel rate of 0.1-0.5 mm/s and hatch spacing between adjacent passes of 1 µm or less. The dimensional and surface characteristics of the patterned surfaces can be precisely tailored as a function of the energy-per-pulse, pulse repetition rate and laser rastering conditions used during femtosecond laser machining.

The state-of-the-art Aerotech ANT95 -50 -XY nMT stage (Figure 12) is a recent addition to femtosecond laser machining facility that greatly enhances our micro and nano fabrication capabilities by providing not only nanometer resolution but also complete control of scan rate over a 50×50 mm² work area. Unlike most nanopositioning systems, this system uses linear DC motors and can be driven with vector commands so that the system can be controlled to the velocity of the moving stage.

![Figure 12: Aerotech ANT95 -50 –XY nMT stage used in the femtosecond laser machining facility.](image)

An example of a chemoattractant gradient forming microfluidic device is shown in Figure 13. In the highlighted gradient forming device, the transition channels connecting the chemoattractant source to the cells are 50 µm long, 7 µm wide and 25 µm deep.

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The device shown in Figure 13 was used to observe the chemotaxis of *Dictyostelium discoideum* in 10 μM folic acid chemoattractant. Figure 14 shows the beginning of cell chemotaxis, 10 minutes after the cells have settled and attached to the bottom surface of the device. Figure 15 shows the progression of cell chemotaxis 10 minutes later, as the cells migrate towards the chemoattractant source.

Another chemoattractant gradient forming microfluidic device with a different design and containing microfluidic channels for biomolecule solution delivery of different sizes is shown in Figure 16.
The concentration gradient forming capabilities of the femtosecond laser machined devices are examined by imaging the concentration gradients formed when Fluorescein dye is added to the biomolecule solution delivery manifold, as shown in Figure 17.

While work is currently underway to make these lab-on-a-chip devices a viable, easy-to-use, and re-usable replacement of standard Gundersen and Barrett based micropipette systems, our ultimate goal is to create devices in which the biomolecule concentration gradients are established exclusively by diffusion and not affected by mass flow. Diffusion driven concentration gradients are inherently stable, a necessary condition to perform precise control, quantification and modeling of the gradients formed and an essential condition when correlating the observed cell responses with the specific concentrations and spatiotemporal profiles of the applied gradients.

Biomolecular gradients are an important signaling mechanism for guiding the migration, growth, and differentiation of cells within living tissues and play important roles in various biological processes, such as tissue development, immune response, cancer metastasis and allergic inflammation. Understanding this process is essential to finding appropriate treatments for a host of diseases.

Principal Investigators: Professor William Hofmeister, Alexander Terekhov and Dr. Lino Costa
Sponsor: Center for Laser Applications
Rapid fabrication of nano-filament templates for nano-imprint lithography

In the recent past\textsuperscript{5}, CLA demonstrated that single-shot femtosecond laser machining of transparent dielectric materials using high numerical aperture micro-objectives can open multi-micrometer long sub-micrometer wide pores on the surface of fused silica substrates. An example of such nano-pores is shown in Figure 18.

![Figure 18: SEM micrograph of a nano-pore filled fused silica substrate surface, after 75 seconds of BOE etching, to be used as a template during the fabrication of polymer nano-filament arrays via the nano-imprint lithography (NIL) route.](image)

The replication technique used previously to evaluate the size and shape of these pores is now being used to fabricate arrays of 10-20 µm long polymer nano-filaments for various applications. So far, replication of nano-pore filled fused silica substrate surfaces has been successfully achieved using cellulose acetate (CA). Here, a 35 µm thick film of cellulose acetate is softened at the nano-pore filled surface by exposure to acetone and forced into the nano-pores by the combined action of gravity and capillarity. Once the acetone has evaporated, the cellulose acetate film containing the nano-filament replicas of the nano-pores is peeled-off the fused silica surface. Examples of CA nano-filaments obtained using this method are shown in Figure 19 and Figure 20.

![Figure 19: Scanning Electron Microscope micrograph of an array of gold-coated cellulose acetate nano-filaments.](image)  
![Figure 20: Scanning Electron Microscope micrograph of gold-coated cellulose acetate nano-filaments.](image)

The various applications for these filaments include the creation of superhydrophobic surfaces, cell traps, and drug and vitamin delivery patches. In the future, the goal is to extend this technique to other polymers of interest, such as PMMA, PDMS, polyethylene, and electroactive polymers such as PEDOT and P3HT. Our current effort has centered on perfecting the replication technique, to allow high aspect ratio nano-filaments to be formed and extracted from these templates with high repeatability, modifying the dimensions and surface properties of the nano-pores via wet chemical etching, and developing methods to surface coat these nano-filaments with thin metal and oxide layers. Gold and Platinum 100 nm thick coatings are routinely applied to the CA replicas via

\textsuperscript{5} CLA 2008 Annual Report
Magnetron Sputtering, while Carbon and Aluminum layers are applied to the CA replicas via vacuum evaporation. We have also succeeded in coating Au-coated CA replicas with a thin layer of SiO$_2$, produced by sol-gel synthesis, as shown in Figure 21.

![SEM micrograph of a Au-coated CA nano-filament coated with a thin layer of SiO$_2$ via the sol-gel route.](image)

The results of this research effort will be presented at the 2010 ICALEO conference.

Principal Investigators: Professors William Hofmeister and Lloyd Davis, Dr. Lino Costa and Kate Lansford
Sponsors: Center for Laser Applications

**Filamentation of Oxide Superconducting Tapes**

ORNL is working on reducing AC losses in YBCO superconducting tapes by filamentation of the tapes. The tapes are made by depositing buffer and superconductor materials on a substrate tape, and then coating the superconductor with a silver stabilization layer. The goal is to ablate parallel channels the silver coating, superconductor, and buffer layers the entire length of the conductor while leaving the substrate intact. The process must be amenable to production in a continuous process.

Since melting of the substrate (or deposited materials) is undesirable, femtosecond ablation was attempted. The femtosecond nanomachining station in the CLA clean room was used to ablate parallel grooves 100 microns wide the length of the conductor. The task is quite challenging due to the mix of optical, thermal and dielectric properties in the conductor. An optical micrograph of a typical ablated line is shown in Figure 25.

![Optical micrograph of an ablated line in a stabilized, coated YBCO superconductor after etching.](image)
Figures 26 and 27 are scanning electron micrographs of the un-etched filament groove shown in Figure 25.

Figure 26: SEM micrograph of laser ablated surface. Silver layer is damaged but not removed. The sample is un-etched and tilted 45 degrees.

Figure 27: This sample was mounted in epoxy and polished at an angle to reveal the interface and depth of laser penetration and material modification. The YBCO layer is cut and some of the substrate melted and re-solidified.

The laser was run at a repetition rate of 250 kHz so the process is not athermal as evidenced by the melting of the substrate. Silver was not removed by the laser, but converted to nanoparticles which can be seen in Figure 27. A mild nitric acid etch was used to remove the nanoparticles to reveal the optical picture in Figure 25.
Future experiments will include oxygen gas injection to remove silver particles and experiments at repetition rates of 1kHz or less to allow time for thermal dissipation between pulses.

Principal Investigators: Professor William Hofmeister  
Sponsor: ORNL Robert Duckworth and Yifei Zhang and Center for Laser Applications

**Laser Machining of “Theta” Samples**

The theta sample was designed for the testing of tensile properties in a scanning electron microscope. Since the sample total size is of the order of one millimeter, femtosecond laser micromachining is a candidate process. Here, dimensional tolerance is important, however, it is very important not to modify the material properties in the fabrication process. Femtosecond process can, in some cases, ablate material without melting.

We have tested the machine path to create the sample in fused silica. The sample in figure 28 was ablated to a depth of 30 microns in the area that appear black in the optical micrograph. The dimensions of this sample are very close (+/- 2 microns) to the desired shape.

![Figure 28: theta sample machined in fused silica to a depth of 30 microns. Black region has been ablated.](image)
We also tested some Cu-Sb-Se material to look at the ablation characteristics as a function of laser power and nanostage travel velocity. At full power (1.3 W average power at 250kHz) the laser cut to considerable depth in the sample, but significant debris and some melting of material was observed. The end of a line cut at this power is shown in figure 29. The melting is probably the source of the cracks that appear in the surface.

![Figure 29: Maximum power cut in Cu-Sb-Se alloy. Note melting and cracks.](image)

At the lower powers (50 mW at 250 kHz) we are able to ablate material cleanly revealing some microstructure of the alloy as shown in Figure 30.

![Figure 30: Low power laser ablation is relatively clean with no cracks. SEM micrograph, no etch.](image)
The results indicate that there will be a range of laser fluency, pulse repetition rate, and laser travel velocity that will ablate material with little or no damage to the specimen.

Principal Investigator: Professor William Hofmeister
Sponsor: ORNL Edgar Lara-Curzio and Paul Majsztrik and Center for Laser Applications

**Thermal Behavior of WC-Co Cermets During the LENS® Process**

LENS® is a solid freeform fabrication (SFF) technology that combines high power laser deposition and powder metallurgy technologies to convert complex CAD solid models to engineering parts. Features of LENS® technology are high cooling/solidification rate, rapid prototyping capability, shape control, and wide material applicability. In this study we used high speed thermal imaging to record the temperature history and gradients during processing and matched that to the 3D finite element code of the simulated process.

![A thermal image from a SS316 line build taken by a high speed camera](Ref: W. Hofmeister et al., JOM, 1999)

![Simulation of a SS410 2D (single-pass wall) part](Ref: Wang et al, Materials Science and Engineering A, 2008)

![SEM images of a WC-Co thick wall sample:](a) image showing alternating sub-layers; (b) cross-sectional image; (c) a boundary area; (d) an image of a large WC particle after etching

Feedstock powder: nanocrystalline WC-12 wt.% Co
Laser power: 200 W;
Traverse speed: 3.2 mm/s;
Powder feed rate: 10 g/min;
Z height increment: 0.2 mm
Working plane: 2 mm higher than the focal plane of the laser beam.

Principal Investigators: Professor William Hofmeister
Sponsors: NSF - J.M. Schoenung, UC Davis, PI, Graduate Research Assistant Y. Xiong
Focus Area: Vision Science Research

Introduction:

The optical physics and design expertise of CLA have been applied to the challenging problem areas of human vision simulation and ocular measurements. The problem of entry for us in this field was support of a company in the development of a vision screening device. In time it became obvious that such development was based on simplistic computations of normal eyes and a strong reliance on empiricism. The essential missing elements included, even for normal eyes, absence of adequate data to characterize population variations of ocular parameters according to gender, race, age, and geographic locations, and for abnormal eyes or ocular diseases, information was sparse. I and my collaborator at that time and now, Dr. J.W.L. Lewis, redirected our efforts to development of the predictive capabilities for abnormal eyes and for population distributions. This research became the bedrock upon which our subsequent instrument development has been based, and the subsequent material describes our current activities in this field.

Customized Eye Model Bank For Virtual Clinical Trials & Education (NIH contract: R21EY018935)

This NIH project, which was granted on 09/01/2009, will develop a ready-to-use computational optical tool-kit that can describe the performance of eyes with normal and abnormal optical structures. The second aim of the project is to demonstrate applications of the established eye bank in Aim 1.

Progress in eye model development

To establish a digital eye bank that contains detailed personalized eye models of both normal and diseased eyes, clinical data have been obtained using patients and state-of-the-art diagnostic ocular instruments at Wang Vision Institute (WVI) in Nashville. Records of 10 mild keratoconus (KC) or FFKC eyes in WVI were selected. Clinical data were processed for the modeling. This group includes 6 mild KC eyes of best corrected visual acuity (BCVA) of 20/30 or better. The control group of 10 eyes includes 3 near-emmetropic and 7 near- and far-sighted eyes that have BCVA of 20/20. Of these 7 ametropic eyes are 3 astigmatic eyes that present clinical features similar to those of keratoconus eyes. The clinical patient data were exported from instruments and then were digitized and transformed into the required ZEMAX formats for modeling using C++ and MatLab programs.

In the past year we have investigated an additional optical simulation program, Advanced Systems Analysis Program (ASAP) to provide a non-sequential simulation option with the powerful capability of modeling the scattering properties of both media and surfaces, including the retina. In March 2010, Dr. Chen attended the ASAP training courses in Tucson with the focus on extending the eye modeling capability for this research project. Shown in Figure 1 are the 3-dimensional non-sequential eye model and one ray-tracing demonstration of a bio-media.

Figure 1: Non-sequential eye modeling using new optical software, ASAP. ASAP has advantage in the investigation and handling of ocular scattering problems in ophthalmic simulation.
Ophthalmic simulation progress
The second aim of the project is the demonstration of the applications of the digital eye bank. In the past months, some of the patient vision simulations were performed with the constructed keratoconus and normal groups of eyes. Shown in Figure 2 are eye models with correcting spectacles at different gazing conditions. Figure 3 is a simulated vision of a keratoconus eye on Snellen Letter E at 20/20 line after trial lens correction. This simulation was performed by tracing 1 million rays. The best-corrected trial lens (second-order correction) is determined by the ZEMAX program through optical optimization and is validated using the clinical measurement of patient record. The visual acuity of this 45 year-old patient is clinically 20/20 with best correction. However, the coma aberration is clearly predicted from the computation.

Figure 2: The CLA eye models with ophthalmic corrections.

Figure 3: Ray-tracing results of Snellen E letter vision simulation of a keratoconus eye using ZEMAX program.
As a second demonstration, the simulation of retinoscopy was initiated and is currently on-going. Initial results of the double-pass diagnostic measurement were obtained, and sample results are provided. Figure 4 is a spot-retinoscope simulation of one myopic eye. The retinal surface of the model in this simulation is assumed to be Lambertian with no specular reflection. The figure shows a traditional spot retinoscope that projects a round-shaped illumination from a distance of 0.5 meter. In contrast, a contemporary retinoscope projects a straight-filament image onto a patient’s eye. A typical computational run uses 100 million rays in each pass to achieve high quality and accurate simulation. Other simulation results using the newly purchased optical program, ASAP, are also performed.

Figure 4: Spot-Retinoscopy double-pass simulation of a myopic eye. The retina is assumed to be a Lambertian surface in this simulation.

The commercial optics code, ZemaxTM (ZEMAX Development Corporation, Bellevue, WA), is a very powerful computer program for the optical system design and optical optimization. For eye modeling work, the optical optimization offered by ZEMAX is especially useful to achieve the detailed optical performance of the patient's eye. Figure 5 shows the wavefront aberration result from a keratoconus eye using Zemax. The addition and inclusion of the ASAP code (Breault Research) in the computation options will significantly extend the range and capability of our study. Specifically, the influence of both single- and multiple-scattering from different ocular surfaces and media can now be theoretically investigated. ASAP is expected to be effective in examining ocular stray light that is essential for performing realistic ophthalmic simulations. With these two parallel computation approaches, not only can we enhance the broad applications, but we can also validate the results through comparison between the results from two programs.

The inclusion of ASAP provides the foundation for expanding the eye modeling to cataract, floaters, and tear films, in the future. The multi-level scattering and surface roughness can be investigated to achieve realistic modeling. This research investment is an important groundwork for the research area and applications.

Figure 5: Wavefront aberration of a keratoconus eye obtained from Zemax modeling.
**Plans for next year**

Using the "forward" eye modules, patient vision simulation will be continuously performed on both keratoconus and normal groups of eyes to demonstrate applications in medical education and patient consultation. Snellen letter chart for distant (20 feet) and near vision (30 cm) will be simulated. In addition, Day and Night Street Visions will be computed. We believe this capability can provide excellent and accurate assessments of the visual acuity and response to a wide variety of occupational environments. All keratoconus vision simulation results will be compared with typical myopic and astigmatic eye vision performance.

Retinoscopy double-pass simulation will continue. This calculation is more time- and effort-consuming. With ZEMAX sequential ray tracing program, the simulation procedure requires two separate simulations using forward and reversed models, respectively. In comparison, when using non-sequential ASAP program, this simulation can be performed with accurate modeling of the scattering properties of retina. The computations will provide estimates of the intra-ocular and fundus reflection for several scattering models. Evaluation of the accuracy of the scattering models will be compared with existing clinical measurements. Using a single-processor computer, to obtain a single simulation image of high quality, the ray tracing time is therefore very long (hours). This computation time can be reduced by using cluster-computing or a multi-processor PC. Although we have access to PC cluster-computing, it is more expedient to minimize implementation time and to use a multi-processor PC. We have just updated our computer system to a 6-core PC this August to make the computation more effective. The computation results from the 2 programs, ZEMAX and ASAP will be compared, and the virtual clinical trial computations will follow.

**Optical Investigation on Early Keratoconus Detection**

This NIH contract project started in August 2009. There are emerging treatment options for keratoconus, and their success increases if detection can be achieved for early-stage keratoconus, or forme fruste keratoconus (FFKC). This research project is to utilize a novel method of detection of early-stage of this disease. The CLA personalized eye modeling technology will be used with contemporary clinical wavefront, topography, and ocular biometry data to provide high-fidelity optical models of FFKC and KC eyes. Using this capability, realistic instrument measurement simulations will guide the optimal design of a low-cost device to approach the high-sensitivity detection.

The specific aims of this research project are:

1. **Computational research**: Use computational predictive medicine to guide the research development -- Construct customized keratoconus eye models that mimic mild keratoconus and FFKC eyes. Simulate with high-fidelity the ophthalmic measurement of patients.
2. **KC detection**: Construct a low-cost KC screening device with CLA patented novel technological advancement.
3. **KC auto-analysis**: Develop a computer-aided-diagnosis (CADx) and user-friendly GUI program.

**Studies and Results/Progress**

In support of the mission of the ARRA (American Recovery and Reinvestment Act of 2009), we hired a researcher through the sub-contract of Wang Vision Institute. This new researcher, Dr. Kevin Baker, is primarily supported with this contract and partially with our NIH/NEI contract R21EY018935. He shares a portion of Dr. Lewis’ workload in planning and documentation and is responsible for the assembly and initial testing of the KC detection device. He also effectively worked and coordinated the activities between the clinical setting at the Wang Vision Institute and the laboratory setting in the Center for Laser Applications at the University. He presented a related poster for FFKC in May this year at the Association for Research in Vision and Ophthalmology (ARVO) annual meeting. This poster examined whether the anterior or posterior irregularity is a
better indicator of FFKC. A second poster publication by Dr. Chen reviewed the age-related lens biometry that is useful for the eye modeling.

**Computational Study Progress**

Records of mild keratoconus (KC) or FFKC eyes in WVI were selected and prepared for the modeling. Each eye is characterized with measurements of the clinical instruments Pentacam (to construct mathematic presentations of cornea and lens surfaces), Master IOL (to obtain axial length), and Wave scan Visx (detailed optical performance as modeling target). The exported data from Pentacam was successfully digitized and then transformed into required ZEMAX and ASAP formats for modeling using C++ and Mat-Lab programs. The recently purchased optical simulation program ASAP provides a non-sequential simulations option with powerful capability of modeling the scattering properties of media and surfaces, including the retina. Shown in Figure 6 is one example ray-tracing result of an eccentric photorefractive (EPR) measurement assuming a Harvey model of the retinal scattering. Figure 7 shows a predictive measurement simulation result of a mild KC eye. This eye has a best-corrected visual acuity of 20/25+2 and refraction of (-5.50S, +2.25C, X173).

![Figure 6: Non-sequential eye modeling and simulation using new optical software, ASAP. ASAP has advantage in the investigation and handling of ocular scattering problems in ocular measurements.](image)

![Figure 7: A predictive simulation of a mild KC eye measurement of the device. This KC eye has manifest refraction of (-5.5S, +2.25C, X173) and BCVA of 20/25+2.](image)

**Progress in Hardware System Construction**

The assembly and testing of the components of the KC imaging system is currently in progress. The system was recently upgraded by incorporating a new digital camera and smaller light sources. The new digital camera provides a faster frame rate of 120Hz, and 50% higher light sensitivity to the NIR light sources that we utilize. Major hardware enhancement will include the testing and optimization of a new computer-controlled camera zoom lens and compact LED light source panel design. The first objective using the new computer controlled camera lens will be to evaluate the possibility of being able to differentiate the crystalline lens and cornea surface as the aberration/scattering sources. Shown in Figure 8 is the configuration of the camera and infrared light source assembly. Also, we are using smaller light sources (3mm in diameter compared to 5mm that were used previously) because they allow a more compact 2-dimensional light source arrangement, which in turn will improve KC detection sensitivity. These critical optical parameters will be tested in the optical software programs with the customized KC eye models before validation with human testing. The initial tests on the new camera, zoom lens, and light sources showed improved performance, and we plan to use a completed prototype for the clinical trial in Wang Vision Institute.
CADx development progress

The development of the computer-aided-diagnosis (CADx) and user-friendly GUI program will start in fall 2010. The CADx software will be developed on the basis of our theoretical evaluation and modeling/simulation results. The CADx programming will create a number of numerical metrics to identify and classify keratoconus and other diseases. We believe the innovative analysis CADx program will not only identify keratoconus from normal group, but also illustrate by a quantitative measure the subtle changes of this disease. The cost-effective nature of our method is intended to provide a reliable tool for a small fraction of cost required using the current approaches.

For eye-modeling studies, ZEMAX optical optimization is especially useful to achieve the detailed optical performance of the patient eye. The inclusion of ASAP, the new optical software, will significantly extend the range of our study. Specifically, the influence of multiple scattering from different ocular surfaces and media can now be hypothetically investigated. ASAP is highly effective in investigating ocular stray light and performing ophthalmic simulations. With these two approaches not only can we improve the expansive applications, but we can also validate the results through assessment between the two approaches.

Principal Investigator: Professor Ying-Ling Chen and Dr. J.W.L. Lewis
Sponsor: National Institutes of Health

Pediatric Vision Screening Research

This pediatric vision screening research project is supported by UT Research Foundation maturation grant 2009-2010 and UTSI/CLA internal research support. CLA Automatic Photoscreening System (APS) Technology– United States Patent # 7,427,135, was granted 09/23/2008. A Continuation-In-Part patent application was submitted during the past year and the patent is pending.

The aim of the APS to perform accurate and rapid vision testing that provides quantitative results within a few minutes of the beginning of the examination. The system is portable, capable of operation without medical professionals and will perform the range of tests required for pediatric vision assessment. Although the system is not limited to pediatric applications, early-age screening is most important because during a specific window of time called the "critical period" when the
The brain is set for aggressive learning, proper binocular visual sensory input is essential. Young brains need the neural activity to mature and to develop plasticity. If the performance of one eye is significantly less effective than the other due to uncorrected refractive errors or strabismus, the brain would cease communication with the problem eye to prevent confusion. After the critical age, the damage in binocular perception is found to be irreversible. This condition is called amblyopia or lazy eye. In the US, the prevalence of amblyopia is 3-5%, and other pediatric vision problems and amblyogenic condition is as high as 25%. Because 85% of a child’s learning is related to sight, the importance and demand of early and frequent vision evaluation is universally acknowledged. To satisfy this need, the APS was designed to perform low-cost, high-quality, ocular tests without requiring either medical professionals or complex manual procedures. The technique objectively determines binocular refractive errors, binocular alignment and motility, and optical opacities, and is both operator- and child-friendly. The successful application of APS will provide a significant benefit to the public, especially those of medically under-served groups.

During the past year, the APS prototype was assembled and the safety evaluation was performed. Institution review board (IRB) approval of human clinical trial was obtained. The first phase of the APS pilot clinical test was performed at the University of Alabama in Birmingham (UAB) School of Optometry in Oct. 25-30, 2009. Clinical eye examinations were performed by optometrists at UAB for 50 volunteers recruited from optometry students of classes of 2011 and 2012, and the clinically measured distribution function of refractive errors are shown in Figure 9. Using the APS prototype, the pilot results of automatic strabismus test and refractive error measurement were obtained and are shown in upper and lower of Figure 10, respectively. The comparison to the clinical comprehensive eye examinations presents promising results. In the human study, we have also identified some problems from these pilot results. First, the human subjects of the UAB pool of students are young adults, and unlike pediatric subjects, the refractive error is biased to the negative refractive error while the targeted pediatric subjects are in the hyperopic region. Also, human factor and variation of retinal scattering and accommodation result in imprecision of measurement. Plans of adjustment in hardware parameters and measurement protocol will be made for 2010 phase II pilot trial. The phase I study provided valuable guidelines for future development.

The most exciting outcome of this phase I trial is the level of enthusiasm and optimistic reactions among the optometry faculty and pediatricians who were present at the clinical trial site and who performed the tests on their own eyes. After the trial, suggestions regarding the design and protocols as well as potential applications in extended research areas were stimulated and continue.

Figure 9: Refractive error distributions of optometry class 2011 and 2012.
Figure 10: APS Phase I clinical trial results. Upper picture shows the strabismus test result from the APS automatic cover-uncover test. Lower picture shows the refractive error test results.

Principal Investigator: Professor Ying-Ling Chen
Sponsor: UT Research Foundation
Focus Area: Ultrasensitive Spectroscopy

Ultrasensitive Fluorescence Spectroscopy / Nanophotonics

In the past year, CLA research in the area of ultrasensitive and single-molecule fluorescence spectroscopy has included several different projects as well as funding from the National Institutes of Health and the National Science Foundation. Research has included collaborations with Louisiana State University, Tulane Health Science Center, and Vanderbilt University. Also, a user proposal with the Center for Nanophase Materials Science at Oak Ridge National Laboratory was successful and work began in February 2010.

As a part of the educational mission of the CLA in this area, 600-level graduate physics courses were taught in Quantum Optics, Non-linear Optics, and Control Theory for Physics. Two students working in the area of ultrasensitive fluorescence spectroscopy (J. Crawford and J. Germann) graduated with MS degrees in physics and one of these students is continuing for the PhD degree and also passed the comprehensive exam. One doctoral student (J. King) presented his research results at the annual meeting of Frontiers in Optics organized by the Optical Society of America in San Jose, California in October 2009; another doctoral student (W. Robinson) co-authored an invited presentation at the 2010 Photonics North conference held in Canada in June; also three graduate students co-authored a presentation at the Single Molecule Spectroscopy and Imaging symposium at the 2010 SPIE Photonics West conference in San Francisco, California, in January.

Also in the research area of ultrasensitive fluorescence spectroscopy, one undergraduate student in physics from the University of the South (J. Simpson) contributed to CLA research to improve laser machining of vias in microfluidic devices for single-molecule measurements and presented his results for his BS Honors project in Spring 2010. Another student (J. Parker) from the BS physics program at Middle Tennessee State University contributed to CLA research in ultrasensitive spectroscopy during Summer 2010 as a co-op student. CLA staff member Dr. Brian Canfield completed a term as postdoctoral fellow and is now continuing to contribute to our research in this area as Research Scientist.

Our research in ultrasensitive fluorescence spectroscopy includes contributions to the development of new experimental techniques and instrumentation, as well as theoretical modeling and computational simulations. Our recent research has included the following:

**Maximum-likelihood multichannel fluorescence microscopy**

In order to extend multichannel fluorescence microscopy methods to the ultrasensitive regime, we constructed several scanning confocal microscopes with pulsed laser excitation using alternating sources of different wavelengths, with collection of fluorescence into spectrally-resolved emission channels, and with time-resolved single-photon detection. We developed novel maximum-likelihood data analysis strategies for quantitatively resolving (un-mixing) the signal contributions from spectroscopically overlapping fluorophores and we used Monte Carlo simulations, and also results from experiments with samples containing known mixtures, to determine technical and fundamental limitations for un-mixing low photon count images obtained from two or three species. We found that maximum-likelihood based un-mixing of multichannel spectroscopic images is superior to least-squares based un-mixing when the numbers of photons within the individual spectroscopic channels are below about 100, and that signals from three fluorescent species with significant spectral overlap can be un-mixed with useful precision even when the total number of photons in all channels is as low as a few hundred. The project has involved design and construction of custom optical set-ups and development of modeling and analysis software.
Results from this research are included in the M.S. thesis of J. Crawford, who graduated in August Summer 2009.

Principal Investigator: Professor Lloyd Davis  
Sponsor: National Institutes of Health

**Single-Molecule Delivery and Trapping in a Nanochannel**

Research from previous years on a DARPA-funded project for the Control of Protein Conformations (CPC) program with the goal of developing advanced tools for the detection and control of single protein molecules has continued over the last year, specifically to improve our techniques and our understanding of the delivery and trapping of fluorescently-labeled proteins within a nano-fluidic device. As single molecules are too small for optical trapping, the method of trapping is instead based on active control of electrokinetic flow in response to position measurements by single-photon detection from the single molecule with time and spatially modulated laser excitation.

Major progress has been made in understanding the physical limitations of photophysical processes, such as triplet blinking and photobleaching, and of instrumental effects, such as feedback latency, the finite electrokinetic flow velocity achievable, and detector dead-time. To this end, a comprehensive physical model and a Monte Carlo computer simulation of all relevant processes have been developed, and these are reported in our recent paper in the Journal of Biomedical Optics, and also The Virtual Journal of Nanoscale Science & Technology. Our studies have provided validation and understanding of past experiments as well as insight on methods to improve future experiments.

For example, Figure X1 shows that as one increases the fluorescence lifetime of the molecule to be trapped, the average number of photons that can be collected and the average occupancy time of a molecule in the trap both decrease, while the percentage of photons with incorrect timing increases. The figure inset shows that the timing delay must be correctly set to within a few nanoseconds to achieve good trapping.

For small molecules with relatively fast diffusion, an improved algorithm for feedback control of the electrokinetic motion has been developed and tested. While accommodating the limited electrokinetic speed and the finite latency of feedback imposed by experimental hardware, the algorithm has been shown to be effective for trapping fast-diffusing single-chromophore molecules within a micron-sized confocal region. Our studies also show that there is an optimum laser power for which loss of molecules from the trap due to either photobleaching or shot-noise fluctuations is minimized.

![Figure 1: Photophysical effects on trapping performance.](image)
In our previous experiments, we have shown that single fluorescent molecules in aqueous solution may be detected within a nanochannel with excellent signal-to-noise and with increased photostability. However, in these experiments, we found that over a course of several hours, the fluorescently labeled molecules stick to the walls of the nanochannel and lead to a steady background of fluorescence. Hence these experiments have required the use of a fresh nanochannel device for each experiment, which has provided a practical limitation on our ability to proceed with more intensive studies.

To address these issues, a user proposal was submitted to the Center for Nanophase Materials Science at Oak Ridge National Laboratory for the purpose of creating a new batch of nanochannel devices to enable studies of surface treatment of nanochannels before the low temperature bonding of the coverslip to attempt to reduce sticking. The scientific questions to be addressed are: (1) Is it possible to create surface-treated nanochannels that prevent molecular sticking and that give low background autofluorescence? (2) How are the photophysical properties of single fluorescent molecules influenced by the nanochannel environment? (3) Can surface-treated nanochannels provide a practical platform for biotechnology applications of single-molecule spectroscopy in which a large number of molecules must be interrogated one by one, and in which other potential advantages of nanochannels may be realized?

Work on the proposed research began with a visit to CNMS by Dr. Lloyd Davis and CLA graduate research assistant Mr. Jason King during the week of March 29 to April 2, 2010. Unfortunately, during this visit, failure of a machine for reactive ion etching prevented us from forming new nanochannels. Wet etching methods were also developed but yielded only limited contrast. Figure 2 shows Mr. Jason King using the CNMS facilities for wet etching. Another visit to CNMS during a week in June also unfortunately met with equipment failures and hence continued work is required.

Principal Investigator: Professor Lloyd Davis
Sponsors: Center for Laser Applications, Oak Ridge National Laboratory Center for Nanophase Materials Science, and the Arthur and Helen Mason Fellowship
Three-Dimensional Single-Molecule Position Sensing and Manipulation

We are working to extend the research on single-molecule trapping in a nanochannel described above to develop new methods for use of a confocal microscope to accurately measure the position of a single emitter in three dimensions (3-D), and also methods for use of microfluidics to manipulate single molecules in solution in 3-D. These developments would enable 3-D trapping of biomolecules that are too small for optical trapping, and it would thereby enable use of the confocal microscope for prolonged spectroscopic investigations of a single molecule freely diffusing in solution.

In wide-field microscopy, the location of a single molecule can be measured to a precision down to about one nanometer by imaging the emitted fluorescence over a number of camera pixels and finding the center of the image. In recent years, methods for super-resolution optical microscopy (i.e., resolution below the diffraction limit of light) that rely on successive position measurements on large numbers of single fluorescent molecules have emerged as a powerful new tool for visualizing the inner molecular workings of cells. Single-emitter localization has been extended to 3-D by a number of techniques, all of which rely on fitting the image of the emitted fluorescence light and they are typically achieved with wide-field illumination. On the other hand, confocal microscopy, which uses a tightly focused laser beam, provides better signal to noise than wide-field microscopy. Furthermore, methods of single-molecule localization that rely on the excitation light rather than emitted light offer improved resolution due to the shorter wavelength. Also, tightly focused laser illumination as used in confocal microscopy is a prerequisite for femtosecond two-photon fluorescence excitation, which offers advantages of lower background for intracellular studies.

With these considerations in mind, over the past year, we have shown that spatially and temporally structured laser excitation with four laser foci in a confocal microscope can provide resolution advantages for 2-D and 3-D single-emitter localization. We have also shown that for conditions under which structured excitation gives comparable localization precision to spatially resolved fluorescence emission, an improvement in resolution can be achieved by using both techniques together, for example, by using four-focus laser excitation and also imaging the fluorescence onto four separate single-photon detectors. As an example, Figure 3 shows maximum-likelihood analysis of results from Monte Carlo simulations showing this to be the case, as reported in our paper titled “Four-focus single-particle position determination in a confocal microscope,” published in the SPIE proceedings in March 2010.

![Figure 3: Position estimates from (a) 4-focus excitation, (b) imaging fluorescence emission to a quadrant detector, (c) both methods; (d) Schematic of imaging the fluorescence to a quadrant detector to yield photocounts \(N_a, N_b, N_c, N_d\) for maximum likelihood analysis.](image)
In order to manipulate a single molecule in 3-D, we are developing a microfluidic device that will enable the adjustment of four voltage levels to control the electro-osmotic and electrokinetic motion of a single molecule in aqueous solution. A mask for the microfluidic device was fabricated in June 2010 during a visit to the Center for Nanophase Materials Science at Oak Ridge National Laboratory. We have been developing facilities for bonding glass microfluidic devices in CLA’s clean room in the past few months. In the year ahead, a microfluidic device will be constructed for studies on this topic as part of the doctoral research of CLA graduate research assistant Mr. Jason King. Also in recent months, CLA graduate student Mr. William Robinson has been developing a computer model to help evaluate methods for controlled manipulation and trapping using the device.

Principal Investigator: Professor Lloyd Davis
Sponsors: Center for Laser Applications, Oak Ridge National Laboratory Center for Nanophase Materials Science, the Arthur and Helen Mason Fellowship, National Science Foundation through a subcontract from Vanderbilt University

**Development of a Nanoparticle Trap for Nano-Spectroscopy**

This work is part of a collaboration with Vanderbilt University and is funded by a National Science Foundation (NSF) Major Research Instrumentation (MURI) grant to Vanderbilt with a subcontract to UTSI. A key goal of the MURI is to build and bring into operation an experimental system at Vanderbilt University for performing temporally and spectrally resolved spectroscopic measurements on trapped, or otherwise isolated, nanoscale-sized particles and molecular constructs. The development phase of the instrument is being used in training and development, as well as in outreach, and as the components of the instrument are completed, it is being used for a variety of experimental studies.

To date, we have designed, assembled and aligned the components of a custom ultrasensitive fluorescence microscope that enables several types of high sensitivity low photon-count measurements to be made on individual nanoscale-sized particles and molecular constructs. Figure 4 shows a block diagram of the microscope. The initial configuration of the camera is shown in Figure 4(a). This configuration enables (1) confocal fluorescence detection (through a 100 μm pinhole) with either (a) a single-photon avalanche diode (SPAD) detector for time-resolved measurements, including sub-nanosecond fluorescence lifetime measurements by time correlated single-photon counting, or with (b) an electron multiplying charge coupled device (EM-CCD) camera, for spectrally resolved confocal measurements, with use of a custom designed high-efficiency prism spectrometer; and (2) wide-field imaging, by directing the collected fluorescence prior to the pinhole directly to the camera, and by insertion of a lens into the laser beam for Kohler (wide-field) illumination. The present configuration for wide-field imaging with the camera is for wide-field spectrally-resolved imaging with a 10° dispersive wedge, and is shown in Figure 4(b).

Initial measurements on ultrasmall (~5 nm) quantum dots from the laboratory of Professor Sandy Rosenthal at Vanderbilt University were conducted using the configurations in Figure 4(a). At this time, the sample was held on an available 2-D nano-translator stage, providing manipulation in x and y, but not in z. These initial experiments observed that samples of ultrasmall quantum dots exhibited weak emission and photobleaching, which made sustained confocal spectral measurements very difficult. In wide field imaging of a sample of many quantum dots, we could observe blinking of individual quantum dots, but spectrally resolved confocal measurements were not achieved.
Ensemble measurements using relatively concentrated solutions (~μM) have observed white light emission from ultrasmall quantum dots and a major question to be addressed with the instrumentation is whether the white light results from (a) broadband emission from each individual quantum dot, or (b) narrowband emission from each individual that fluctuates in wavelength as a function of time, resulting in a time-integrated white-light signal from each individual, i.e., a homogeneously broadened white light spectrum, or (c) steady narrowband emission from each individual, with different center wavelengths for different individuals, resulting in a heterogeneously broadened white-light spectrum.

To address this question, we decided to rebuild a part of the microscope to achieve wide-field spectrally-resolved imaging, so that many individuals could be studied simultaneously. Also, to account for the very weak emission and improve the signal to background, the spectrometer was redesigned to disperse the white light spectrum (from ~400 to ~700 nm) over a smaller number of camera pixels (~30 rather than ~400) by replacing the dispersion prism with a 10° wedge made from low dispersion BK7 glass. Zemax optical design software was used to select the wedge angle.

In our preliminary experiments with this reconfiguration, movies have been collected from a 128 × 128 pixel field at a frame rate of ~100 Hertz using several different samples of ultrasmall quantum dots with slightly different synthesis procedures and dilutions. The samples are prepared in toluene and evaporated onto glass coverslips. Results so far indicate that steady white light emission is observed from samples that appear to be aggregates, because they do not exhibit blinking and they fade slowly rather than photobleaching in one step. Individual particles/aggregates give images that are ~1 pixel tall (magnification resulting in 200 nm/pixel and diffraction limited point spread function of ~200 nm) and ~20 pixels wide (emission bandwidth of ~250 nm, yet to be calibrated). Samples prepared at lower concentrations, which do exhibit blinking and hence are defensibly

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Figure 4: Ultrasensitive fluorescence microscope with (a) Initial configuration of camera, for wide-field imaging and spectrally-resolved confocal imaging; (b) Present configuration of camera for wide-field spectrally-resolved imaging of quantum dots. (The removable mirror is the same as that in (a).)
single quantum dots, have been observed to exhibit narrowband emission. It appears that the emission wavelength of some dots fluctuates in time. However, experiments have not yet conclusively determined if this is the case for the following reason:

During the collection of the data for these experiments, the piezo stage developed a failure such that motion in one axis exhibited random jumps in time and motion in the other ceased completely, making it very difficult to position and hold a sample. The stage has very recently been replaced with a new 3-D piezo stage. The front end of the microscope has been rebuilt and is shown in the photograph in Figure 5. The EM-CCD camera and 10° wedge are at the back of the photo. The 3-D piezo stage will enable 20 μm of nanometer precision translation and 4 mm of manual adjustment in each dimension, and will be used for sample positioning and for confocal trapping and tracking experiments. In the months ahead, it will also be fitted with temperature and environment control for live cell imaging.

In the experiments above, the sample is illuminated by just a single laser beam, but for confocal trapping/tracking experiments, the pulsed laser beam is split into four temporally interleaved pulses, to create a temporally and spatially modulated excitation profile. The beam paths for doing this are shown in Figure 6. Also shown in Figure 6 are two small lasers, a He-Ne 633 nm laser (red dotted line) and a Gre-Ne 543 nm laser (green dotted line). These are used for alignment, or can be attenuated and used for registration of correct focusing of the fluorescence microscope, or can be
used with Kohler illumination to image scattered monochromatic light from individual quantum
dots, so that the fluorescence emission wavelengths of each dot can be determined from a
comparison of images.

Principal Investigator: Professor Lloyd Davis
Sponsor: National Science Foundation through a subcontract from Vanderbilt University

High Throughput Modular Microfluidic Systems for Drug Discovery

One important part of CLA’s research into ultra-sensitive laser fluorescence measurements covers
pharmaceutical drug discovery research and associated biotechnology applications. Toward this
end we are part of a four-year collaboration begun in 2007 with Professor Steven Soper at
Louisiana State University and Professor Prescott Deininger at Tulane University Health Science
Center, with funding from the National Institutes of Health. The project goal aims to develop an
ultra-sensitive, high-throughput, rapid-readout microfluidic platform for drug discovery and
evaluation and demonstrate its use in screening for inhibitors of L1-endonuclease (L1-EN), an
enzyme that is implicated in cancer.

CLA’s major contribution to this collaborative project concerns the development of ultra-sensitive
fluorescence assay readout methods to determine molecular species concentrations within
microfluidic channels constructed from polymeric materials. These methods are necessary to
monitor small changes in the concentrations of fluorescently labeled molecules resulting from
enzyme activity induced by potential new pharmaceutical compounds under investigation.
However, because autofluorescence of the polymer fluidic devices themselves is an issue,
fluorophores emitting in the deep red must be used to reduce the background signal.

We have designed an experimental apparatus for multi-point detection in polymer microchannel
devices over a wide field of view (FoV). The apparatus, which has been revised from its original
construction, is shown in Figures 7 and 8. Features of this custom-built microscope include a
Köhler epi-illumination scheme using an angle-tuned longpass filter, a high-NA objective, and
detection with an electron-multiplying CCD camera. The original construction used a 660 nm
diode laser exhibiting a circular, Gaussian beam profile as the light source for generating a
fluorescence response. This situation necessitated a complex system of beam-shaping optical
components in order to obtain an ellipsoidal approximation of the desired rectangular illumination
profile. However, the initial Gaussian profile was still propagated to the focus, resulting in
significantly lower intensities toward the edges of the focal region.

Figure 7: Custom microscope for wide-field, high-throughput readout. The line-generating diode laser is located
at the far right.
The major improvement of the modified configuration was replacing the circular Gaussian beam with a line-generating diode laser containing a diffractive optical element. The line laser operates at the same wavelength of 660 nm, but it produces a linear beam exhibiting a uniform ‘top hat’ intensity profile. This substitution not only eliminates the beam-shaping optics, allowing a much simpler and more compact optical system, but allows a nearly ideal rectangular focused spot with uniform intensity over the FoV.

As shown in Figure 7, a single spherical lens is used to collimate the beam emitted by the line laser, and in Figure 8, a cylindrical lens is used to achieve the Köhler illumination condition, where the beam is focused at the back conjugate plane of the objective. Rather than being focused to a diffraction-limited spot, the light is then approximately collimated as it emerges from the objective, effectively mapping a miniaturized rectangular illumination profile to the microscope’s FoV. The focused rectangle is approximately 2 microns by 500 microns.

The objective is a water-immersion apochromat with NA 1.2, field number of FN = 26.5, a magnification of M = 60, and also has an adjustable correction collar. It is thus capable of providing a flat-field image on a camera over a region of diameter FN/M = 0.44 mm. Careful, compact placement of the optics as seen in Figure 8 has allowed us to achieve a FoV >0.5 mm, with only minimal image curvature at the far edges. This FoV is sufficient for imaging a polymer device with ~200 microfluidic channels, each 1.0 micron wide with 1.0 micron spacing, onto the camera.
Because the apparatus uses epi-illumination, the fluorescence is imaged onto the camera with the same 1.2 NA objective, allowing for excellent collection efficiency. The microfluidic device is aligned on the stage above the objective so that the 0.5 mm dimension of the rectangular illumination zone intercepts all microchannels. The angle-tuned longpass filter immediately beneath the objective fulfills a double purpose as a mirror to the excitation wavelength, directing the pump beam into the objective and rejecting any collected backscatter from the sample, but transmitting the longer-wavelength fluorescence. In addition, appropriate choice of the filter’s cut-on wavelength (680 nm) addresses even small Stokes shifts of ~10 nm, as the passband shifts significantly toward shorter wavelength with increasing angle of incidence.

The lenses are chosen to provide the full FoV while maintaining 1:1 mapping between CCD pixel size (16 microns) and sample space. A slit placed at the focus of the lens below the filter in the detection arm provides additional spatial filtering to image the excitation region onto only a single row of pixels on the camera. By reducing the active imaging region of the camera we can therefore maximize the speed of data collection and readout. A second longpass filter immediately before the CCD ensures complete removal of any residual laser light.

Preliminary experiments have been conducted using a low-background PMMA microfluidic device with a small number of large-dimensioned (100 micron) channels. The key constraint on the microchannels is not their width, however, but their shallowness. The channel depth must be limited to 1–2 microns so that fluorescently labeled molecules remain within the objective’s depth of focus during transit. We are currently preparing to study ultra-sensitive fluorescence detection from Alexa 660-labeled molecules in prototype multichannel polymeric microfluidic devices. The optimal camera parameters such as exposure and readout times, maximum measurable flow rate, and appropriate electron multiplying gain will need to be investigated. A comprehensive computer simulation that models the experiment is under development and this will be used in the year ahead to help select optimum operating parameters.

Principal Investigators: Professors Lloyd Davis and Brian Canfield
Sponsor: National Institutes of Health through a subcontract from Louisiana State University

**Laser-Induced Ignition Studies of Solid Aluminum Particles**

Collaboration with The University of New Mexico at Las Cruces and Sandia National Laboratories at Albuquerque, addressed experimental studies of laser-ignition characteristics for solid aluminum ignition. Recent developments in AMO (Atomic, Molecular, Optical) Physics show feasibility and success of laser-induced breakdown spectroscopy methods for application in laser-induced ignition, and here, laser-induced ignition of solid propellants. Application of time-resolved atomic spectroscopy, molecular spectroscopy, and high-speed photography was conducted in an experimental effort at UTSI’s Center for Laser Applications, augmented by addition of a used “work-horse” Nd:YAG laser equipment for several parametric tests.

Fundamental molecular spectroscopy work at The University of Tennessee Space Institute comprises development of accurate data bases for selected molecular transitions of several diatomic molecules. Historically, these spectroscopic studies aimed at characterization of micro-plasma, including detailed description of laser-induced optical breakdown (LIOB) phenomena. Early in the plasma generation and decay, atomic species dominate spectroscopic signatures, followed by occurrence of diatomic recombination molecular emission spectra. In some applications, obviously, excitation of molecular species occurs without LIOB, and the generated accurate molecular data base can be applied for identification purposes as well. Figures 9 and 10 illustrate an AlO spectrum at T = 3000 K, and a previously measured AlO spectrum during laser ablation. Spectra of this kind are expected to be measured in laser-induced ignition of aluminum.
Standoff applications extend remote, fiber-type small to reasonable size laboratory applications, but are not limited to these kind of “laboratory” distances that generally fall in the category of remote sensing. Applications include diagnostics applications in combustion, in laser-ignition and formation of macro-carbon molecules. At the University of Tennessee Space Institute, theoretical descriptions of molecular spectra have been of interest for the last several decades. Some of this interest derives from characterization of plumes of various origins, including specific signatures of propulsion systems. Laboratory scale experiments were conducted to validate theoretical descriptions. Along these efforts in molecular spectroscopy, significant theoretical and experimental work was performed in atomic spectroscopy for purpose of determination of physics and chemistry phenomena. Here, our expertise in atomic, molecular, and optical physics is extended for characterization of aluminum particle ignition, including time-resolved measurements and analysis of molecular signatures with goal of investigating the laser-induced combustion process.

Figure 9: Theoretical AlO spectrum of the AlO $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ Band.

Figure 10: Measured and fitted AlO spectrum of the AlO $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ Band.

Principal Investigator: Professor Christian Parigger
Sponsor: Center for Laser Applications
Ultra-sensitive Diagnostics Instrumentation for Research

Research efforts at the Center for Laser Applications require a healthy cycle of research instrumentation. Approximately fifteen (15) years ago, major instrumentation additions occurred in part funded by the National Science Foundation for ultra-high speed diagnostics. Elements included high speed camera, equipment for time-resolved measurements, an ultrashort laser providing nominal 60-fs laser radiation, a high-repetition Copper-Vapor laser radiation, and computer instrumentation. These additions spawned several sponsored research projects. The 60-fs laser continues to be of use in materials research with a recently acquired amplifier, yet other areas require investment. For that purpose an extensive proposal was prepared and submitted to the National Science Foundation.

The aims of the Research and Development (R&D) proposal to the NSF are focused on promoting collaboration amongst a multi-disciplinary group of researchers working in fundamental Mathematical and Physical Sciences, Applied Physics, and Materials Science and Engineering. The proposal request is for coherent light sources/laser-beam-shaping equipment and spectroscopy/microscopy diagnostics instruments needed to enable specific experimental projects and both inter- and intra-disciplinary research activities at The University of Tennessee Space Institute / Center for Laser Application (UTSI/CLA). This major equipment request is perfectly aligned with the long-range mission of the University of Tennessee (UT): Invigorate Applied Physics and Materials research and outreach at UTSI and CLA. Objectives include in-situ and remote diagnostics using coherent radiation, an approach that can be extended to diagnostics in the field of airborne sciences. Existing collaborations with National Laboratories will be increased, for instance with Oak Ridge National Laboratories and with Sandia National Laboratories. International collaboration in Condensed Matter Science and in Applied Chemistry will strongly benefit from the proposed research and training efforts.

The intellectual merit of this request is substantial. The equipment requested will enable much needed studies in femto- pico- and nano- physics and chemistry, nano-scale materials modifications, and nano-scale structures that impart novel functional properties to materials, partly through coating, surface and/or bulk modifications. Figure 11 shows images of ablated saw-tooth structures on silicon and single crystal nanodiamond surfaces. The program’s interests further extend to diagnostic applications that derive from AMO (atomic/molecular/optical) Physics that involve cold-temperature applications. These are primarily based on the use of appropriately shaped coherent radiation both in temporal and spatial domains. Additional focus areas include the testing of particular hypotheses arising in the diagnostics of chemically reacting flows, turbulent swirling flows, and non-equilibrium fluid physics. Figure 12 illustrates counter-rotating vortices generated by aircraft. Experimental studies and numerical modeling are already intrinsic to research applications at UTSI’s Center for Laser Applications, and the equipment requested will bolster in significant ways UTSI’s abilities to carry out modern research while seeking out secondary collaborations with industry. Finally, amongst the proposed activities are investigative studies that encompass biomaterials and micro-fluidics that hold the potential of opening up new lines of inquiry in medical diagnostics research.

The proposed efforts will have a direct impact on society by exposing high school, college, and graduate students to vital research experiments and equipment in Applied Physics, Materials Science and Engineering. This will be accomplished through strategically planned short courses, summer internships, and competitive design activities. The inherent safety of laser diagnostics permits testing in lively demonstrations and courses on the subject. It will be applied to attract students from several public schools in conjunction with UTSI’s active involvement in recruiting and educating K-12 and under-represented groups. This program will therefore (1.) complement and extend UTSI’s reach into Material Science and Engineering; (2.) help to promote graduate research; (3.) enhance the diagnostic and development capabilities of UTSI and the Center for
Laser Applications; (4.) provide new testing platforms for UTSI’s competition teams; (5.) help to interface with national and international collaborators; (6.) involve high schools in alluring scientific research; (7.) offer new courses on femto- pico- and nano- physics; (8) offer short courses on the subject both at UTSI and professional conferences; (9.) preserve the role of the Center for Laser Applications as a critical national asset; and (10.) strengthen the outreach and research programs that are shared between UTSI, Oak Ridge, and the nearby Arnold Engineering Center.

Figure 11: Ablation of saw-toothstructures on (a) silicon and (c) single crystal nanodiamond surfaces. b, and d, SEM non-destructive replication for estimating the dimensions of the saw-tooth has been demonstrated.

Figure 11: Example of counter-rotating vortices generated by aircraft.

Principal Investigators: Professor Christian Parigger and other faculty members of CLA and UTSI
Sponsor: The Center for Laser Application
International Collaboration on Laser Spectroscopy

Time resolved experimental studies and numerical modeling of laser-induced plasma processes were presented at the annual Plasma Physics Conference at Zvenigorod, just outside of Moscow, in February. Dr. Parigger was invited by the organizers who greatly showed their hospitality to the two invited international attendees in 2010, one from Belgium and one from the U.S.A. Figure 13 shows the “Pensionat” of the Russian National Academy of Science in Zvenigorodski. Figure 14 exhibits a section of the “Watching Hill” monastery some 50 km outside of Moscow. Figure 15 depicts the frozen Moscow River with Cross-Country Skiing tracks. The interest in Plasma Physics extends to the establishment of ITER (International Thermonuclear Experimental Reactor) that is an international magnetic confinement fusion research/engineering project that could help to make the transition from today’s studies of plasma physics to future electricity-producing fusion power plants. While the research interest at UTSI is in the nominal optical region with energies of the order of a few eV, in our laser-induced studies, fusion plasma energies are in the order of 20 MeV; nevertheless, diagnostic applications extend to the study of plasma boundaries/edges.

The contents of the invited presentation are summarized by the abstract: “Transient microplasma is generated by laser-induced optical breakdown (LIOB). Here we are interested in the characterization of laser-induced plasma using time-resolved atomic and molecular spectroscopy. A detailed review will be presented of use of hydrogen Balmer series H-alpha, H-beta, and H-gamma, atomic lines for diagnostic purposes. Early in the plasma decay, Boltzmann plots are applied to determine the excitation temperature in the range of 100,000 to 7,000 Kelvin. The corresponding electron densities in the range of $10^{19}$ to $10^{16}$ cm$^{-3}$ are inferred using Stark shift and width measurements. Laser-induced breakdown spectroscopy (LIBS) techniques are further investigated in the analysis of molecular recombination emission spectra, for example diatomic CN and C$_2$ Swan bands. Usually highly excited molecular spectra are recorded indicating equilibrium temperature in excess of 7,000 Kelvin. Computation of diatomic molecular spectra includes use of accurate rotational line strengths. Optical breakdown processes are also investigated using ultra-high speed photography methods. Recent advances in theory of atomic and molecular spectra are discussed,
including modeling and simulation of highly excited atomic, molecular species following laser-induced optical breakdown in various applications.

Figure 14: Frozen Moscow river in Zvenigorod with Cross-Country Skiing tracks on left.

Following this visit communication exchanges occurred on subject of future collaborations on laser-induced spectroscopy and other physics areas. As an example, one of these areas includes study of fractal nature at cosmic scales. An understanding of the fractal composition of the Universe will allows us to also address: (i) Why the visible mass in space amounts to only a few percents of the mass in the Universe; (ii) Why galaxies may be formed in a relatively short time compared to the age of the Universe; (iii) Why cosmic objects such as planetary nebulas or galaxies show a typically narrow size distribution. The idea behind formation of galaxies and perhaps the universe is fracture of fractal filaments of dark matter. Figure 16 and 17 illustrates interacting galaxies and the mentioned fracture.

Figure 15: Images of Interacting galaxies UGC 06471 and UGC 06472. b. Image-enhanced schematic. c. Enhanced image at a magnified scale

Figure 16: A. Two interacting galaxies NGC 4038/4039. B&C. Enhanced images.

Principal Investigator: Professor Christian Parigger
Sponsor: The Center for Laser Applications
Characterization and Modeling of Spark-induced Breakdown Plasmas

Active collaborations continued between the University of Denver and the University of Tennessee Space Institute. The goal of this collaboration is to perform an in-detail characterization and modeling exercise on the plasma formation conditions in spark-induced breakdown spectroscopy (SIBS). SIBS is an analytical technique that provides elemental composition information and has been applied to a variety of environment and process-line samples. SIBS appears to be especially promising in the analysis of airborne particulate, now a measurement of importance because of the connection between increased human morbidity and mortality and ambient airborne particulate material. Additionally, SIBS has been demonstrated to be a useful component in systems to detect airborne bio-aerosols and is therefore of interest to homeland security concerns. In spite of the promising results obtained in these applications, SIBS remains an immature analytical method. This is partially due to the lack of fundamental data on the relationship between the SIBS electrical input and the resultant analytical plasma, as well the association between plasma conditions and analytical signals. Figure 18 shows typical atomic and molecular CN emissions. Figure 19 illustrates measured spark appearance. And Figure 20 shows the diagnostics applications of both experimental and theoretical application of fundamental studies of selected diatomic molecular transitions.

A focus of this collaboration will be the study of excitation process and its relationship to the observed signals. This should allow us an in-detail analysis of important measurements, with optimistic results in many cases. A more complete understanding between electrical input and the overall plasma evolution, including the initial streamer formation, the expansion and shape at various times during excitation and cooling, is critical to better and more widespread use of this interesting analytical technique. Spark discharges have been successfully used for decades to measure metals in conductive samples, typically under a purge gas; the relationship between power supply output and plasma formation is well known in this case. However, the SIBS spark is instead similar to a flash lamp excitation event, except that the analytical discharge is struck in air, rather than in Xe or Kr. Such a discharge has not been used in an analytical capacity before now. This effort is projected to aid in the development of instrumentation that will be useful for monitoring airborne particulate material, and will contribute both in the areas of health and security. Besides the opportunity to support and train students, this collaborative research effort encompasses three principal arenas: domestic security, environmental and economic.

A better understanding of the basic SIBS process will positively affect the development of the instrumentation of interest to the U.S. government dedicated to monitoring for biological warfare agents. The SIBS technique has also been applied to measurements of environmental interest, namely the detection of toxic metals in soils and airborne particles. The initial detection limits for metals such as Pb and Cr in soil are better than those required to meet regulatory requirements, both in the U.S. and in many foreign countries. The analyses are simple and the results available in minutes, rather than the days required to analyze a soil sample using traditional wet lab methods.
Development of an on-site SIBS soil analyzer would simplify and speed remediation of hazardous waste sites. Data on metal loading of fumes and process aerosols can be available on a minute-by-minute basis with SIBS. Lastly, development of new analytical equipment in both sectors will provide the Nation with jobs and sales.

Figure 19: Pseudo-color rendering of the iCCD spark shape image.

Figure 20: Measured and simulated emission spectrum.

**CN \( B^2\Sigma^+ \rightarrow X^2\Sigma^+ \) Violet System**

- **T=7940K**
- CLA line-strength data
- Experiment: 1:1 CO\(_2\)/N\(_2\) atm mixture
  - FWHM = 2.0 cm\(^{-1}\)
  - 0.4 \( \mu \)s time delay

Principal Investigators: Professor Christian Parigger and Dr. Amy Bauer of Denver University
Sponsor: The Center for Laser Applications
Mössbauer spectra of glasses and nanoparticles

A Mössbauer spectrometer has been installed and successfully commissioned. Both $^{57}$Co and $^{151}$Sm sources are available for $^{57}$Fe and $^{151}$Eu measurements respectively.

The primary aim is to analyze and characterize europium nanocrystals doped into ZBLAN glasses made at UTSI by Dr J.A. Johnson. This material is being developed here for application as a digital x-ray detector for medical imaging, and requires that the majority of the europium is in the divalent Eu$^{2+}$ state. The Mössbauer Effect provides a simple and non-destructive method for distinguishing between oxidation states. Data so far show that most of the europium is Eu$^{3+}$ and there is no clear indication of Eu$^{2+}$. This is partly because the Mössbauer $f$-factor of Eu$^{2+}$ is lower than for Eu$^{3+}$, and partly because dilute Eu$^{2+}$ shows line-broadening due to magnetic relaxation. To increase the sensitivity requires measurements at low temperatures and it is planned to purchase a closed cycle refrigerator to operate down to 5 K.

Other measurements on Eu not requiring low temperatures are in progress and include (i) Eu-P glasses (in collaboration with MST, the Missouri University of Science and Technology) (ii) nanoparticles of CaF$_2$ doped with Eu (in collaboration with Clemson University) and (iii) EuS nanoparticles (in collaboration with Vanderbilt University). The latter material is magnetic with a $T_c$ of 18 K and is being studied at low temperatures at Argonne National Laboratory. Measurements with $^{57}$Fe are being made on (i) Fe-P glasses (in collaboration with MST) (ii) nanoparticles of Fe-Co, Fe-Ni and other iron alloys (in collaboration with the Russian Academy of Sciences, Moscow).

Sb Mössbauer spectra of a Sb$_2$O$_3$ glass made at the University of Warwick by roller-quenching were measured at Argonne, and showed that the antimony was pure 3+. Previous attempts to make the glass always had Sb$^{5+}$ impurities.

Principal Investigator: Professor Charles Johnson
Sponsor: The Center for Laser Applications
Enrichment Programs

UTSI/CLA Computational Science Camp for Middle and High School Students
Thirty area middle and high school students and six teachers attended a workshop and were exposing the technologies, techniques, and tools of computational science and the close relationship between math and science. Bob Gotwals has been the instructor the last four years and returned this year to continue this very popular outreach program.

As in the previous year’s workshops, students were taught how to use models, modify existing models, and how to create models from scratch. Topics that were studied included computational astrophysics, meteorology, agriculture, genomics, epidemiology, pharmacokinetics, and drug design and quantum chemistry. Students had an opportunity to write their own computer programs, using languages such as gnuplot, perl, and NetLogo. All the materials used in the class are available at no cost to students and teachers. The teachers involved in the workshop learned how to deliver these materials in their own classrooms. This collaboration is a continuing activity and will spread with the involvement of these dedicated teachers.

Bob Gotwals conducting a team building exercise involving the observation of rope tricks.

Peyback Foundation Grant
UTSI and the Hands-On Science Center received funding through Peyton Manning’s Peyback Foundation to serve at-risk alternative school students in Franklin and Coffee Counties. The graduate research assistants brought various science programs to the students each month. One program was provided by the Optical Society of America. The “Optics Briefcase” gave the students an opportunity to investigate how optics and photonics impact daily life – computer screens, cell phones, car headlights, and emerging technologies.

Joel Thompson and Jason King engage students with the “Optics Briefcase”
Science Camp for Fourth and Fifth Grade Students
The Hands-On Science Center hosted the UTSI Science Camp this year. Twenty six students learned how exciting science can be during the week full of engaging activities. The students learned about Isaac Newton’s Laws of Motion, built rockets from straws, and experimented with microscopes.

These programs were developed at UTSI four years ago and since then it has been determined that it is more appropriate for the students to meet at the Hands-On Science Center, therefore, UTSI is assisting in the management and delivery of science camp for younger learners.

Outreach Coordinator: Carole Thomas
Sponsor: Center for Laser Applications

Bill Boss from the Hands-On Science Center engaging students and teachers in electricity.
Awarded Grants and Contracts 2009-2010

R02-4007014 - $896,569 expended in FY 2010
“The Center for Laser Applications”
State Appropriations, Professor William Hofmeister, Director of CLA
Contract period: July 1, 2009 – June 2010
Total grant for FY 2009: $965,200

R02-4411031 - $13,093 expended in FY 2010
“Closed-Loop Process Control for Electron Beam Direct Manufacturing”
Sciaky Corporation, Professor William Hofmeister
Total award: $30,000

R02-4411032 – $35,845 expended in FY 2010
“Exploratory LISI Coating of Transportation Rails”
Transportation Technology Center, Inc., Professor William Hofmeister
Contract period: October 15, 2009 – April 30, 2010
Total award: $35,845

R02-4411033 - $0 expended in FY 2010
“Laser Induced Surface Improvement for Superior Wear Resistance in Extreme Conditions”
AFOSR STTR Phase I Subcontract, Professor William Hofmeister
Contract period: June 1, 2010 – March 31, 2011
Contract award: $50,000

R02-4334020 - $44,951 expended in FY 2010
“Laser Ignition of Solid Propellants: Aluminum Particle Ignition”
Sandia National Laboratory, Professor Christian Parigger
Contract period: July 21, 2009 – September 30, 2009
Contract award: $44,951

R02-4380029 - $27,532 expended in FY 2010
“ATA Internship”
Arnold Engineering Development Center, Professor Christian Parigger
Contract period: October 7, 2009 – September 30, 2010
Contract award: $40,259

R02-4318031 – $105,826 expended in FY 2010
“High Throughput Microfluidic Systems for Drug Discovery/Development of Assays for High Throughput Drug Discovery,”
Louisiana State University subcontracts to UTSI
Contract awarded: $559,438

R02-4318033 - $19,081 expended in FY 2010
“Development of a Nanoparticle Trap for Student Training and Nano-Spectroscopy,”
Vanderbilt University, Professor Lloyd Davis
Contract period: April 1, 2009 – August 31, 2010
Total award: $36,535
R02-4417020 - $524,259 expended in FY 2010
“Advanced High-Resolution Two-Dimensional X-Ray Detector for Mammography”
National Institute of Health, Professor Jackie Johnson
Contract period: February 1, 2008 – November 30, 2009
Total award: $1,394,613

R02-4419020 – $86,325 expended in FY 2010
“IMPACT (Imprinted Polymer Array for Counter Terrorism): A Simple, Low-power Approach to Explosives Detection”
NSF, John Hopkins APL, Professor George Murray
Contract period: November 4, 2008 – July 31, 2010
Total award: $150,000

R02-4419021 - $69,624 expended in FY 2010
“Uranium Sensors for Y-12 Plant at Oak Ridge”
B&W Technical ServicesY-12, Professor George Murray
Contract period: March 2, 2009 – September 2009
Total award: $75,000

R02-4419022 - $17,371 expended in FY 2010
“Electro-active Polymers for Explosives Detection”
Raptor Detection, Inc., Professor George Murray
Contract period: February 17, 2010 – February 17, 2012
Total award: $399,805

R02-4348023- $57,282 expended in FY 2010
“Electronic Propulsion Vertical Thrust Stand”
AEDC Task Order, Professor Trevor Moeller
Contract period: July 31, 2006 – April 30, 2010
Total award: $310,000

R02-4348025- $35,431 expended in FY 2010
“Multi mega watt Electronic Power System (MEPS) Thermal Management”
General Autonomics, Professor Trevor Moeller
Contract period: November 21, 2006 – November 15, 2009
Total award: $760,153

R02-4348026 - $55,600 expended in FY 2010
“Cryo Deposition Research”
AEDC Task Order, Professor Trevor Moeller
Contract period: November 21, 2008 – November 20, 2011
Total award: $200,000

R02-4348028 - $31,049 expended in FY 2010
“Combined Recover Factor Model”
AEDC Task Order, Professor Trevor Moeller
Total award: $35,000

R02-4348031 - $7,359 expended in FY 2010
“GTL/ATK Moeller Effort,” Professor Trevor Moeller
Contract period: January 22, 2010 – February 28, 2010
Total award: $7,359
R02-4348029 – 52,631 expended in FY 2010
“Space Engineering and Planning Study”
AEDC Task Order, Professor Trevor Moeller
Contract period: May 20, 2009 – May 20, 2010
Total award: $60,000

R024313025 - $22,245 expended in FY 2010
“Pilot Clinical Test of Adaptive Photoscreening System (APS)”
University of TN Research Foundation, Professor Ying-Ling Chen
Contract period: February 1, 2009 – November 1, 2009
Total award: $22,245

R02-4313026 – $136,132 expended in FY 2010
“Optical Investigation of Early Keratoconus Detection”
National Institutes of Health – Wang Vision Institute
Contract period: August 1, 2009 – July 31, 2011
Total award: $187,362

R02-4313027 - $124,240 expended in FY 2010
“Keratoconus eye model bank for virtual clinical trials and medical educations”
National Institute of Health – National Eye Institute
Contract period: August 1, 2009 – August 31, 2010
Total award: $187,500

Total Research funds expended in FY 2010 = $2,362,445
Graduate Research Assistants and Summer Interns

**Graduates in 2009 - 2010**
Sarah Cothran, Master of Science, Mechanical Engineering, Non-Thesis

Richard Joel Thompson, Master of Science, Mechanical Engineering, “Computational Investigations of Characteristic Performance Improvements for Subkilogram Laser Micropropulsion”

Nicholas Lister, Master of Science, Mechanical Engineering,


James Germann, Master of Science, Physics, “Three Dimensional Localization with Time-gated Photon Counting and Maximum-likelihood Analysis”

**Enrolled in 2009-2010**
Lei Shi, MS     Physics                           Professor Chen
Nicholas Lister, MS   Mechanical Engineering  Professor Moeller
James Germann, MS   Physics                           Professor Davis
Jason King, PhD      Physics                           Professor Davis
Richard Joel Thompson, MS   Mechanical Engineering  Professor Moeller
Nehemiah Williams, MS   Aerospace Engineering  Professor Moeller
Densu Aktas, MS   Mechanical Engineering  Professor Moeller
Russell Gardner, MS   Mechanical Engineering  Professor Moeller
Deepak Rajput, PhD      Material Science  Professor Hofmeister
William Robinson, PhD      Physics                           Professor Davis
Manh Vu, MS     Material Science  Professor Johnson
Mathew Dede, MS     Material Science  Professor Murray
James Rogers, MS   Mechanical Engineering  Professor Moeller
Russell Gardner, M.S.    Mechanical Engineering  Professor Moeller
Alexander Williams, M.S.    Physics                           Professor Parigger
Gregory Boyadjian, PhD      Physics                           Professor Parigger
Jesse Labello, PhD      Physics                           Professor Parigger
Jesse Ogle, PhD     Physics                           Professor Parigger
William Ring, PhD     Physics                           Professor Parigger
Alexander Woods, PhD     Physics                           Professor Parigger

**New Students Recruited in FY 2009/2010**
Kent Wilcher, M.S.    Mechanical Engineering  Professor Moeller
Marcus Conner, M.S.    Mechanical Engineering  Professor Moeller
Russell Gardner, MS   Mechanical Engineering  Professor Moeller
Chris Foerester, M.S.    Materials Science  Professor Murray
Alexander Williams, M.S.    Physics                           Professor Parigger
Gregory Boyadjian, PhD      Physics                           Professor Parigger

**Student Awards**
In Spring 2010, Jason King received an Award for UTSI outstanding Graduate Research Assistant for academic year 2009-2010.

**Interns Employed 2009-2010**
Summer Interns
Ellen Bomar, Tennessee Tech
Claire Murphy, Tennessee Tech
Jeremy Simpson, University of the South
Bradley Tucker, Tullahoma High School
Julia Shi, Tullahoma High School
Brittany Ramos-Janeway, Tennessee Governor’s Academy
Nickolas Dueber, Tennessee Governor’s Academy
Josh Parker, Middle Tennessee State University
Publications, Presentations and Patents

**Reviewed Journal Publications Published in FY 2009-2010**


**Journal Articles Submitted**


“Simulation of single-molecule trapping in a nanochannel,” W.N. Robinson and Lloyd M. Davis, J. Biomed. Opt. 15, 045006 (August 2010); doi:10.1117/1.3477320; [This paper was been selected for inclusion in the August 23, 2010 issue of The Virtual Journal of Nanoscale Science & Engineering].
Technology. The Virtual Journal, which is published by the American Institute of Physics and the American Physical Society in cooperation with numerous other societies and publishers, is an edited compilation of links to articles from participating publishers, covering a focused area of frontier research. You can access the Virtual Journal at [http://www.vjnano.org](http://www.vjnano.org).


**Other Publications**


“A secondary ion mass spectroscopy (SIMS) and Mössbauer study of modified ZBLAN glasses,” Manh Vu, Alexander Terekhov, George Murray, Stefan Schweizer, Rick Weber, Charles Johnson and Jacqueline Johnson. The American Ceramic Society, Glass and Optical Materials Division Meeting (Corning, USA, May 2010).

Presentations at universities and national laboratories


“Physics at UT Space Institute,” L.M. Davis; Presentation at the Department of Physics, UT Knoxville, November 11, 2009.

“Fluorescence detection of single molecules near interfaces and in sub-micron fluidic channels,” L.M. Davis; Invited presentation, Polymers Division, National Institute of Standards and Technology, Gaithersburg, MD, November 2, 2009.


“Ionic Imprinting of Conductive Polymer Films,” Murray, G. M., University of Tennessee Space Institute, October 22, 2009.


Book chapters:


**Patents and disclosures:**


“Molecularly Imprinted Polymer Sensor Device,” Murray, G. M. Published Application 20090197297, August 6, 2009.


“Capillary perfused bioreactors with multiple chambers.” Wikswo; John P., Baudenbacher; Franz J., Prokop; Alex, Leboeuf; Eugene J., Chung; Chang Y., Cliffel; David, Haselton; Frederick R., Hofmeister; William H., Lin; Charles P., McCawley; Lisa J., Reiserer; Randall S., Stremler; Mark A., US Patent number 7,534,601, granted May 19, 2009.


“Wide Field of View, Multispectral Scene Generation,” William Hofmeister, UTSI, filed with UTRF on August 18, 2010.
**Honors**

**Lloyd Davis**

In May 2010, the Optical Society of America (OSA) Board of Directors approved an inaugural class of 162 OSA Senior Members. Included among these was Professor Lloyd Davis. OSA Senior Members are well-established individuals with a designation that recognizes their experience and professional accomplishments or service within their field that sets them apart from their peers. For further details, see [http://launch.osa.org/membership/MemberNewsletter/2010/June_2010/default.asp#headline1](http://launch.osa.org/membership/MemberNewsletter/2010/June_2010/default.asp#headline1).

In February 2010, Dr. Lloyd Davis was awarded a Visiting Fellow position from JILA, the University of Colorado Boulder. JILA, formerly known as the Joint Institute for Laboratory Astrophysics, is one of the leading physical science research institutes in the United States. JILA's faculty includes three Nobel laureates—Eric Cornell, Carl Wieman, and John L. Hall—and two John D. and Catherine T. MacArthur Fellows—Deborah S. Jin and Margaret Murnane. Each year, JILA scientists publish more than 200 original research papers in national and international scientific journals and conference proceedings. Creative collaborations among JILA Fellows and their groups play a key role in generating the pioneering research JILA is known for around the world. Dr. Davis will be on sabbatical leave at JILA during the Fall semester of 2010. Dr. Davis has been with the Center for Laser Applications since April 1985 and this will be his first sabbatical leave.

In March 2010, Dr. Davis was awarded an Honorary Appointment at Auckland University, where he will continue his sabbatical leave during the Spring semester of 2011. In Auckland, Dr. Davis will collaborate with the departments of Chemistry and Physics and participate in research in The Photon Factory, a new facility for high pulse energy femtosecond laser physics and materials science.

[http://sites.google.com/site/utsiosa/Home](http://sites.google.com/site/utsiosa/Home)

Over the last year, CLA students have continued activities for the UTSI Student Chapter of the Optical Society of America (OSA). Jason King, President of the UTSI Student Chapter, attended a workshop at the OSA annual meeting, held in October 2009 in San Jose, CA. The UTSI Student Chapter was awarded an Education Outreach Grant of $1,000 from OSA, which has been used using to provide supplies and travel for local outreach programs in optics and laser applications aimed at middle and high school students.
Visitors to the Laboratory FY 2009-2010

UT Knoxville
Chancellor Jimmy Cheek
Rita Sanders Geier, Associate to the Chancellor and Senior Fellow

UT Trustees
George Cates
Charles Wharton

Arnold Engineering Development Center
Col Michael Panarisi, Commander, AEDC
Col Eugene Mittuch, Vice Commander, AEDC
Dr. Ed Kraft, Chief Technologist, AEDC
Dr. Dan Stewart, Associate Vice President for Research, UT

Institute for Public Service
Paul Jennings
Chuck Shoopman
Bill Wiley
Beth Phillips

Vanderbilt University
Professor Melissa Skala

California State University
UT Thomas Jefferson Lecturer, Dr. Richard A. Samuelson, Assistant Professor of History

Western Connecticut State University
UT Thomas Jefferson Lecturer, Dr. Kevin Gutzman, Associate Professor of History

The Aerospace Corporation, Los Angeles, CA
Quick-Goethert Lecturer, Dr. Wanda Austin, President and Chief Executive Officer

Materials Development Incorporated
Rick Weber

“Engineers for a day” Coffee County High School
Katherine Calvin & Katey Neuffer

Fifty Forward Martin Center, Brentwood TN
Chris Bettes, Ruth Mateheson, Sally Proder, Camille Bruno, Helen Neal, Barbara Rahrer, Madeline DeCuyper, F.A. DeCuyper, Genetry, Belthy Jackson, George Jackson, Doroty Swanner, Helen Landry, Lynn Chultan, Kris Hagen, Sharon Hohman, Rich Hohman, Julie Collins, Mary Lou Caldwell, Ernestine Lynfoot
Arnold/ATA University Programs
Chris Davis
Colin Loudermil
Shawn Shehee
Charles Roberts
Phillip Terry

Coffee County Junior/Youth Leaders
Leia Hudson, Roshelle Johnson, Alanna Keele, Jenna Peterson, Rachel Sain, Christopher Taylor, Casey Vincent, Emily West, Jonathan Blackwell, Brittany Brunner, Jordan Burton, Emma Chessor, Brian Green, Kelsie Hull, Brian Linderode, Alonna Morrison Sara Beth Nelius, Sara Norris, Emily Pearson, Hannah Quick, Alivia Shasteen, Jack Vance, Tozia Ware, Deb Bryant, Eric Elwell, Kerri Meeks, Laura Jent, Jon Bell, Jr. and Louis Baldwin, Jr.
## Schedule 7

### CENTERS OF EXCELLENCE/CENTERS OF EMPHASIS

**ACTUAL, PROPOSED, AND REQUESTED BUDGET**

<table>
<thead>
<tr>
<th>Institution</th>
<th>U T Space Institute</th>
<th>Center</th>
<th>Center for Laser Applications</th>
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<tbody>
<tr>
<td><strong>Expenditures</strong></td>
<td></td>
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<tr>
<td></td>
<td>FY 2009-10 Actual</td>
<td>FY 2010-11 Proposed</td>
<td>FY 2011-12 Requested</td>
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<td>Matching</td>
<td>Appropriation</td>
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<td>Matching Appropriation</td>
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<td>1,497,513</td>
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<tr>
<td><strong>Salaries</strong></td>
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<td>Faculty</td>
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<td>117,120</td>
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<td>103,063</td>
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<td>132,009</td>
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<td><strong>Total Salaries</strong></td>
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<td>712,619</td>
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<td><strong>Fringe Benefits</strong></td>
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<td>166,684</td>
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<td><strong>Total Personnel</strong></td>
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<td>588,167</td>
<td>879,303</td>
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<td><strong>Non-Personnel</strong></td>
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<td>18,226</td>
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<td>Books &amp; Journals</td>
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<td>Consultants</td>
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<tr>
<td>Renovation</td>
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<td>Other (Student Fees)</td>
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<td>28,671</td>
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<td>Other (Cost Share)</td>
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<td><strong>Total Non-Personnel</strong></td>
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<td>308,402</td>
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<td><strong>GRAND TOTAL</strong></td>
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### Revenue

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<tr>
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<th>FY 2009-10</th>
<th>FY 2010-11</th>
<th>FY 2011-12</th>
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<td>New State Appropriation</td>
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<td>118,344</td>
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<tr>
<td>Carryover from Previous Matching Funds</td>
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<td>0</td>
</tr>
<tr>
<td><strong>Total Revenue</strong></td>
<td>482,600</td>
<td>1,014,913</td>
<td>1,497,513</td>
</tr>
</tbody>
</table>