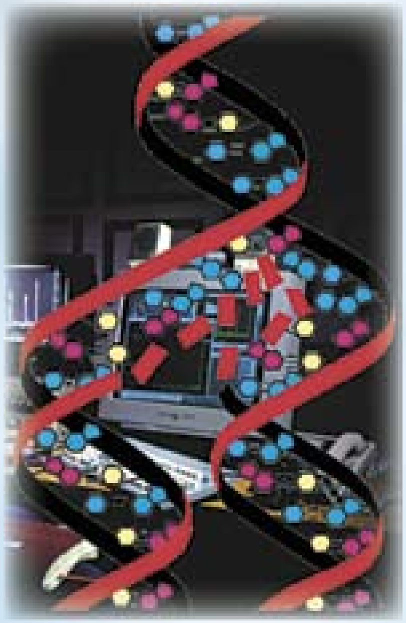
Center for Laser Applications

Annual Report 2004 - 2005



THE UNIVERSITY of TENNESSEE UT

SPACE INSTITUTE

Tullahoma, Tennessee

Center for Laser Applications

An Accomplished Center of Excellence

Administrative Council

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THE UNIVERSITY of TENNESSEE
SPACE INSTITUTE
Tullahoma, Tennessee

Executive Summary

The Center for Laser Applications (CLA) was established at the University of Tennessee Space institute in 1984 as one of the original THEC Centers of Excellence, and was named one of the original Accomplished Centers in 1989. Its mission is to provide a multidisciplinary research center environment for the training of masters and doctoral graduate students in specialized science and engineering topics through participation in internationally recognized research.

From its formation, the Center successfully used a consensus management structure consisting of an Administrative Council composed of Senior Faculty and an annually rotating Chair selected from the Council members. Several senior faculty members have retired during the past few years, seriously diminishing the Center's corporate memory and experience base. It became evident that the future success of the Center required a change in the management approach. The required changes were carefully considered by the Council with approval by the UTSI Chief Operating Officer, and were implemented during this fiscal year (FY05). The new administrative structure consists of a permanent Center Director with the Council serving in a strong advisory capacity. Dr. James W. L. Lewis served as Interim Director during FY05 while the search for a permanent Director was conducted. Dr. William Hofmeister was appointed Director of CLA September 12, 2005.

The most critical problem currently facing the Center is revitalization of the laser materials processing program after several senior researchers retired. This is particularly important at this time, since the overall recovery plan for UTSI identified materials research as one of two major areas of emphasis. A workshop was held in Knoxville during July 2005 with the participation of ORNL and UTK to chart the future direction of the UTSI materials research activities. It is expected that CLA laser materials processing will play a major part in the UTSI plan for materials research. An important part of this revitalization is the establishment of an ORNL-UTSI-UT Joint Center for Advanced Photonics Processing Center (JCAPP) at ORNL. A proposal with letters of support from the appropriate leadership of the three institutions was submitted to UTK seeking formal approval.

Searches for senior faculty in the areas of plasma science and laser materials processing were conducted during FY05. Several candidates were interviewed for the laser materials processing positions, and one excellent candidate, Dr. William Hofmeister, was identified. Negotiations with Dr. Hofmeister resulted in a half-time appointment at UTSI that began February 2005 in a collaborative agreement with Vanderbilt University. Negotiations continued throughout the year, and Dr. Hofmeister become a full-time CLA Faculty member September 1, 2005.

Two successful candidates were identified for the plasma science position. An offer was made to the first candidate, but after due consideration the offer was declined. An offer was made to the second candidate and was also declined for family reasons, but the candidate indicated a strong interest in joining the Center at a later date. This candidate has had continued contact with center faculty and is collaborating on research and joint proposals.

Center research activities remained strong. Twenty papers were published in refereed journals and 18 presentations were made at national scientific meetings. Strong contract support for research continued. The nonequilibrium fluids area received $1.113M during FY05 for new projects and additional funding for existing contracts. The ultrafast spectroscopy area received $285,600 during FY05 for new projects and additional funding for existing contracts. The materials processing area received $86,400 from an addition to an existing contract and small short term projects.

Recently, Dr. Davis was notified by the National Institutes of Biomedical Imaging and Bioengineering (NIBIB) that his proposal to develop an innovative ultrasensitive method for multi-dimensional spectroscopic fluorescence imaging would be accepted. A collaborative agreement with the Cell Imaging Resource at Vanderbilt University Medical Center was established to facilitate applications of the new techniques to samples and problems relevant to the biomedical imaging community. This grant, which begins August 2005, is the first project led by UTSI to receive funding from the National Institutes of Health (NIH).

Building on Dr. Davis' NIH success, a proposal entitled, "Multiphoton Fabrication and Sensing in Nanofluidic Devices" was prepared by Professors William Hofmeister and Lloyd Davis of the University of Tennessee Space Institute; Professor Narendra B. Dahotre of the University of Tennessee-Knoxville; and Professors John Wikswo and Deyu Li of Vanderbilt University in response to NSF's Active Nanostructures and Nanosystems (ANN) solicitation for a Nanoscale Interdisciplinary Research Team (NIRT) and was submitted November 29, 2005.

Some highlights of the Center research activities and accomplishments for the past year follow. More detailed discussions are available in the body of the report.

Laser Materials Processing

Dr. Dahotre has continued to spearhead innovative research in the area of laser surface modification for both industrial and biological materials. The surface modifications serve to enhance wear and corrosion resistance in metals and to increase longevity and successful implantation of biological materials.

Major activities continued for the three-year project in the area of high-speed laser synthesis of amorphous and ultra-fine surface structures. This project is an international collaboration between the University of Tennessee (UT), and The Indian Institute of Technology-Kharagpur (IIT-KGP), India.

Research investigations into the morphological changes of the structure of in situ laser dressed abrasive grinding wheels has shown an improvement in the grain structure which leads to better performance than is obtained with conventional dressing methods.

Ti and its alloys are excellent biomaterials that are often used for medical implants, but to provide effective osseointegration, hard and wear-resistant bioceramic materials such as zirconia are coated on implant surfaces. These surfaces are textured at various length scales to promote effective tissue integration. Laser surface modification has been used to provide simultaneous coating and texturing of bio-metallic materials. By carefully modulating the laser optics and processing parameters, it is possible to produce tailor made surfaces for various applications.

A new book co-authored by Dr. Dahotre, "Materials Science in Manufacturing" (pp. 560, ISBN: 0-7506-7716-3), is scheduled for publication by Academic/Elsevier Press, New York, in March 2006.

A new, state of the art Ytterbium fiber laser was acquired from IPG. This 1kW laser will be used in support of surface modification work and in planned activities in laser additive manufacturing. High-power, solid-state fiber laser technology has had a significant impact the laser materials processing community by increasing energy efficiency to near 20% (wall plug to beam) and providing up to 10000 hours operational service life.

Professor Hofmeister continues to collaborate with Vanderbilt colleagues and has used CLA facilities to contribute to the fabrication of microfluidic devices for Prof. Wikswo's Vanderbilt Institute for Integrative Biomedical Research and Education and to laser machine diamond field emission devices for Prof. Davidson's Diamond Microelectronics Group.

Ultrafast Laser Spectroscopy

Dr. Lloyd Davis has a long history of seminal contributions to the development of techniques and applications for ultrasensitive detection of laser-induced fluorescence, down to the single-molecule level. These laser techniques are now enabling cutting edge biophysics discovery and revolutionary biotechnology applications, such as whole-genome DNA-sequencing at speeds and costs orders of magnitude faster and cheaper than before. The pharmaceutical company Abbott Laboratories has continued to support a significant component of CLA's research in this area.

Over the course of the past year, the CLA expertise in single-molecule spectroscopy provided important collaborative support for a large NIH P-31 grant application in collaboration with Louisiana State University, and for an NSF grant application to the Sensors program in collaboration with Tennessee Technological University. The combination of ultrasensitive fluorescence detection methodology and laser materials modification research will provide opportunities for interdisciplinary research within CLA and with other institutions on new nanotechnology and biotechnology device applications that are being vigorously pursued in the year ahead.

Nonequilibrium Fluid Physics

Dr. Trevor Moeller is conducting research in pulsed high power electric propulsion devices for applications in nuclear fission powered future space missions. Experiments have been conducted on a locally designed pulsed plasma accelerator. These experiments utilized laser diagnostics to develop experimental results that can be compared with computer simulations using the existing MACH2 code and a new code, GEMS, being developed in collaboration with Purdue University. This work is funded by Arnold Engineering Development Center, and a new task was added to this project in FY05. The new project requires the design, fabrication and testing of a new vertical thrust stand to be installed in the AEDC 12-V test chamber to enable testing of high powered electric propulsion thrusters.

Dr. Moeller is also continuing his research in hypersonic vehicle electric power systems (HVEPS). During the past year, facility upgrades were initiated that will permit increased flow rates and higher electrical conductivities required for future MHD generator testing, combustion facility flow field characterization, and facility preparation for the installation of a subscale MHD generator with superconducting magnet.

Biomedical Applications

During the past several years, the CLA vision science team has developed human eye models and computer simulations for other than the normal, average human eye. These models can include abnormal conditions as well as statistical, age, gender and racial variations. The models can then be used to evaluate and improve surgical procedures, diagnostic methods and instrumentation. Applications of these models and simulations have led to improved pediatric vision screening through telemedicine, screening for keratoconus prior to refractive laser surgery, such as LASIK, and individual tailored modeling.

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Focus Area

Laser Materials Processing

Introduction

The materials research within CLA continues to be strong in the area of laser based surface modifications of a variety of materials systems. The extent of research in this area is shown by the of publications in refereed technical journals in the past year. Dr. Dahotre continues to hold joint appointment with UTSI/CLA, UTK and ORNL that has been instrumental for many joint research activities in the area of materials processing and provides opportunities to conduct several research tasks related to materials analysis at ORNL using unique and state-of-the–art facilities. Several graduate students in materials area were resident at ORNL for substantial period of time in the past year. The recognition of the materials research is clearly indicated by hiring of recent graduates by nationally known employers such as Intel, Milwaukee Tools and Chromalloy and election of Dr. Dahotre to the Class of 2004 Fellows of ASM International for his pioneering contributions to research and development of surface engineering and laser processing of materials. In addition to surface modifications, materials research is also positioning to explore new areas such as nano, bio, and flexible electronic materials. The exploration into new areas of research will be pursued through the recent hire of Dr. William Hofmeister as Research Professor of Materials Science.

High Temperature Oxidation of Laser *In-Situ* Combinatorial Carbide Coating on Steel

A 2.5 kW Nd:YAG laser was employed to modify the surface of a AISI 1010 steel deposited with a precursor powder mixture of Fe, Ti, Cr and C. With the help of laser surface engineering, an *in-situ* combinatorial carbide (Ti and Cr carbide) composite coating on the surface of plain C steel was achieved.

Titanium carbide is a refractory carbide with exceptional hardness (2800 kg/mm^2), excellent wear and abrasion resistance and superior thermal stability (decomposition temperature 3065ºC). It has been extensively used as reinforcing particles in bulk composites. Introduction of hard particles in a metal can considerably decrease the amount of abrasive wear. Similarly, chromium carbides are also known to impart hardness and wear resistance to white cast irons and high-speed steels. The carbides, like M_7C_3 (M=Fe,Cr) in high-Cr white irons are hard (1500-1800 HV), which makes them an attractive class of material for wear applications. Composites with steel matrix and metallic carbides offer high hardness and sufficient fracture toughness. By careful selection of the type of carbide, it is possible to design a composite for severe abrasive conditions. But, during high temperature conditions, the oxidation of these carbides could be detrimental to the properties, which necessitates the investigation of thermal oxidation behavior of the materials and these phases.

High-temperature oxidation behavior of TiC single crystals has been the subject of many studies in the past. It has been reported that the major phases observed through the formation of two subscales are Ti_3O_5 (inner subscale) and TiO_2 (outer one). A correlation between TiO_2 orientations and the TiC crystal face has been reported. Similarly, thermal oxidation studies of the Fe-Cr alloys have been done and the major oxidation product reported is Fe_2O_3. But, all these studies were done on individual monolithic materials which is different from behavior of these materials in the presence of each other, especially as a surface composite coating layer. It is therefore essential to evaluate the high-temperature oxidation behavior of the carbide composite coating.

TiC particles have been used as reinforcements on various metallic substrates using several processes such as surface modification of steel and Al by laser cladding and by electron-beam and plasma-transferred arc. In the current study, carbide particles were grown *in-situ* using the laser surface engineering technique. The extremely high flux of energy, applied by a laser to a very thin surface layer of a specimen, produces a highly localized heat source capable of altering the microstructure and hence the properties of various materials. Moreover, the localized melting of the surface material during laser treatment makes it possible to treat small surface areas without affecting bulk properties, thus making expensive alloying of the entire component unnecessary. The high temperature gradients and heat sink effect (of the rest of the components) result in a very high cooling rate or rapid self quench, exceeding $10^{4\text{-}6}$ K/s. The processing parameters (laser power, laser scan speed, beam size, laser optics) can be easily modified to tailor the surface as required. Also, *in-situ* grown particles have the inherent advantage of being uncontaminated and well bonded to the matrix, and hence have superior properties.

The temperature range of formation of these phases and thermal stability of the coating have been proven using differential scanning calorimetry (DSC) in previous efforts. The current study addresses the elevated temperature behavior of this surface composite coating. The high temperature isothermal oxidation behavior and the oxidation kinetics of coatings processed at different laser powers were investigated as part of the present effort. For a thorough understanding, quantitative analysis of the oxidation reaction was done using a thermogravimetric analyzer (TGA).

The oxidation rate for the *in-situ* carbide composite coating was found to be parabolic at 700 and 1000ºC (Figure 1) . Variation in the oxidation products is observed with laser processing power and temperature used for the oxidation behavior investigations. The rate of oxidation was slowest for samples processed at 2100 W laser power (Table 1). Phase identification of the oxides formed during elevated temperature heating of samples in air suggested Fe_2O_3, Ti_2O_3, TiO2, Fe-Cr, TiC and M_7C_3 as the major phases at 700ºC and Fe_2O_3, Ti_2O_3, Fe-Cr and M_7C_3 at 1000ºC (Table 2). The oxidation is more severe at 1000ºC in comparison with 700ºC (Figure 1 and Table 1).

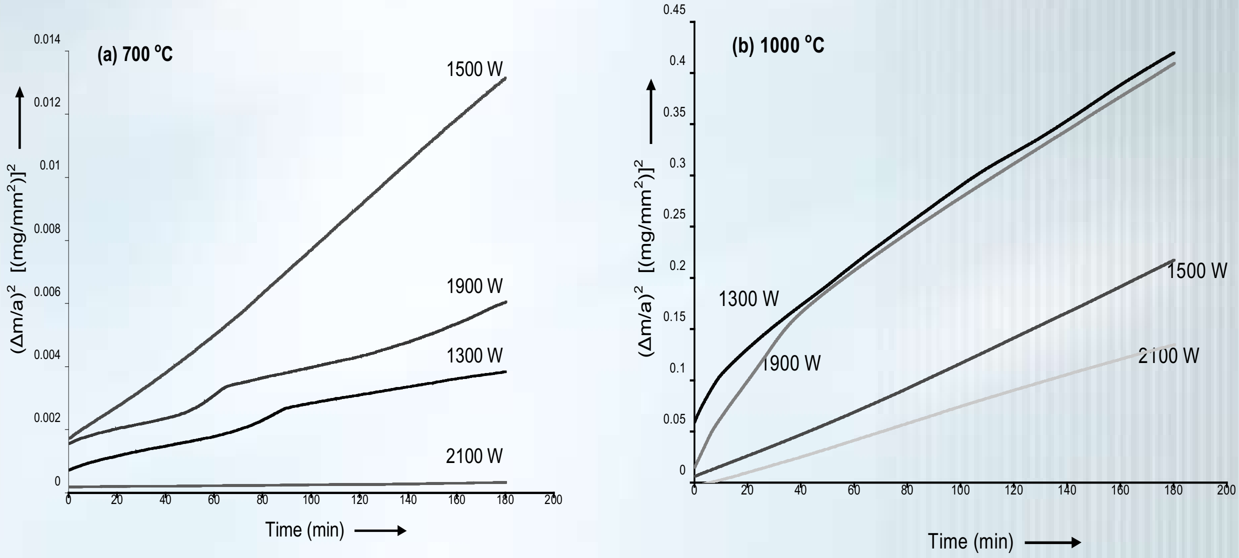


Figure 1. Oxidation kinetics for composite coatings at (a) 700ºC and (b) 1000ºC

Table 1. Oxidation kinetic constants for composite coatings at 700ºC and 1000ºC

Temperature of Exposure (ºC)	Power (W)	K ($mg^2 mm^{-4} min^{-1}$)	C ($mg^2 mm^{-4}$)
700	1300	20 x10^{-5}	8 x10^{-4}
	1500	70 x10^{-6}	13 x10^{-4}
	1900	20 x10^{-6}	16 x10^{-4}
	2100	0.7 x10^{-6}	2 x10^{-4}
1000	1300	1.9 x10^{-3}	9.6 x10^{-3}
	1500	1.2 x10^{-3}	3.5 x10^{-3}
	1900	2.0 x10^{-3}	79.6 x10^{-3}
	2100	0.7 x10^{-3}	6.5 x10^{-3}

Table 2. Summary of phases evolved during isothermal oxidation at 700 and 1000ºC

Processing Power(W)	Phases Observed at 700 °C	Phases Observed at 1000 °C
1300	TiO_2, TiC, Fe-Cr	Ti_2O_3, Fe_2O_3, Fe-Cr
1500	TiO_2, TiC, Ti_2O_3, Fe_2O_3, Fe-Cr, M_7C_3	Ti_2O_3, Fe_2O_3, Fe-Cr, M_7C_3
1900	Ti_2O_3, Fe_2O_3, Fe-Cr	Ti_2O_3, Fe_2O_3, Fe-Cr
2100	TiC, Fe-Cr, TiO_2, Fe_2O_3	Fe-Cr, Ti_2O_3, Fe_2O_3

Investigator: Dr. Narendra B. Dahotre
Sponsor: Center for Laser Applications

Morphological Modification of Laser-Dressed Alumina Grinding Wheel Material for Microscale Grinding

Abrasive grinding wheels are used for grinding materials with poor machinability because of their longer life, high grinding efficiency, and dimensional stability. Alumina ceramics offer a great potential as materials for tribologically loaded parts owing to their unique combination of low weight, high stiffness, strength, temperature stability, and corrosion resistance. However, the grinding wheel needs to be dressed to maintain its form tolerance and dimensional stability over a large number of grinding passes. The wheel also needs to be cleaned of the clogged metal chip particles that get loaded into the grinding wheel surface during grinding. The conventional processes such as mechanical diamond dressing result in excessive wheel material loss and also reduce the number of effective cutting edges present on the surface of the wheel. In the light of this, high-power lasers that are currently used as efficient non-contact type machining tools for various manufacturing applications like cutting, drilling, welding etc., have also been explored for use as a dressing tool. Some of the earlier studies, though useful, did not deal with the nature of the morphological changes taking place in the grinding wheel during interaction with laser energy, which happens to be a fundamental aspect contributing to its dressing performance. Unlike the previous studies, this paper does not intend to compare laser dressing with conventional methods like mechanical dressing; instead it is an effort to show the feasibility of the laser as a dressing tool.

In the present study, a high-power, continuous-wave laser was used as a non-contact type dressing tool for alumina grinding wheels. Several initial experiments have been conducted to investigate the feasibility of the laser-dressing process and the results have been reported elsewhere. Cooling rate during laser dressing governs the microstructure formed, the effect of which has been studied. Surface processing of ceramics by laser irradiation offers potential advantages such as, precise control over high input of thermal energy at spatial and depth levels, rapid processing speed and unique modification of microstructure due to rapid heating, remelting, solidification and cooling. Focused laser radiation produces enormous power densities in a very small region of the wheel surface and thus can cause a localized modification either of the exposed grain or of the bonding constituents. Since the focused spot size can be made much smaller than the nominal size of the abrasive grain, it can penetrate through abrasive grain and produce multiple cutting edges on the same grain. Depending upon the laser processing parameters used, melting (followed by resolidification) and/or vaporization results in modification of surface topography (morphology and composition). Refinement of grain size, densification of the surface layer, and evolution of multifaceted grains with cutting edges and vertices are the main morphological modifications taking place on the surface of the wheel. (Figure 2). These morphological modifications are expected to improve cutting efficiency.

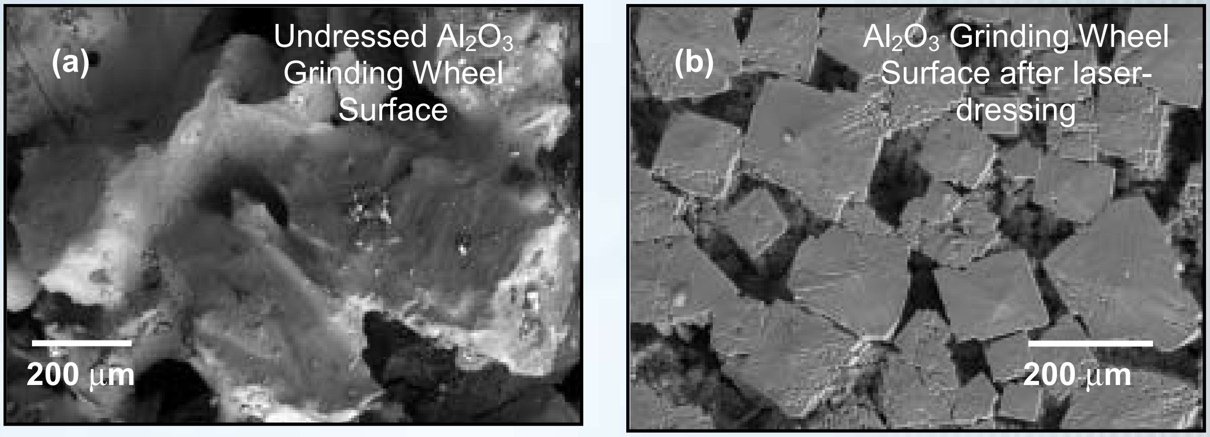


Figure 2. Microstructure of the grinding wheel surface (a) undressed and (b) post laser-dressed (750 W) showing refined equiaxed and faceted grains

It was intriguing to see well-defined facets in the laser processed samples. It is akin to non-metallic crystals found in the nature. X-ray diffraction experiments indicated formation of crystallographic texture on the surface of the dressed wheel (Figure 3). In this work, pole figure analysis was used to investigate the planar textures formed by laser-dressing. The efficiency of the grinding process for the laser-dressed wheel in comparison with undressed grinding wheel was evaluated using a grinding apparatus. The surface finish on the ground workpiece is quantified using surface roughness parameters.

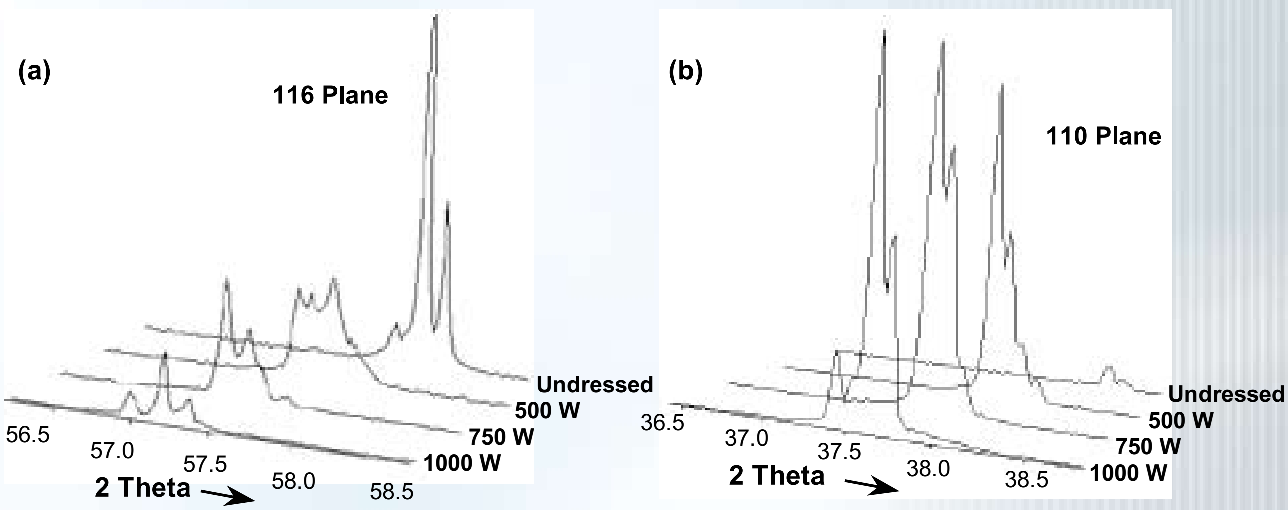


Figure 3. XRD spectra as a function of laser power for (a) (116) plane and (b) (110) plane indicating the variation of the texture

Post laser-dressing pole-figure analysis indicated evolution of planar crystallographic textures in the particles of the resolidified surface layer. Evolution of refined and preferably oriented crystallographic planes ((110) and (214)) (Figures 4 and 5) resulted in formation of individual particles (grains) with sharp vertices and cutting edges in the laser-modified surface. The surface roughness of the dressed wheel sample was a manifestation of the new morphologically modified surface. This modification in morphological features on the surface helps maintain a high grinding efficiency. The performance of the laser-dressed grinding wheel sample was evaluated in comparison to the undressed wheel sample using a grinding apparatus. Because of the above-mentioned specific and uniform particle morphology, during the grinding test a substantially less weight loss and higher grinding ratios for the laser-dressed grinding wheel samples compared to the undressed wheel sample were observed (Table 3). Microscale grinding can be done efficiently using the laser-dressed wheels to produce a smooth surface finish on the workpiece material.

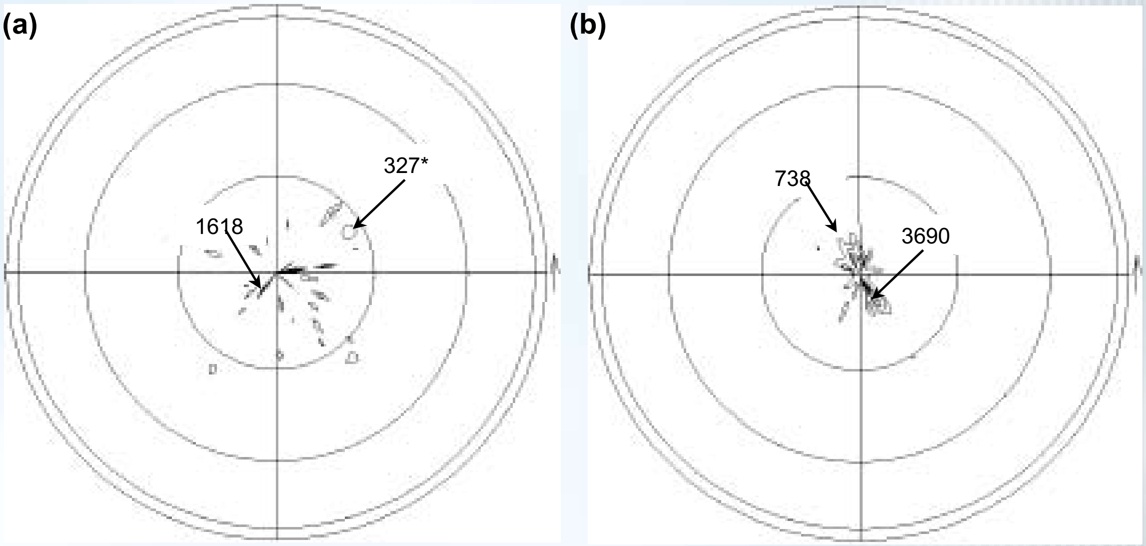


Figure 4. Pole figure for (110) plane in (a) undressed sample and (b) laser-dressed sample (Denotes intensity)*

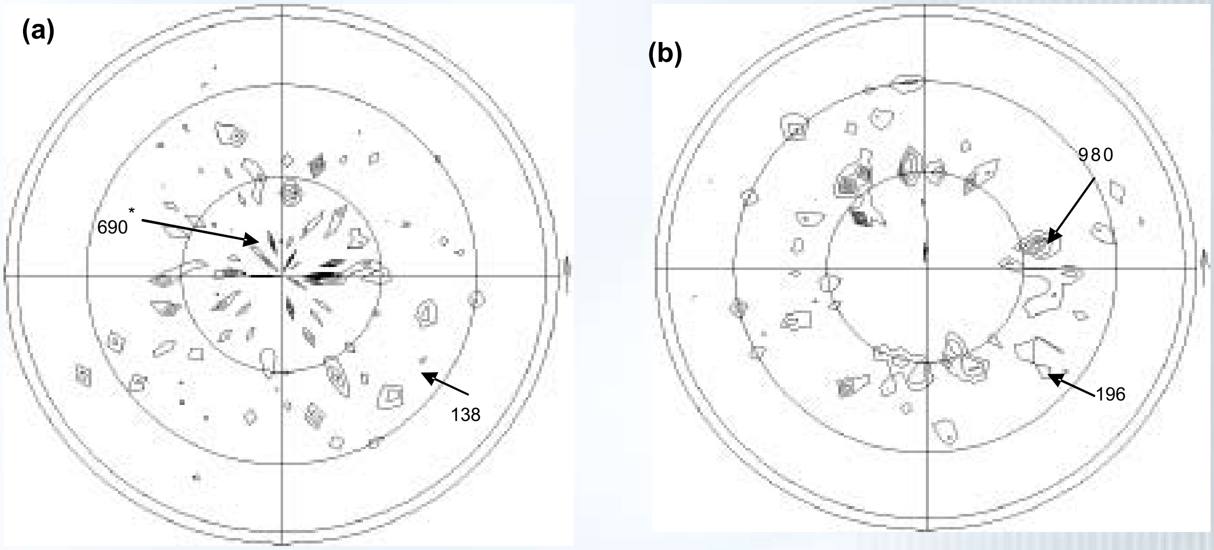


Figure 5. Pole figure for (214) plane in (a) undressed sample and (b) laser-dressed sample (Denotes intensity)*

Table 3. Grinding ratio for high-speed grinding test at varying laser power

Sample	Undressed Wheel	Laser-dressed Wheel		
		500 W	750 W	1000 W
Time (minutes)	0.2	10	10	10
Cumulative Weight Loss in Grinding Wheel G (grams/unit contact area)	0.0444	0.0257	0.0203	0.0091
Cumulative Weight Loss in Pin P (grams/unit contact area)	0.00515	0.02017	0.0055	0.00922
Ratio of weight loss in Pin to weight loss in Grinding Wheel: P/G	0.115991	0.784825	0.270936	1.013187

Investigator: Dr. Narendra B. Dahotre
Sponsor: Center for Laser Applications

High-Energy-Density Coating of High Temperature Advanced Materials for Energy Efficient Performance

The 3-year project that ended in December 2004 involved development of the technique and materials systems for coatings on ferrous (steel) and nonferrous (Al-alloy) structural alloys for high temperature wear and corrosion applications. Such coatings were ceramic-based (TiC, and TiB_2) and intermetallic (Fe-Al) materials systems. The laser-based and infrared plasma-based techniques were developed to deposit coatings on metal substrates. The use of laser, infrared plasma, singly and in combination, allows coating of various surface geometries in a selective manner with generation of novel and nontraditional microstructures within the coating and subsurface region. Due to control of processing parameters during both laser and infrared processing, various thermal conditions, ranging from equilibrium to near- or non-equilibrium, can be achieved to tailor the microstructure and both chemical and physical properties of the coatings.

Processing was investigated as a function of material and processing parameters, such as type of the material, energy density, mode of deposition of energy (pulse versus continuous), speed, etc. The microstructures within the modified surface and the interface (between the modified surface and the substrate) were characterized. Computational modeling based on thermodynamic calculations for evolution of phases during coating allowed prediction and design of microstructure as a function of processing conditions. The functionality and effectiveness of coatings produced with experimental and theoretical approaches were evaluated through testing for dry sliding block-on-disc wear, high-temperature furnace exposure oxidation, thermogravimetric (TGA) dynamic weigh change oxidation, and potentiometric aqueous corrosion. These evaluations of coated materials indicated substantial improvements, compared to the substrate, in wear, oxidation, and corrosion performance. Such inexpensive substrate materials (steel and aluminum) coated with high performance material systems are highly economical for improved and efficient performance as structural materials in a broad range of applications such as hydro turbines, heat exchangers, die-casting dies and inserts, continuous steel casting rolls, transfer rolls for flat glass, cutting and casting tools, combustion chambers in diesel engines, components for chemical processes, components for processing of pulp and paper, and auto engines. The improved and longer lasting performance of these surface modified materials in a wide variety of applications hold tremendous potential in energy savings (up to 250 x 10^{12} BTU/year). Although friendly commitments for industrial implementation of these materials systems and processing (engineering) techniques were obtained from industrial organizations in various sectors, the time and lack of funding did not include the efforts on commercialization.

The specific observations of the present project included:

1) Plasma-arc high-density IR lamps can be used to coat Fe-Al alloys on 4340 steel. Process conditions and composition of the precursor coating have to be carefully selected to retain iron aluminides on the surfaces of the samples. Under appropriate processing conditions, coatings free of porosity and cracks can be obtained using this technique.

2) Hardnesses of the coating and the heat-affected zone are a strong function of the processing parameters and hence can be tailor-made for an application. In the case of the samples processed with the IR plasma arc lamp, the hardness varies with the processing conditions.

The processing conducted at lower energy density (2025 W/cm^2) with the IR lamp produced the harder (> 1.5 times) coating layer than those processed at higher energy density (2350 W/cm^2). Similar trends for hardness of the coatings produced by the laser-based technique were observed (Figure 6). The hardness values within the coating were much larger (Knoop hardness values > 400) than that obtained for the base material (Knoop hardness values < 300). Also, the laser processing conducted at higher power (1750 W) produced coatings of lower hardness compared to the coatings produced at lower power (1200 W). Accordingly both IR and laser produced coatings at lower energies indicated higher wear resistance compared to the coatings produced at higher energies. Intermetallic compounds (stoichiometry) evolved in the coating were considered to be responsible for these changes. At higher energy of processing, the coating stoichiometry was observed to be rich in Al compared that processed at lower energy thereby providing inferior hardness and wear properties (Figure 7).

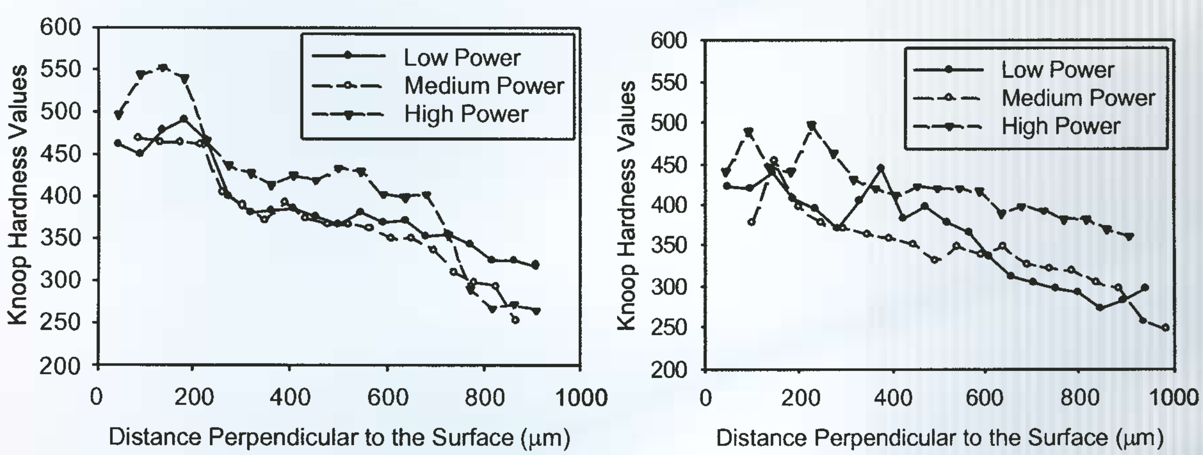


Figure 6. Variations in Knoop hardness values with laser power as a function of distance perpendicular to the surface in coatings prepared with (a) precursor layer with 43.5 mole % Al, and (b) precursor layer with 75 mole % Al

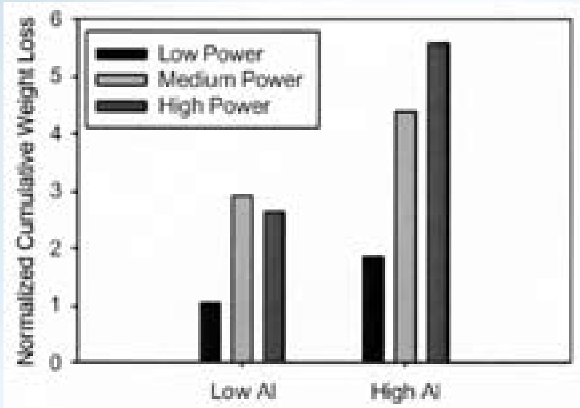


Figure 7. Variation in the normalized cumulative weight loss as a function of precursor Al-content and laser power

3) Better corrosion resistance of laser coated iron-aluminide than the base steel may possibly be attributable to the superior oxide layer offered by mixed oxides. The aluminide in the composite coating was responsible for reduced corrosion and oxidation. The variation of corrosion current and oxidation resistance clearly indicates the influence of laser parameters in improving the corrosion resistance. It was observed that the Fe-Al coated samples exhibited significantly lower corrosion current (I_{corr}) in both sulfuric acid (Figure 8) and sodium chloride (Figure 9) solutions. The corrosion current roughly translates to corrosion rate. In other words, the laser-coated samples are significantly more corrosion resistant than the base materials.

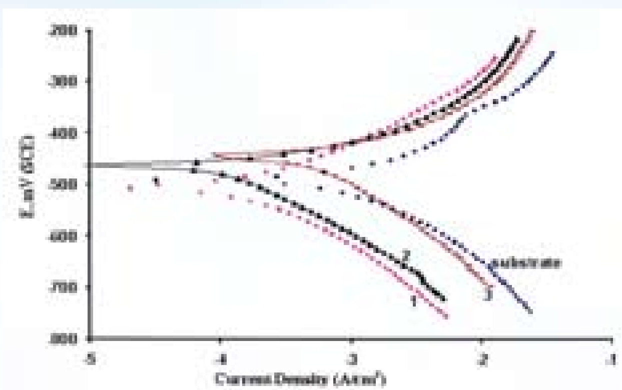


Figure 8. Tafel plots of laser Fe-Al coated 4340 steel including base material in 1N sulfuric acid solution

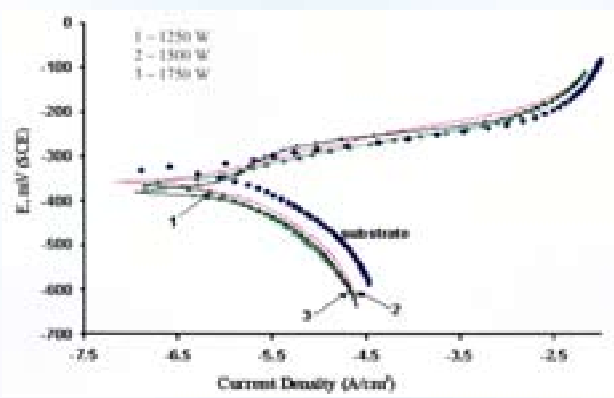


Figure 9. Tafel plots of laser Fe-Al coated 4340 steel including base material in 1% NaCl solution

4) Experiments involving oxidation in air, done in thermogravitometric analysis (TGA), indicated that laser-processed samples were more oxidation resistant than the substrate. All the time-weight gain/area relation followed either cubic (mostly) or parabolic relationships. In other words, there is some extent of intrinsic oxidation resistance in the coating as well as the substrate.

In light of the above-mentioned specific observations and in relation to the project objectives, several project accomplishments have been achieved. Reliable, efficient and economic methods based on high-energy laser and IR plasma lamp for coating ceramic and intermetallic materials on ferrous materials were developed. The techniques were mostly proved for intermetallic coatings on structural steel (AISI 4340); they also proved their feasibility for coating ceramic systems such as TiC and TiB_2 on ferrous (steels) and nonferrous (Al) metals. The coating microstructures were thoroughly studied to understand their improved chemical (corrosion, oxidation) and physical (hardness and wear) properties as function of processing parameters. The coating techniques (laser and IR plasma lamps) were configured to process components of a variety of sizes and shapes and are ready for processing industrial components in a production environment.

Investigator: Dr. Narendra B. Dahotre
Sponsor: DOE, Industrial Materials of Future Program

Laser-Induced Multi-scale Textured Ceramic Coating on Bio-Metallic Material

Ti and its alloys are excellent biomaterials because of their good biocompatibility and corrosion resistance. The spontaneous formation of a passive TiO_2 layer provides the necessary inertness and biocompatibility. However this TiO_2 layer has inferior mechanical properties and fractures easily under wearing conditions. This results in detrimental accumulation of wear debris and eventual ion release into the biosystems. To overcome this problem and to provide effective osseointegration, hard and wear-resistant bioceramic materials are coated on implant surfaces. Bioceramics like zirconia have good fracture toughness and bending strength, along with excellent biocompatibility, and have been coated on Titanium alloys.

The other surface processing for implant surfaces involves texturing the surfaces to make the tissues grow into the surface and adhere better. Physical texturing is now recognized to play a major role in the way cells respond to surfaces and thus many studies were dedicated to correlating the proliferation, adhesion, migration and differentiation. Surfaces textured at micro and nano scales met with certain success. At this point it is worth remembering that in nature materials are organized at various length scales ranging from nano to micro level. Thus a synthetic material designed to survive and effectively integrate into a bio environment might be expected to show compatibility at multi-scales rather than at a single scale. Hence the present emphasis is on developing materials that are functionally active and hierarchically organized at various length scales. So far, efforts to produce integrated micro to nano features for bio applications are limited and rare. There exist many techniques to provide either efficient coatings or textures but so far there has been no effort to integrate effectively both coatings and texture together to produce the desired surface.

This work is focused on the concept of simultaneous coating and texturing using a laser source. The use of a laser for surface engineering offers great flexibility and presents manifold advantages. By carefully modulating the laser optics and processing parameters, it is possible to produce tailor made surfaces for various applications.

However, a major problem associated with engineered surfaces like coatings or textures for bio applications is their physical characterization. Generally, a surface is characterized by a large number of length scales mutually superimposed into one another. The arithmetic average roughness, R_a, or the root mean square average, R_q (rms), commonly used to characterize the surface roughness do not convey information on the range of length scales over which different topographic features exist. The roughness measuring instruments often provide different values for surfaces at different scales depending on the resolution and the filtering capabilities of the instrument at that length scale. Therefore, surfaces should be characterized in a way such that the structural information at all scales is retained. Over the last few decades, researchers have tried to characterize multi-scaled surfaces using the mathematical concept of fractals which are invariant with respect to scale. Fractals are unique because of their extreme fragmentation bounded by non–euclidean geometry instead of topological dimensions. These fractals are quantified by fractal dimension, D_f, which permits distinguishing fractals at any scale. Typically the calculation of fractal dimensions of engineering surfaces is a complicated process since it involves not only a number of mathematical models but also surface topography image processing. These fractal dimension calculators are built into commercial surface instruments, such as atomic force microscope (AFM) and Talysurf PG I. Apart from being costly the fractal dimension calculators attached with these instruments cannot be used to calculate the surface fractal dimension of data acquired by other equipment. In light of this, the present work reports a laser based technique to simultaneously coat and texture surfaces with potential for bio applications and deals with simple fractal based analysis to characterize surfaces for their multi-scale nature using a free public domain software package called ImageJ (available from National Institutes of Health, USA).

A textured coating of zirconia on Ti-6Al-4V alloy was produced using a pulsed-laser processing technique. Scanning electron microscope observations coupled with fractal analysis revealed the multi-scale nature of the textured coating (Figure 10). Both stylus based profilometric measurements and fractal analysis indicated the non-linear nature of the relationship between laser processing speed at constant pulse frequency (10 kHz) and roughness of the textured coating (Figure 11).

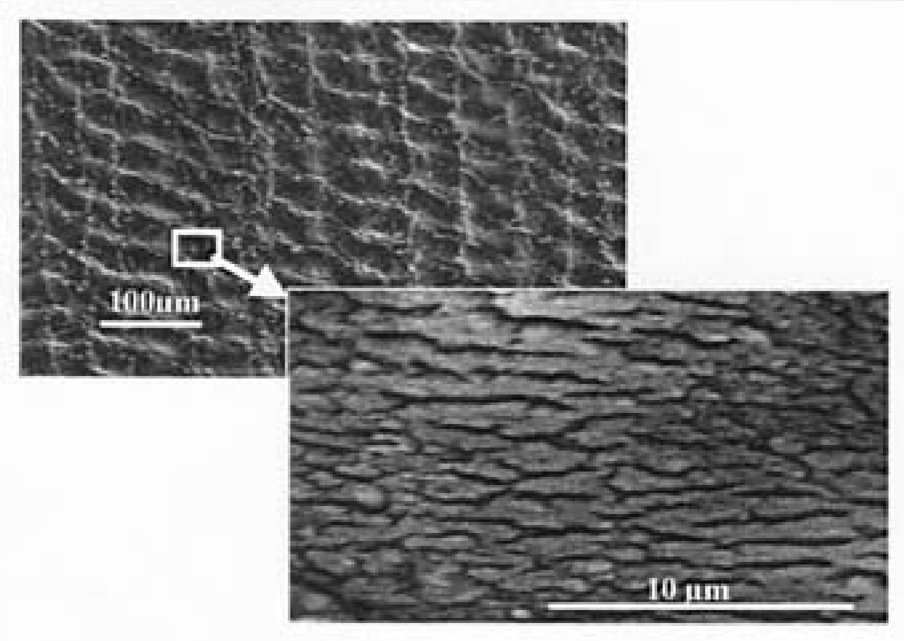


Figure 10. Multi-scale features delineated under scanning electron microscopic observation for the sample processed at 40 cm/min.

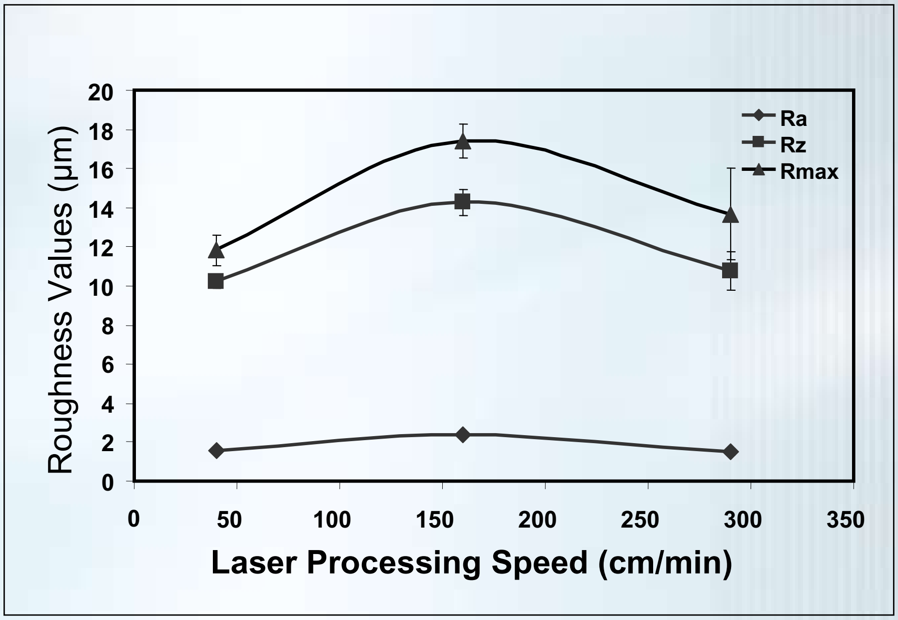


Figure 11. Variation of roughness parameters based on laser processing speed

The textured coatings produced with all the three processing speeds (40, 160, 290 cm/min) were fractal over certain length scales. Processing at 40 cm/min resulted in structures that are fractal across a large number of length scales as where higher processing speeds resulted in fractality over fewer length scales (Figure 12). The processing speed influenced the zirconia content in the coating and the phase transformation within the Ti-matrix of the coating. Within the coating, while zirconia content decreased, the amount of retained ß-Ti increased with increase in processing speed (Figure 13). Such physical and chemical transformations are desired in a titanium bio-implant for effective contact with protein, cells and tissues at various length scales and its effective chemical performance in the bio-environment.

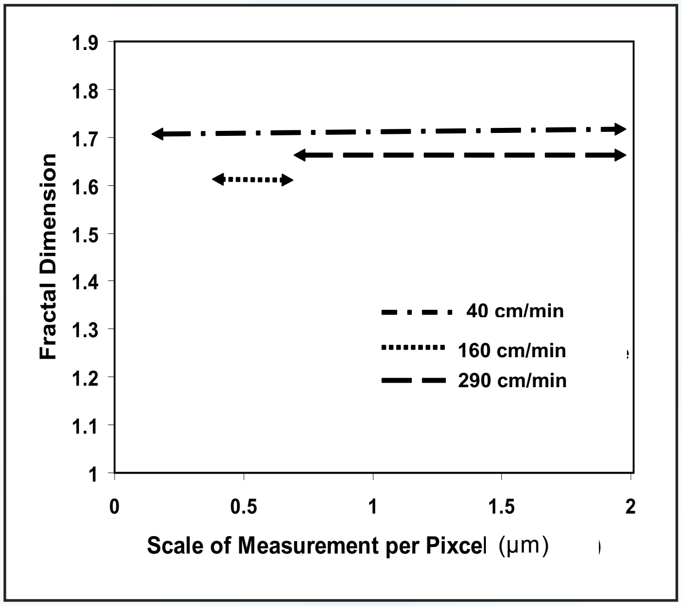


Figure 12. Variation in fractal dimension at various length scales

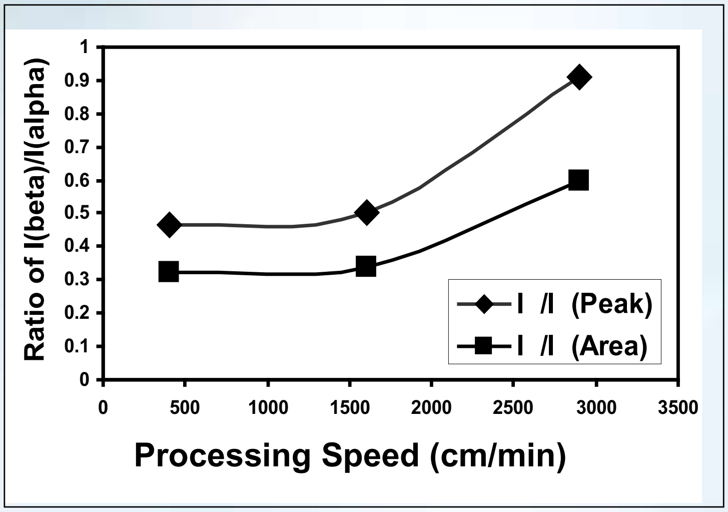


Figure 13. Figure showing the ratio of retained ß-Ti to a-Ti at various processing speeds

Investigator: Dr. Narendra B. Dahotre
Sponsor: Center for Laser Applications

Laser Synthesis of Amorphous/Glass Forming Surface Structures

In the preliminary study, an attempt was made to explore deposition of a Fe-based amorphous/glassy layer on plain carbon (AISI 1010) steel by laser surface cladding (LSC) to improve resistance of the substrate to wear and corrosion. Unlike crystalline alloys, the amorphous state is devoid of long-range periodicity, restricted equilibrium solid solubility and dislocations that allow plastic deformation at a stress level significantly lower than the theoretical shear strength of the material. As a result, amorphous or glassy solids offer extremely high hardness and elastic modulus but poor ductility and toughness. Laser surface cladding (LSC) allows developing a surface coating with different microstructure and composition using a high power laser beam with concomitant rapid self-quenching and re-solidification. The extremely fast cooling rate in LSC is ideal to retain or develop a non-equilibrium microstructure in the cladding including extended solid solution with amorphous/glassy state on a chosen crystalline substrate.

Three known glass-forming powder blends (under rapid solidification conditions) with nominal compositions of 94Fe4B2C, 75Fe15B10Si and 78Fe10BC9Si2Al1C (all in wt.%) were deposited by LSC using a continuous wave Nd:YAG laser under optimum processing conditions determined by preliminary trials. Despite the rapid quenching accompanying LSC, none of the coatings developed/retained amorphous/glassy cladding, possibly due to large-scale solute redistribution in the clad zone and/or between the clad layer and substrate. The clad microstructure is characterized by a fine dispersion of nano/microcrystalline intermetallic and interstitial compounds/phases in a ferritic matrix. All three compositions led to extreme refinement (31-52 nm average grain size) of ferritic grains formation and dispersion of precipitates of $Fe_{23}(B,C)_6$ in 94Fe4B2C clad; Fe_2B and Fe_3B in 75Fe15B10Si clad; $Fe_{23}(B,C)_6$ and Fe_3Si in 78Fe10BC9Si2Al1C clad. Both microhardness and wear resistance showed a significant improvement, particularly after LSC with 94Fe4B2C (Figures 14 and 15).

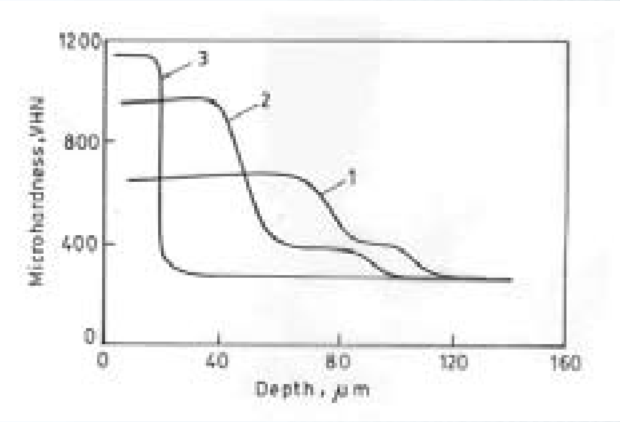


Figure 14. Microhardness profile with depth along the cross sectional plane (perpendicular to the clad/top surface for laser surface clad AISI 1010 steel with (1) 75Fe15B10Si, (2) 94Fe4B2C and (3) 78Fe10BC9Si2Al1C respectively. Note that degree of hardening is the maximum after LSC with 78Fe10BC9Si2Al1C

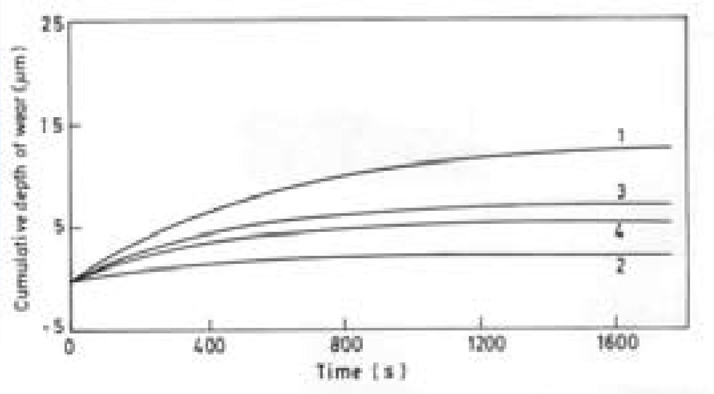


Figure 15. Kinetics of wear as a function of time (against a diamond indenter with 1 kg applied load) for (1) as-received vis -à-vis laser surface clad AISI 1010 steel with (2) 94Fe4B2C, (3) 75Fe15B10Si and (4) 87Fe10BC9Si2Al1C, respectively. Note that laser cladding with 94Fe4B2C induces the highest wear resistance

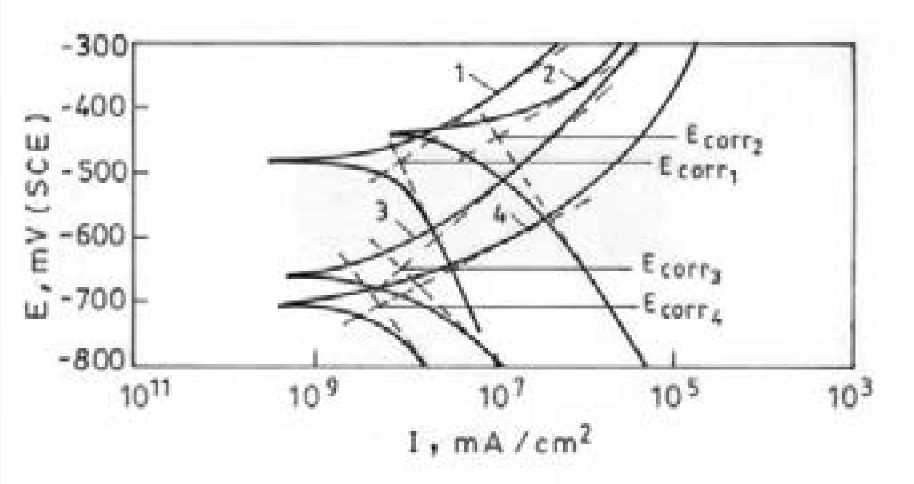


Figure 16. Variation of current density with potential in potentiodynamic polarization study in 3.56 wt.% NaCl solution for (1) as received and laser surface clad AISI 1010 steel with, (2) 75Fe15B10Si, (3) 78Fe10BC9Si2Al1C and (4) 94Fe4B2C

Potentiodynamic polarization studies in 3.56 wt.% NaCl solution showed that corrosion resistance of the substrate was remarkably improved by LSC with 94Fe4B2C, but slightly deteriorated after LSC with the other two coatings. Thus, it appears that LSC with 94Fe4B2C, among the present coatings, significantly enhances hardness and resistance to wear and corrosion of the substrate, though it fails to develop/retain amorphous microstructure under the present laser-processing conditions.

Investigator: Dr. Narendra B. Dahotre
Sponsor: National Science Foundation

Laser Surface Modification of Bio-Metallic Materials

Stainless steel (SS) 316L and Ti6Al4V are amongst the frequently considered materials for bio-applications. Their popularity is primarily due to unique combination of mechanical and corrosion resistance properties. These materials have been extensively studied with regard to their corrosion behavior in industrial and aerospace environments where they showed excellent or satisfactory performance. Physiological solution is one of the extremely aggressive environments that poses challenges to existing biomaterials. This has led to a development and use of several ceramics and polymers as substitute materials for biomedical applications; these were expected to be less toxic than the metallic materials. However, both ceramic and polymers materials have limited mechanical properties which restricts their use in the biomedical field.

In order to increase the corrosion resistance of metallic materials in physiological solutions, change in material's composition (includes development of new materials) or improvement in the functional surfaces using coatings by suitable methods are the only options. There are numerous surface modification methods, such as plasma-ion implantation, laser-melting and laser-surface alloying, physical and chemical vapor deposition (PVD and CVD), thermal oxidation, electrochemical surface modification/ anodizing, etc., that are currently used for improving corrosion resistance and biocompatibility of biomaterials. However, each of these methods has limitations in regard to the performance of tailored surfaces and their complex operating procedures. A few advanced surface-modification techniques, such as plasma-based techniques and laser treatments, have been developed and increasingly used to produce tailored surfaces suitable for bio-applications. They overcome the limitations of conventional coating methods such as electroplating, electroless plating, anodizing, etc. The uniqueness of these methods is that they offer desired surface properties either by alloying or by changing the microstructure of the outer surface, while keeping properties of the bulk material intact. In addition to increasing corrosion resistance, surface-modification techniques are also used to design surfaces for easy and faster bone formation and growth in living bodies.

Laser surface treatment has advantages over other methods as it is associated with extremely high cooling rates to obtain a non-equilibrium surface, simple operation, short processing time, good coating adherence, and high melt/coating depth. Laser surface treatment has been employed to desensitize the surface (to improve intergranular corrosion resistance) of sensitized stainless steels 316L (due to faulty heat treatment in the range 500 – 700ºC). Laser treatment has often been used to improve the corrosion and wear resistance of steels either by surface melting or suitable surface coating. However, the open-literature available on capabilities of the laser surface treatment methods to modify the corrosion resistance of biomaterials is limited. The recent efforts on the modification of titanium and titanium alloy (Ti6Al4V) surface using laser surface treatment have been shown to offer promising functional surfaces for biomedical application. The work so far has addressed improvements in wear performance of titanium with TiN on the surface obtained by laser melting in nitrogen atmosphere. A few of these studies have attempted to show the effects of excimer laser treatment, with its UV radiation and extremely short pulse duration, on the corrosion resistance and microstructure of Ti surfaces. The laser surface melting (LSM) has been carried out in the presence of argon or nitrogen as shielding gas at constant treatment conditions. During these efforts, the laser nitrided surfaces showed favorable changes in corrosion resistance while others showed contradictory results in different chloride containing solutions. The laser treatment of Ti-alloy in presence of argon showed significant improvement in the corrosion resistance. However, the laser melting in the absence of inert gases (in ambient atmosphere) could be advantageous due to formation of an oxide layer (TiO_2) on Ti surfaces, which is extremely important for biocompatibility. This will likely change the corrosion behavior of materials. While aiming at biomedical applications, laser-treated surfaces should be studied in simulated or in-vivo environments.

Influence of Laser Surface Modification on Corrosion Behavior of Stainless Steel 316L and Ti6Al4V in Simulated Bio Fluid

Laser surface engineering has been explored as a possible method for improving the functional surface properties of biomedical materials such as stainless steels and titanium alloys. This study emphasizes the influence of laser surface processing, carried out in the range of laser powers from 500-1500 W in ambient atmosphere, on the surface microstructure, corrosion behavior of SS316L and Ti6Al4V, and metal ion released during the corrosion process. A homogeneous surface microstructure includes columnar dendrites and fine grains in the re-solidified region of SS316L (Figure 17). The gradual increase in grain size from processed surface towards the base substrate was revealed. The laser processing of Ti6Al4V was found to develop a surface full of dendrites followed by acicular martensite in the interface region (Figure 18).

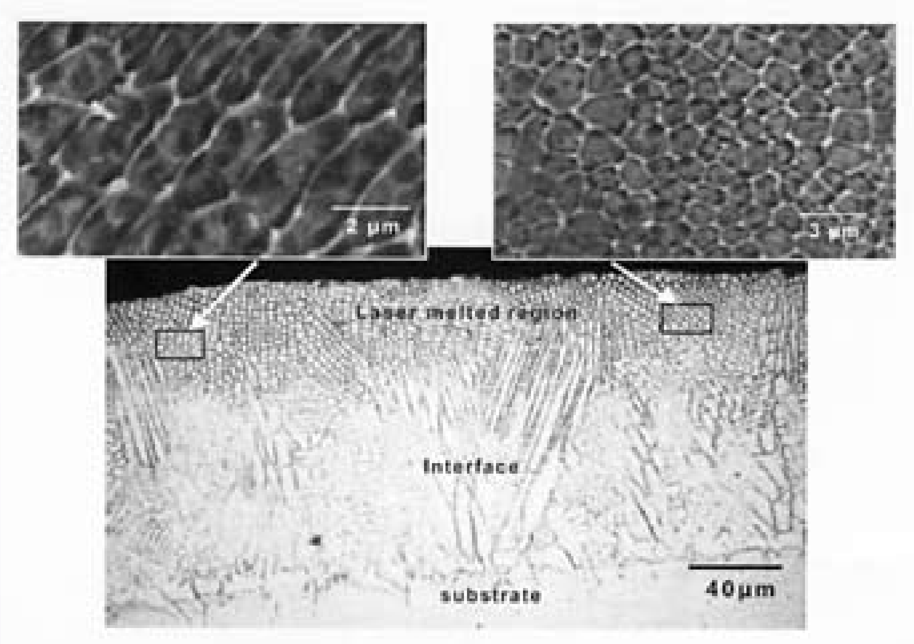


Figure 17. Microstructure of SS316L after laser surface treatment at 1500 W

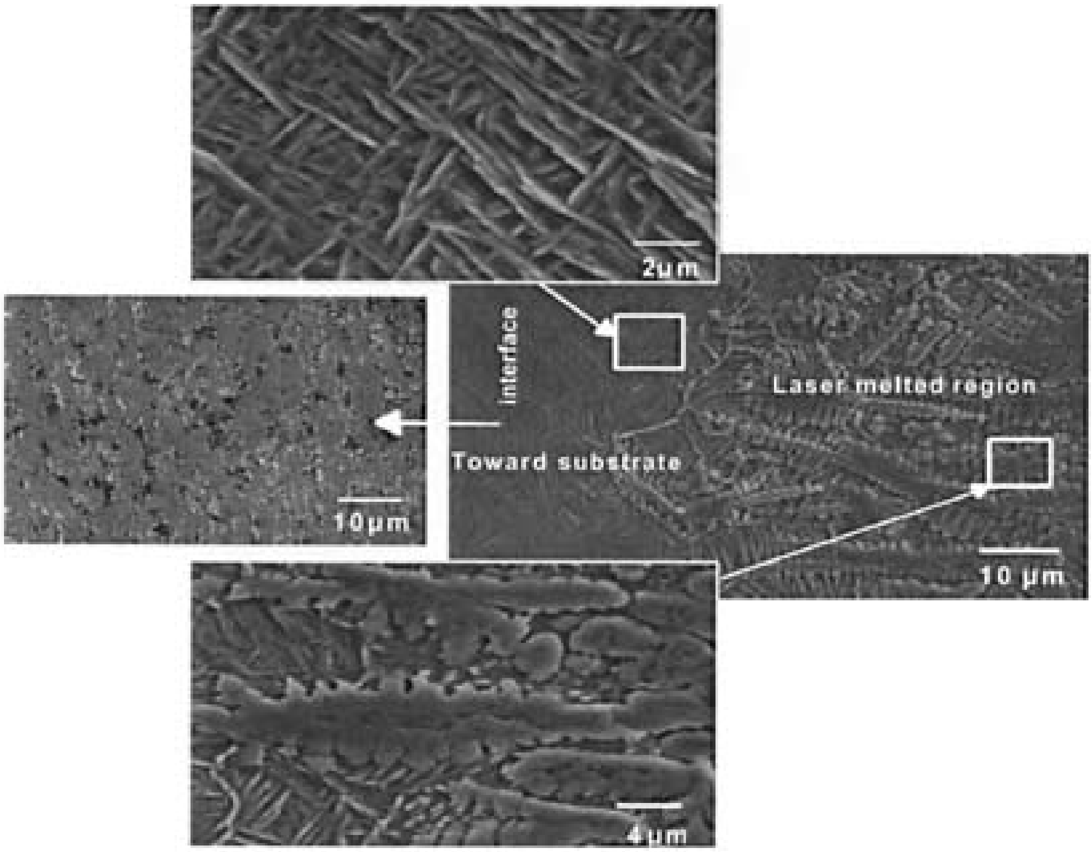
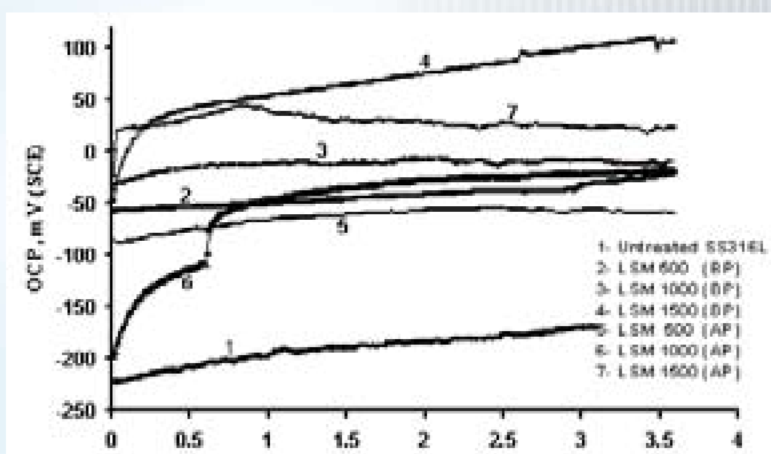


Figure 18. Microstructure of Ti6Al4V before and after laser surface treatment at 1500 W

The corrosion studies in Ringer's physiological solution showed increase (more noble than untreated) in the open circuit potential (OCP) as a result of laser surface treatment of both SS316L (Figure 19) and Ti6Al4V alloys (Figure 20). After laser processing, the corrosion properties of SS316L were observed to deteriorate while Ti6Al4V showed improvement as compared to their respective untreated counterparts. The variation of laser powers influenced the corrosion resistance of SS316L while that of Ti6Al4V did not vary significantly. Laser surface treatments at higher powers (> 1000 W) reduced the leaching of specific metallic ions from SS316L and Ti6Al4V during corrosion in Ringer's physiological solution.

Figure 19. OCP versus time curves obtained for untreated and laser treated SS316L in the Ringer's solution at 37ºC



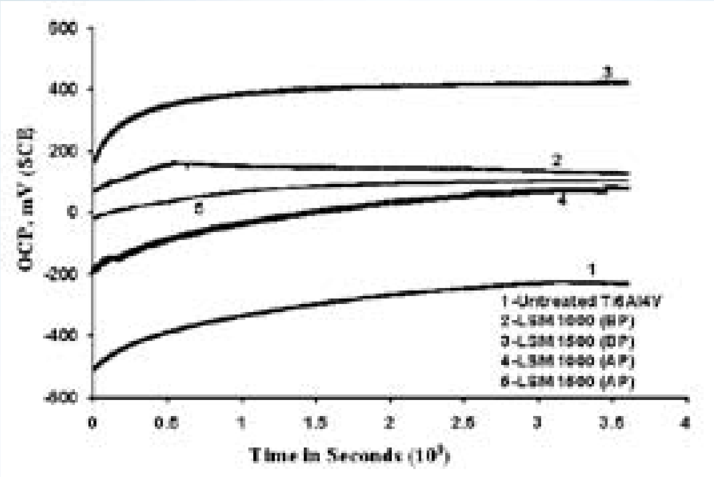


Figure 20. OCP versus time curves obtained for untreated and laser treated Ti6Al4V in the Ringer's solution at 37ºC

Corrosive Wear in Laser Surface Modified Ti-6Al-4V in Simulated Bio Fluid

The laser surface melting (LSM) of Ti-6Al-4V was performed in argon to improve its properties such as microstructure, corrosion, and wear for biomedical applications. Corrosion behavior was investigated by conducting electrochemical polarization experiments in simulated body fluid (Ringer's solution) at 37ºC. Wear properties were evaluated in Ringer's solution using pin-on-disc apparatus at slow speed.

The untreated Ti-6Al-4V contains a + ß phase. After laser surface melting, it transformed to acicular a embedded in the prior ß matrix (Figure 21). Growth in the range of 65 – 89 µm with increase in laser power from 800-1500 W (due to increase in associated temperature) was observed (Figure 21).

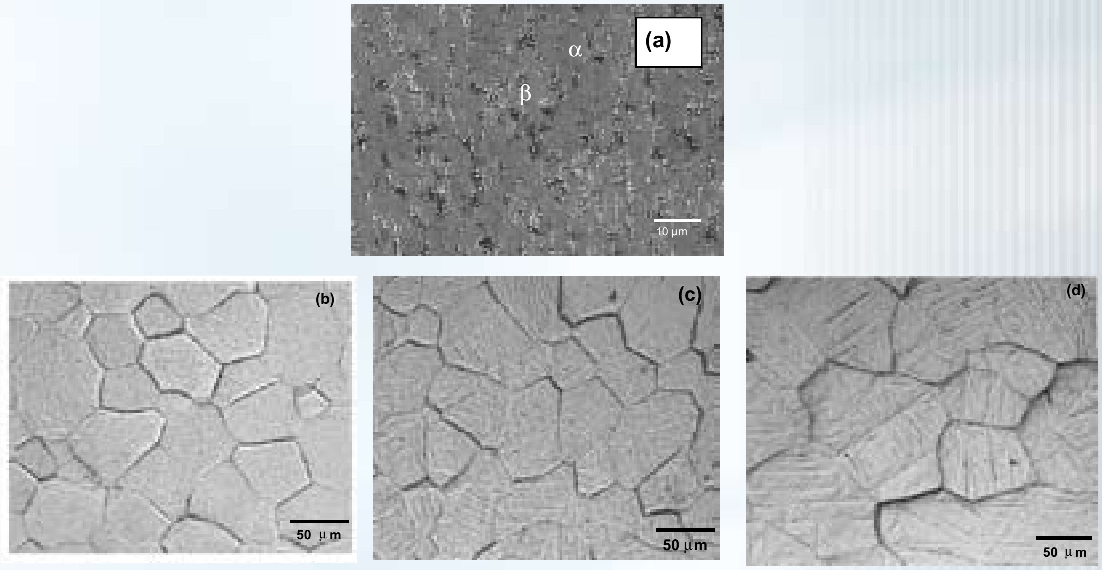


Figure 21. Microstructure of Ti-6Al-4V (a) as-received and after laser surface treated at (b) 800 W, (c) 1200 W, and (d) 1500 W powers

The hardness of as-laser-processed Ti-6Al-4V alloy was more (275-297 HV) than the untreated alloy (254 HV). Passivation currents were significantly reduced to < 4.3 μA/cm^2 after laser treatment compared to untreated Ti-6Al-4V (~ 12 μA/cm^2) (Figure 22). The wear resistance of laser-treated Ti-6Al-4V in simulated body fluid was enhanced compared to untreated one. It was highest for the one that was processed at 800W laser power (Figure 23). Typical micro-cutting features of abrasive wear were the prominent mechanism of wear in both untreated and laser-treated Ti-6Al-4V. Fragmentation of wear debris assisted by micro-cracking was responsible for mass-loss during the wear of untreated Ti-6Al-4V in Ringer's solution.

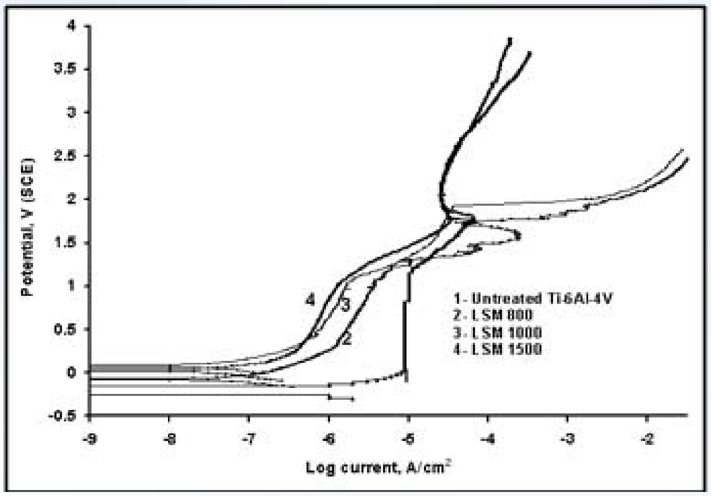


Figure 22. Anodic polarization behavior of untreated and laser-treated Ti-6Al-4V in Ringer's solution

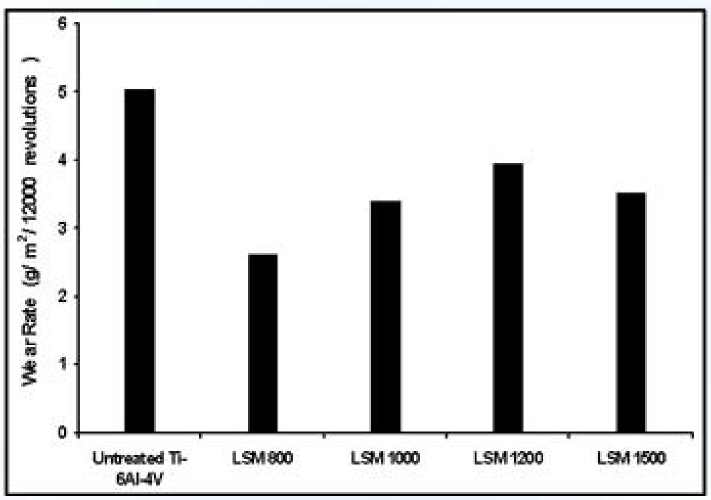


Figure 23. Wear rate of untreated and laser surface treated due to wear after sliding 450 m distance in Ringer's solution

Investigator: Dr. Narendra B. Dahotre
Sponsor: Center for Laser Applications

Laser Induced Surface Improvement Applications, AEDC Task Order Project; DoD Applications of LISI Technology

The objectives of this effort are to seek out applications in DoD where LISI technology can be implemented on an industrial scale with improved manufacturing and process control. The surface problems targeted will be those that currently result in extensive repair or replacement of the component during maintenance. The LISI process will also be applied to unique identification marking of critical components for tracking purposes where conventional marking methods are not applicable.

Principal Investigators: Dr. Dennis Keefer and Dr. Narendra Dahotre
Sponsor: Arnold Engineering Development Center

UTK LISI Wear Surface Fatigue Investigation

Very successful surfaces have been alloyed on steel and aluminum; however the high thermal quench rates in the LISI process produce residual stresses in the alloy layer. Post processing techniques such as shot peening have been demonstrated to restore fatigue life of the LISI wear surfaces. A very careful series of fatigue tests have been conducted by Dr. Liaw at UTK on 4340 steel with LISI wear surfaces to evaluate fatigue life reduction. Shot peening post processing effects have been evaluated for their effectiveness in restoring fatigue life. Baseline tests were completed and the evaluation of reduced fatigue life from the as-processed LISI wear surfaces was documented. Results confirm the significant reduction in wear surface fatigue life when the resulting surface stresses are not reduced by post processing. If the LISI wear surface contains surface cracks caused by improper processing parameters or alloy selection, the reduction in fatigue life may be unacceptable. Although the chrome and chrome-diboride wear surface on steel substrate has proven to be an exceptionally good wear surface, the potential reduction in fatigue life must be considered and addressed with post processing techniques.

Principal Investigators: Dr. Dennis Keefer and Dr. Narendra Dahotre
Sponsor: Arnold Engineering Development Center

Titanium Flaw Repair with LISI

Very successful surfaces have been alloyed on steel and aluminum; however the high thermal quench rates in the LISI process produce residual stresses in the alloy layer. Post processing techniques such as shot peening have been demonstrated to restore fatigue life of the LISI wear surfaces. A very careful series of fatigue tests have been conducted by Dr. Liaw at UTK on 4340 steel with LISI wear surfaces to evaluate fatigue life reduction. Shot peening post processing effects have been evaluated for their effectiveness in restoring fatigue life. Baseline tests were completed and the evaluation of reduced fatigue life from the as-processed LISI wear surfaces was documented. Results confirm the significant reduction in wear surface fatigue life when the resulting surface stresses are not reduced by post processing. If the LISI wear surface contains surface cracks caused by improper processing parameters or alloy selection, the reduction in fatigue life may be unacceptable. Although the chrome and chrome-diboride wear surface on steel substrate has proven to be an exceptionally good wear surface, the potential reduction in fatigue life must be considered and addressed with post processing techniques.

Principal Investigators: Dr. Dennis Keefer and Dr. Narendra Dahotre
Sponsor: Arnold Engineering Development Center

Unique Identification Matrix Marks

A DoD requirement for the unique identification for tracking of some DoD parts over a specific value and those for critical missions have been placed on all new procurements. UTSI has been working with a matrix mark reader company to validate various marking techniques, including GALE and LISI which are UTSI developed. The LISI and GALE marks have the durability for application in harsh environments. Marking of turbine engine parts has proved difficult without using deep engraving or dot peening which can have serious fatigue life impact. UTSI started a project to evaluate LISI and GALE marks on turbine blade materials for fatigue life impact. The GALE mark has no fatigue impact, and the LISI mark has some fatigue life reduction but much less than dot peening. Both LISI and GALE matrix marks have been applied to turbine engine parts received from both Solar Turbine and the Naval Aviation Depot at Cherry Point, NC. The parts have been returned for evaluation during normal overhaul processes. UTSI has been funded for purchase of a galvo-driven marking head for the higher power lasers to allow true deep LISI matrix marking. The deep LISI marks should demonstrate good survivability on the turbine engine parts.

Principal Investigators: Dr. Dennis Keefer and Dr. Narendra Dahotre
Sponsor: Arnold Engineering Development Center

Army TACOM SBIR Project with C-K Engineering

The US Army is funding research on development of high-temperature cylinder wall operation in diesel engines for improved fuel economy. UTSI is supporting C-K Engineering in developing a high-temperature LISI surface on steel cylinder inserts for wear testing. New LISI precursor materials containing moly are being investigated which may have broad application to DoD high temperature wear problems. A moly-moly boride precursor mix was selected for the cylinder LISI surface. Wear samples were processed for evaluation, and the engine cylinder spraying and processing fixtures were developed. Engine cylinders will be processed and tested in diesel engines next year.

Principal Investigator: Mr. Fred Schwartz
Sponsor: C-K Technologies, LLC

EJ Company TiN Coating Analysis Report

The purpose of this testing was to hopefully bring business back to Tennessee (Creative Coating Solutions, Inc. of Smyrna, TN) that had been taken out of state. The EJ company of Woodbury, TN. Remanufactures tool bits for the Nissan plants in Tennessee and has used Creative Coatings until recently. The reason for the loss of this business was due to improved performance by the out of state competitor of TiN plated tool bits that have silver soldered WC inserts. Tool bits incorporating silver solder are the only bits affected. Removal of Freon by the EPA from cleaning techniques has brought on this problem so new techniques for cleaning before plating were required. Both Creative and the out of state plating company have employed these new techniques but the out of state company has apparently developed an additional technique that extends their coating lifetime by up to a factor of 10 over Creative Coatings. UTSI, in an effort to support Tennessee industries, has assisted Creative in trying to develop a solution to their problem using the materials lab at UTSI.

First we visited Creative Coating's complex to gather information and discuss possible changes to enhance their coating process. Some immediate actions were recommended to their vacuum system which resulted in a decreased pump down time of 7 minutes. This did not correct the coating problem but increased their throughput. Next we had the EJ Company remanufacture four tool bits which were identical in all aspects for comparison purposes. Next we sent two to Creative for coating and two out of state for coating. They were then sent to UTSI for comparative analysis. We identified these bits as Creative © and out of state (B). We took pictures of the delivered bits (Picture A) and right away noticed that bit B was a much brighter gold color and the surface texture was smoother than (C). This may be due to a post plated cleaning process done to (B) indicated by the removal of the silver solder heat discoloration areas next to the plated areas. Next we sectioned each tool bit and mounted them for polishing which allows for hardness measurements and examination under high magnification microscopes. Microscope examination revealed very little differences between samples. We looked at both the pure WC plated area and base metal plated area. The plating is so thin it is almost impossible to see with a microscope and polishing techniques seem to remove the plating. Most of what was seen seems to be silver solder. Hardness measurements were taken and the average hardness of the base metal revealed that (B) is softer than (C). This could be contributed to (B) being plated at a higher temperature than (C) causing an annealing of the base metal just as Creative Coatings suspected. Next we performed SEM analysis using the X-Ray mapping to look for elemental differences. The most significant difference was a 5:1 difference in the Zn content in the silver solder areas. This could also be attributed to plating at a higher temperature because Zinc has a low melting point (419ºC) and boiling point of (907ºC).

A summary of the analysis is that we cannot declare what process the out of state company is using to improve their plating process but we can say that it appears to be tied to the plating temperature. Jim Clay from Creative Coatings says that the Zinc content of the solder is very important to the plating process. This is probably due to out gassing of the zinc during plating because of its low boiling point. Higher temperatures would deplete the Zinc allowing for better adherence.

The EJ Company is currently using Aufhauser SilverAlloy A-50Ni2 solder which contains 26-30% Zinc. I would recommend a trial set of bit soldered with Aufhauser SilverAlloy B-56Ni2 which contains no Zinc. This solder is similar in all other aspects and should otherwise perform well. This could be a solution to plating at higher temperatures for Creative Coatings but may also yield better wear properties in all plating applications.

Picture A: Elemental analysis for sample bits B and C

Elt.	Line	Intensity (c/s)	Error 2-sig	Conc		
Si	Ka	3.16	0.230	0.191	wt.%	
Ti	Ka	4.19	0.264	0.281	wt.%	
Cr	Ka	10.04	0.409	0.744	wt.%	
Fe	Ka	545.02	3.014	64.643	wt.%	
Ni	Ka	1.94	0.180	0.337	wt.%	
Cu	Ka	68.78	1.071	15.475	wt.%	
Zn	Ka	6.52	0.330	1.806	wt.%	←
Ag	La	110.49	1.357	16.523	wt.%	
				100.000	wt.%	Total

kV 18.4
Takeoff Angle 46.7°
Elapsed Livetime 240.0

EJ-B Elemental Analysis

Hardness chart for sample bit B

Elt.	Line	Intensity (c/s)	Error 2-sig	Conc		
Al	Ka	4.19	0.264	0.160	wt.%	
Si	Ka	5.29	0.297	0.149	wt.%	
Ti	Ka	131.45	1.480	4.709	wt.%	
V	Ka	0.00	0.000	0.000	wt.%	
Cr	Ka	10.68	0.422	0.446	wt.%	
Mn	Ka	2.28	0.195	0.108	wt.%	
Fe	Ka	599.44	3.161	34.133	wt.%	
Ni	Ka	6.58	0.331	0.525	wt.%	
Cu	Ka	117.33	1.398	12.068	wt.%	
Zn	Ka	80.84	1.161	10.405	wt.%	←
Ag	La	476.12	2.817	37.298	wt.%	
				100.000	wt.%	Total

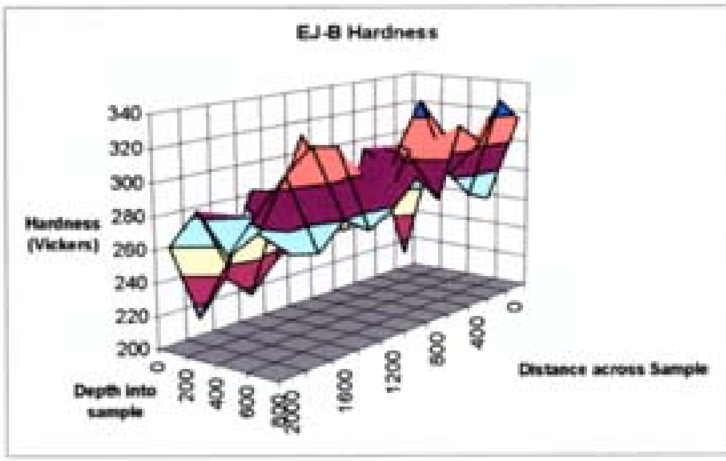
kV 18.4
Takeoff Angle 46.7°
Elapsed Livetime 240.0

EJ-C Elemental Analysis

Sample 1 7/29/2004 9:46 EJ-B

	0	200	400	600	800	1000	1200	1400	1600	1800	2000
0	210.619	261.822	294.131	240.051	255.939	241.244	233.328	215.312	231.072	210.68	259.804
200	286.264	295.694	276.299	258.173	287.807	273.166	317.124	277.479	289.474	248.414	284.588
400	288.135	308.716	330.15	303.57	261.697	277.236	280.327	274.644	291.017	280.344	261
600	259.883	286.403	283.252	295.45	303.731	274.75	287.966	317.578	320.805	307.173	277.331
800	317.074	331.786	307.212	320.803	277.415	294.175	278.97	270.257	280.048	265.159	269.079
Average	272.395	292.8842	298.2086	283.6094	277.3178	272.1142	279.543	271.054	282.4832	262.354	270.3604

Total Average 278.3931

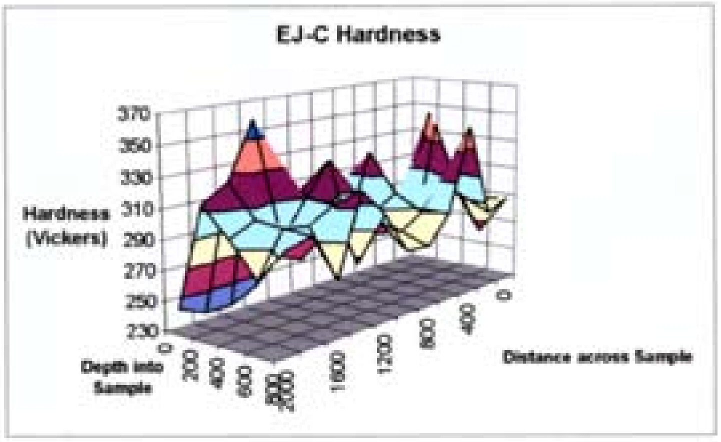


Hardness Chart for Sample Bit C

Sample 1 7/28/2004 14:18 EJ-C 500 gm load

	0	200	400	600	800	1000	1200	1400	1600	1800	2000
0	259.645	253.258	258.017	284.402	288.537	251.843	258.505	242.334	234.335	234.299	242.332
200	345.468	286.07	284.809	324.82	277.291	277.474	310.495	287.838	361.873	324.586	313.702
400	292.318	341.24	267.674	298.724	288.091	308.772	331.54	309.694	286.369	303.523	295.537
600	262.342	292.329	307.173	287.935	278.709	289.571	264.852	308.765	269.147	301.784	273.162
800	289.404	283.449	347.193	290.713	271.757	272.887	301.669	320.857	267.831	300.36	296.717
Average	289.8354	291.2692	293.0132	297.3188	280.877	280.1094	293.4122	293.9376	289.911	292.9104	284.09

Total Average 289.6986



Principal Investigator: Mr. Fred Schwartz
Sponsor: EJ Company

Focus Area

Ultrasensitive Fluorescence Spectroscopy

Introduction

The CLA was one of the first few laboratories in the world to develop experimental techniques for the detection of single fluorescent molecules in solution. As described in previous CLA annual reports, our research contributions in this area have included seminal advancements in single-photon detector technology, and development of single-molecule fluorescence imaging instrumentation in support of industry efforts to create new methods for very high-speed DNA sequencing. The pace of innovation and applications for ultrasensitive fluorescence detection has been phenomenal: For example, in the DNA sequencing application, the human genome was first sequenced in draft form using bulk fluorescence detection in year 2000 at a cost of about $800M, but just this summer private industry has begun selling $500K machines that employ ultrasensitive fluorescence detection to rapidly sequence entire genomes for as little as $20K (New York Times, August 9). While molecular fluorescence detection has become a key component in many present day biomedical applications, there remains a critical need for further development of the capabilities of ultrasensitive fluorescence spectroscopy. A detailed scientific understanding of the underlying molecular photophysics, stochastic processes, statistical effects, optical physics, and instrumental limitations is needed in order to push back the envelope to enable future technological advancements and applications. Over the past year, the CLA research in this area has aimed to continue making important contributions that address these needs with a multifaceted program, which has included theoretical developments, computational modeling, and interdisciplinary collaborations on various biophysics topics and biotechnology applications. Our recent research encompasses the following areas:

Theoretical Developments for Excitation Saturation Experiments

Single-molecule detection (SMD) and fluorescence correlation spectroscopy (FCS) are increasingly popular methods for chemical and biological sample characterization. For many applications, including intracellular biophysics studies and high throughput pharmaceutical drug screening, it is becoming increasingly important to reduce the measurement times for sample characterization. While an increase in laser power can yield more photons and can decrease the time required to achieve the desired statistics, excitation saturation and other photophysical processes modify the correlation functions and the single-molecule photon statistics. For correct interpretation of the data, the usual approximations must be abandoned and it becomes essential to form a detailed understanding of saturation and photophysics, and to include them in the data analysis models. Recently, we have melded theoretical considerations from non-linear optics with those from single-molecule fluorescence to develop a detailed model for excitation saturation effects in ultrasensitive fluorescence experiments. Our model, which was presented at the January 2005 Photonic West symposium in San Jose, CA, together with supporting experiment and computer simulation results, predicts that there are differences in the saturation behavior that occur with femtosecond-pulsed, picosecond-pulsed, and continuous-wave laser excitation. Fig. 1 some shows a result from an experiment conducted in our lab that characterizes some of those differences.

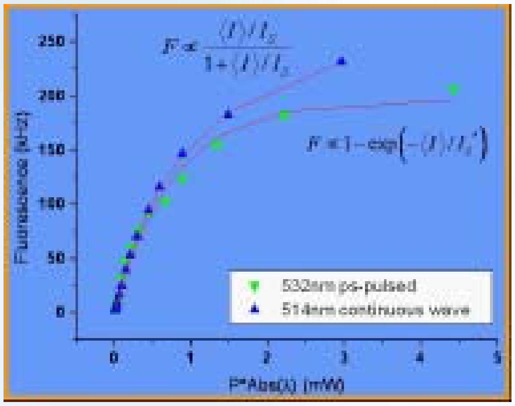


Figure 1. Saturation of fluorescence signal with increasing laser power showing the different power-dependence for picosecond-pulsed and continuous-wave laser excitation

In recent months, we have extended our theoretical model to also include triplet-state kinetics and we presented theory and preliminary experimental results at the July 2005 6th International Weber Symposium on Innovative Fluorescence Methodologies in Biochemistry and Medicine. There is considerable interest in this topic from the fluorescence community because triplet-state effects are very often evident even in experimental results collected at low laser powers, and our results show that in such cases the previously available data analysis models lead to incorrect predictions of the concentrations of the fluorescent species. We are currently working to collect experimental results that carefully distinguish the triplet-state saturation effects from other effects that can influence molecule concentrations, such as photobleaching and sample loss due to non-specific binding of molecules to the glass surfaces.

Principal Investigator: Dr. Lloyd Davis
Sponsor: Abbott Laboratories

Scanning Fluorescence Fluctuation Spectroscopy

In Fluorescence Fluctuation Spectroscopy (FFS), a tightly-focused laser beam and confocal pinhole are used to define a femto-liter sized probe-volume; fluctuations in the weak fluorescence signal from the small numbers of sample molecules in solution that pass in and out of the probe volume are measured using single-photon counting instrumentation; and statistical analysis of the photon counts is performed to obtain the concentrations and dynamic properties of the various molecular species contained within the sample. The first form of FFS, fluorescence correlation spectroscopy (FCS), was invented in 1972, but FFS has become an important and practical tool only since the development of single-molecule detection capability. Whereas bulk fluorescence measurements provide information only on the net fluorescence properties of the mixture, FFS methods enable the sample constituents to be individually quantified and studied. In effect, only one or two molecules are probed at any given time, so that the make-up of the sample can eventually be determined after many of the constituent molecules diffuse individually in and out of the probe volume.

For pharmaceutical drug discovery applications that involve large bio-molecules such as fluorescently-labeled protein complexes, enzymes, and antibodies, undesirably long data collection times are needed to obtain statistically significant FCS results, in part because of the slow molecular diffusion. For high-throughput screening (HTS) of bio-molecules, there is a need to reduce the measurement time per sample. An obvious way to interrogate molecules more rapidly is to translate the sample container so that the laser beam scans through the solution.

Figure 2 shows one example of photon burst data collected in this way using a commercial $400K instrument during a CLA visit to the sponsor's facility at Abbott Labs, North Chicago. Although the photon bursts appear similar to those obtained in a static experiment, new methods for statistical analysis of the fluorescence fluctuations are needed in order to extract molecular species parameters while accounting for the known molecular motion. Also, for data from repetitive scans across several different samples, such as that shown in Fig. 2, the data segments from each sample must be extracted from the total data set and then combined. Over the past year, we have developed new data analysis tools that can be applied in such experiments. We have also experimentally studied photobleaching and other photophysical effects that are effectively modified by the paths that molecules take as they are transported through the focused laser beam.

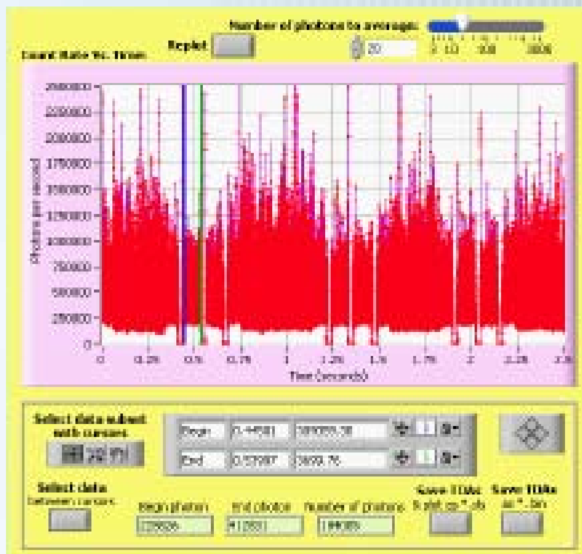


Figure 2. Data collected by CLA at Abbott Laboratories showing fluorescence fluctuations obtained in a scanning FFS experiment from several adjacently-placed samples

Principal Investigator: Dr. Lloyd Davis
Sponsor: Abbott Laboratories

Capillary Flow System

For FFS analysis of large bio-molecules with slow diffusion, in addition to the sample-scanning method described above, the sequential detection of large numbers of individual molecules in a short time can also be accomplished by causing molecules to flow through a stationary tightly focused laser beam. Micro-fluidic and nano-fluidic systems are of particular interest for investigation of tiny-sized drops of precious bio-samples. In recent work, we have investigated several capillary-based systems that can be easily retrofitted to existing microscopes and drug-screening platforms. Our studies have considered the capillary material (glass or quartz), fabrication cost and re-usability, background luminescence from the capillary, non-specific adsorption of molecules to the capillary, influence of detergents commonly used in HTS applications, course and precise position adjustability, mechanical stability, and the initiation, control, stability, and measurement of the flow rate. Figure 3 shows one of the capillary systems under study mounted on CLA's custom-built single-molecule fluorescence microscope. The side-mounted syringe is used to initiate a stable siphoning flow of the sample droplet up into the capillary. The laser beam is focused microns below the tip of the capillary and bio-molecules are carried by flow axially along the laser beam, up into the capillary, so that they traverse the long axis of the elliptically shaped laser probe region.

A capillary system similar to that shown in Figure 3 was delivered to the sponsor at Abbott Labs for experiments in their drug discovery laboratory. CLA student Mr. David Ball accompanied Dr. Lloyd Davis to install the system on Abbott's instrument and to conduct experiments together with Abbott staff to demonstrate the capabilities and performance of the capillary system in control experiments. The research on this topic will form part of the doctoral dissertation of Mr. Ball. CLA will continue to collaborate with Abbott scientists in the year ahead on the application of this system to drug discovery experiments.

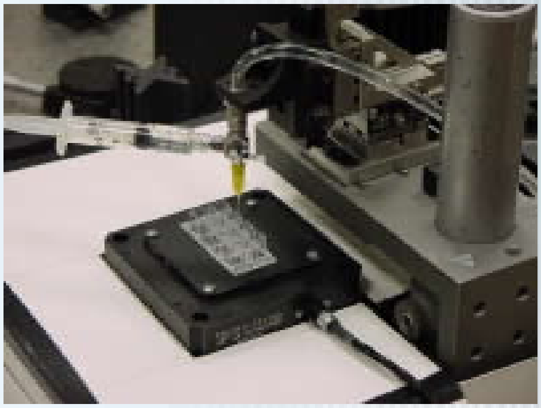


Figure 3. Capillary-based system and 8-unit micro-liter sample holder, mounted on CLA's custom-built single-molecule fluorescence microscope. (The microscope optics are out of view, below the sample stage.)

Principal Investigator: Dr. Lloyd Davis
Sponsor: Abbott Laboratories

Molecular Brightness Assays for Monitoring Drug-Binding Equilibriums

Fluorescence fluctuation spectroscopy has proven to be a useful technique for monitoring different molecular species in very dilute solution mixtures, for applications such as competitive drug-binding assays and high throughput pharmaceutical drug screening. This past year, we have developed a new data analysis method applicable to cases where different types of molecules have different fluorescent brightness, and where molecules are actively transported through the laser beam. The time of arrival of each detected photon is recorded by photon counting instrumentation and the data stream is processed by a digital filter that is matched to the determined rate of transport, to accentuate photon bursts from individual molecules. The distribution of the resulting burst amplitudes is then modeled by an empirical function, and maximum entropy methods are used to extract fitting parameters, which give a measure of the mean molecular brightness, for the given laser power and other experimental conditions. With the same experimental conditions, mixtures of molecules with different effective molecular brightness values may then be analyzed by maximum likelihood estimation. We presented details and application examples of this new analysis method at the February 2005 Biophysical Society annual meeting.

Figure 4 shows the performance of the method in analyzing data from a simulated competitive drug-binding assay in which a non-fluorescent drug-like molecule (D) displaces a fluorescently-labeled ligand (L) from a fluorescently-labeled target molecule (T). Although the net fluorescence signal remains constant through the titration, the fluorescence signal per particle decreases with ligand-target dissociation. The new data analysis method is able to recover the binding equilibrium with a measurement time of only 10 seconds per titration point.

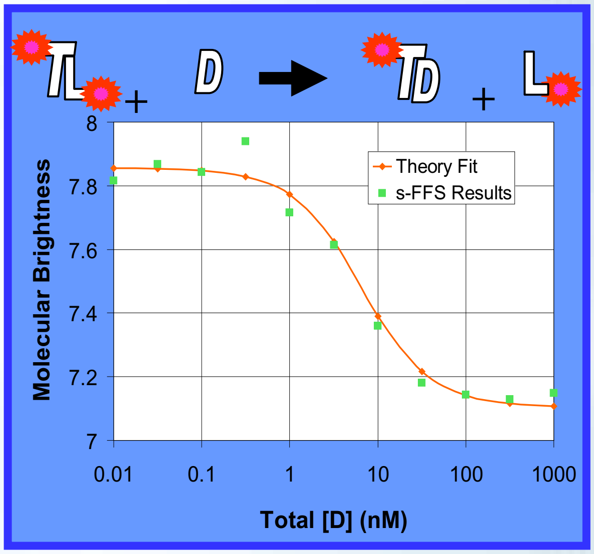


Figure 4. Results of FFS data analysis from a model competitive drug-binding titration

Principal Investigator: Dr. Lloyd Davis
Sponsor: Abbott Laboratories

Computer Modeling and Simulations

A sophisticated computer simulation of single-molecule detection developed by CLA over the course of several years has been further developed and extended this past year. The simulation has been invaluable in designing experiments and evaluating new data analysis strategies. One version of the simulation now includes modeling and analysis of a new form of fluorescence fluctuation spectroscopy (FFS) described above, that aims to quantify molecular species that have differences in fluorescent brightness. Figure 5 displays a screen shot of the LabView interface for that simulation. The "Burst Amplitude Probability Density" graph in the center of the figure includes a model fit (green line) of the histogram of digitally-filtered photon bursts. The model uses maximum-likelihood estimation techniques to characterize the fluorescence brightness of individual molecules. Other simulation studies conducted over the past year have played a key role in improving our understanding of the effects of excitation saturation and photophysics in ultrasensitive fluorescence spectroscopy experiments.

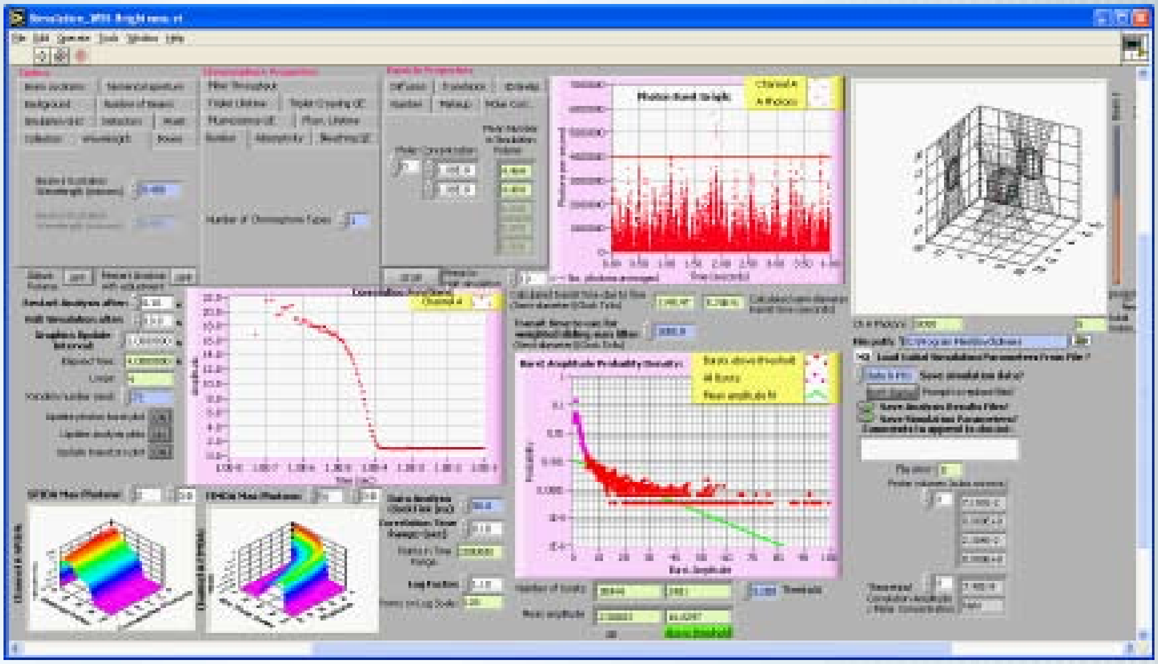
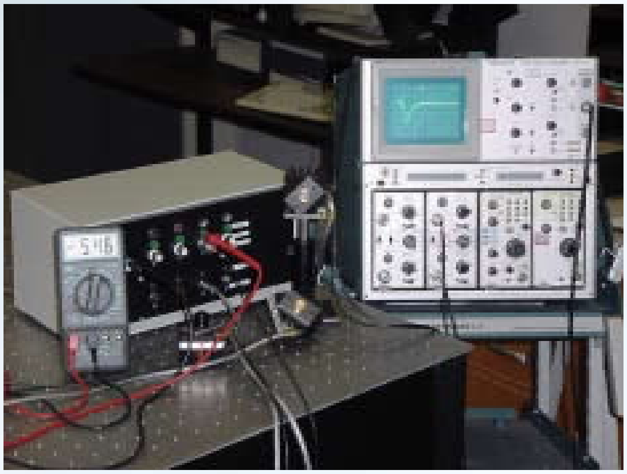


Figure 5. Screen shot of the LabView interface of a new computer simulation of a scanning fluorescence fluctuation spectroscopy experiment

Principal Investigator: Dr. Lloyd Davis
Sponsor: Abbott Laboratories

Avalanche Photodiodes for High Efficiency Single-Photon Detection with Picosecond Timing

Ultrasensitive fluorescence spectroscopy generally requires efficient detection of bursts of single photons. For many applications, including those in which molecular species are to be characterized by their fluorescence lifetimes, it is necessary to record the arrival time of each detected photon to within sub-nanosecond precision. In a past collaboration with EG&G Optoelectronics, Canada, CLA contributed to the development of single-photon avalanche diodes (SPADs) for high efficiency, high-time resolution single-photon detection. EG&G Optoelectronics was subsequently acquired by Perkin Elmer, and the detectors are now exclusively packaged with “active-quenching” circuits that provide low dead-time or fast recovery, so that closely-spaced photons within a burst may be recorded. The Perkin-Elmer detector modules, which cost ~$8K each, are now widely found in ultrasensitive fluorescence applications throughout the world. Unfortunately, the active-quenching circuits now in use result in a loss of sub-nanosecond timing precision. In particular, the photon timing has a strong dependence on count rate, which is detrimental to single-molecule fluorescence lifetime applications. A 4-channel SPAD detector newly available from Perkin Elmer was provided to CLA on loan and was also found to have this same deficiency. This past year, we have used other SPAD detectors donated to us by Perkin Elmer with custom circuitry built by CLA in a study aimed at improving detector timing capabilities. This study will continue in the year



ahead. Figure 6 shows CLA's custom mounted SPAD detectors and control electronics.

Figure 6. CLA-built control electronics and single-photon avalanche diodes

Principal Investigators: Dr. Lloyd Davis and Mr. Newton Wright
Sponsor: Center for Laser Applications with detectors donated by Perkin Elmer

Multi-wavelength Excitation for Ultrasensitive Fluorescence Experiments

At the end of last year, we faced several major problems with the lasers that are used in our ultrasensitive fluorescence spectroscopy research. Over the course of the year, we have solved these various problems and have now set up a very versatile configuration of lasers with excellent stability and beam focusability. Figure 7 shows the two picosecond pulsed dye lasers (foreground), tunable from 560—6 10 nm and 605—660 nm, which we have recently set up for simultaneous operation, synchronously-pumped by a new picosecond 532 nm modelocked frequency-doubled Nd:YAG laser (Spectra Physics, Vanguard; at left). The pulses from this system may be "Lock-to-clock" synchronized with the 700—950 nm femtosecond pulses provided by the Ti-Sapphire laser (Spectra Physics, Tsunami; background), which is pumped by the continuous-wave beam from the argon ion laser (Spectra Physics, BeamLok; mid-ground). We have set up spectrometer and autocorrelator diagnostics and a configuration of switchable mirrors to select the beam paths for a variety of experiments. We have used the femtosecond pulses from the Ti-Sapphire laser for various experiments using two-photon excitation of fluorescence, including FCS and FFS experiments with the previously described capillary system. We have also set up a BBO laser-frequency doubler, which is shown in the foreground of Figure 8, for experiments that require excitation wavelengths in the 350—475 nm range. In recent months, this has been used for collaborative experiments with visiting professor K.H. Lee to measure nanosecond fluorescence lifetimes of blue luminescence from light-emitting devices that contain nanostructure features etched in silicon.

Figure 7. CLA's modelocked laser system provides a versatile multiple-wavelength excitation source with continuous wave, or femtosecond or pico-second pulse durations

Figure 8. A BBO laser frequency doubler has been set up to provide blue wavelength sub-picosecond pulses

Principal Investigators: Dr. Lloyd Davis, CLA staff,
Visiting Professor K. H. Lee
Sponsor: Center for Laser Applications

Maximum Likelihood Multi-Channel Fluorescence Microscopy

Multi-channel spectroscopic imaging is a developing method that uses multiple excitation wavelengths, detection wavelengths, and time-resolved detection for detailed sample characterization. Over the past year, we have used computer simulations to study the extension of such methods to imaging applications with low signal levels. Simulation results and preliminary experimental results obtained with a 4-channel SPAD detector were used to support a proposal to the National Institute of Biomedical Imaging and Bioengineering with the stated goal of advancing the scope of multi-channel spectroscopy to address ultra-sensitive fluorescence detection applications. The proposal has resulted in a two-year grant, which began August 1, 2005, from the National Institutes of Health. The abstract of the research, which will involve collaborations with Professor David Piston of the Molecular Physiology & Biophysics Department at Vanderbilt University, follows:

The objective of this work is to develop a new approach to multichannel fluorescence spectroscopy that will result in extended sensitivity for a number of imaging applications in biomedical research, including high-speed multiplexed read-out of bio-chips, rapid DNA sequencing, fluorescence lifetime imaging microscopy, and cell imaging experiments that require separation of fluorescent labels with overlapping excitation and/or emission spectra, such as green fluorescent protein and its variations. The aims include implementation of a scanning confocal microscope with multiple excitation wavelengths, multiple emission wavelength bands, and time-resolved single-photon detection, and also implementation of statistically efficient maximum-likelihood based methods for the resolution of the resultant multi-channel data sets into the fractional components corresponding to each fluorophore present, and background. Numerical methods will be used to solve the analytically intractable maximum-likelihood equations to determine the component fractions and their errors and co-dependence. Analysis software will be made available for internet download. Also, a procedure will be developed for the optimal selection of the excitation wavelengths and emission bands for given fluorophores and experimental conditions. The maximum-likelihood based approach will be evaluated using experimental test data. Monte Carlo simulations will also be developed to validate the new approach using the spectra of commonly-used fluorophores and to determine its capabilities in terms of the accuracy (lack of bias), statistical precision, and covariance of parameters for given signal and background levels, particularly for photon-starved imaging applications. The performance range of the maximum-likelihood based approached will be compared with that of existing least-squares curve-fitting-based "linear un-mixing", which is expected to become statistically invalid for low-count data sets.

Principal Investigator: Dr. Lloyd Davis
Sponsor: National Institutes of Health

Other Activities in the Ultrasensitive Fluorescence Spectroscopy Focus Area

In September 2004, Dr. Davis presented research results at the 10th International Workshop on Single Molecule Detection and Ultrasensitive Analysis in Life Sciences, held in Berlin, Germany. As this was the 10-th workshop, several of the pioneers of single-molecule detection were in attendance (see Figure 9). Contacts were renewed with several researchers from Europe, including Emeritus Professor Rudolf Rigler, a pioneer of Fluorescence Correlation Spectroscopy, who is from the Royal KTH Institute in Sweden, which had invited Dr. Davis to visit as a consultant the year before. Prof. Rigler is now with the group of Dr. Theo Lasser in Switzerland. Dr. Steve Soper, from Louisiana State University, Baton Rouge, who had been a postdoc with Dr. Richard Keller's group at Los Alamos National Laboratory when Dr. Davis coauthored the first successful single-molecule detection experiment at LANL in 1990, was also in attendance. Dr. Soper invited Dr. Davis to submit a presentation to the "Pittcon" symposium on "15 years of Single-Molecule Detection," to be held in Orlando, FL, February 27—March 4, 2005.

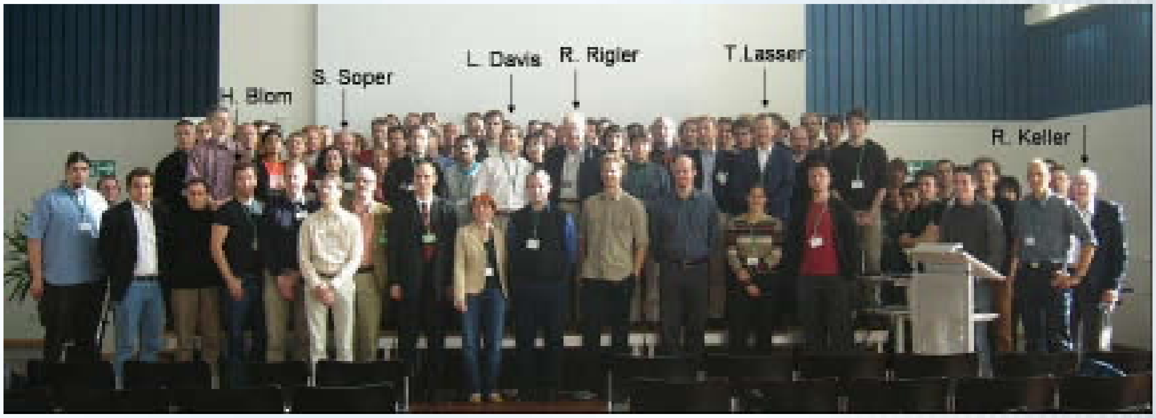


Figure 9. Attendees at the 10th International Workshop on "Single Molecule Detection and Ultrasensitive Analysis in Life Sciences," held September 2004 in Berlin, Germany

In November 2004, Dr. Davis presented an invited seminar at Tennessee Technological University, Cookeville, TN, after being contacted by Dr. M. Wells, who had just been recruited to Tennessee from the research group of Dr. Lasser in Switzerland. Dr. Wells' research involves biologically-engineered cells that may be used in bio-availability and environmental bio-sensing applications. Drs. Davis and Wells initiated a collaboration on the application of ultrasensitive fluorescence spectroscopy methodology to environmental bio-sensors. A joint proposal was submitted in February 2005 to the NSF "Sensors and Sensor Networks (Sensors)" program. This proposal was not successful but will be refocused with additional preliminary experimental results and resubmitted to funding agencies in the year ahead.

Following his presentation at the Pittcon symposium in Spring 2005, Dr. Davis was invited by Dr. Soper to collaborate on a National Institutes of Health P-31 Center grant application for an interdisciplinary "Biotechnology Resource Center", to be affiliated with the Louisiana State University Center for Advanced Microstructures and Devices (CAMD). On April 5-6, 2005, Dr. Davis visited LSU for the NIH site visit for the review of the $5M+ 5-year proposal. Although the UTSI/CLA component of the proposal was highly rated, the proposal as a whole received a priority score that placed it below the recommended level, and it was not funded. LSU intends to resubmit the Center grant application next year, again with UTSI/CLA as a collaborator. Since then, Dr. Davis has joined with Dr. Soper and others in preparing an NIH R-01 grant application to the NIBIB "Bioengineering Research Grants" Program. The interdisciplinary proposal will combine LSU's expertise in micro-fabrication and in near-infrared fluorescent dye synthesis, UTSI/CLA expertise in ultrasensitive fluorescence detection for screening of pharmaceutical drug interactions, and particular biological screening application needs of another collaborator. That other collaborator, who is from the Tulane University Cancer Center in New Orleans, has temporarily relocated to LSU following hurricane Katrina. NIH has granted us an extension for submittal of this proposal.

Dr. Davis has also begun another research collaboration over the past year with Dr. Hans Blom, also pictured in Figure 9. Dr. Blom has recently returned to the KTH (Kungliga Teknishka Hogskolan—Royal Institute of Technology) in Stockholm, Sweden, after a postdoctoral appointment in Germany. He is presently setting up to perform biophysics experiments using total-internal reflection FCS.

Much of the research conducted in ultrasensitive fluorescence spectroscopy area by CLA also falls within the general area of Chemical Physics and over the past year CLA has continued its involvement with the UT Center in Chemical Physics (http://www.phys.utk.edu/chemphys.htm). Dr. Davis and his group attended the annual three-day workshop in Chemical Physics held at Knoxville in February 2005 and CLA student Mr. David Ball gave the only student presentation at the workshop. This past year, the Chemical Physics Center also awarded a $500 travel grant in support of the sabbatical visit to CLA/UTSI of Professor Ki-Hwan Lee, of Kongju National University, South Korea. The remaining financial support for Professor Lee's one-year sabbatical appointment with CLA was provided by Kongju National University. Professor Lee, who is an established researcher in photophysical and photochemical processes, presented a symposium to CLA titled "Photoluminescent Properties of Porous Silicon and Porous Silicon Carbide, and Synthesis of a Novel Fluorescent Macrocyclic Molecule and Its Fluorescence Behavior." While with CLA, he engaged in collaborative experiments on the characterization of luminescence from nanometer-sized features created by chemical etching of silicon substrates and also fluorescence from DNA oligomers affixed to gold nanoparticles, and he learned about experimental techniques used in single-molecule detection.

Focus Area

Nonequilibrium Fluid Physics

Nuclear Fission Electric Power and Propulsion, AEDC TASK 03-01

UTSI has just started the third year of an on-going project to provide detailed experimental diagnostics and advanced computational simulations of the physical behavior and performance of high-power plasma thrusters for possible applications in nuclear electric propulsion systems, such as envisioned in Project Prometheus. Nuclear Electric Propulsion will provide much larger available electric power for electric propulsion (EP) applications than has been possible in the past. Conventional EP thrusters, such as ion engines, Hall thrusters and arcjets, are well suited for lower power applications, but have not been scaled to the power levels anticipated with fission-based space nuclear electric power systems. These smaller thrusters utilize electrostatic and thermal processes to provide thrust from a plasma propellant. Electromagnetic acceleration of plasmas for propulsion has long been seen as a means to efficient high-specific-impulse propulsion systems. However, development of this class of accelerators has languished because they are efficient only at power levels that were then unavailable.

Two types of electromagnetic thrusters have been suggested: Magnetoplasmadynamic (MPD) thrusters that are steady flow devices, and Pulsed Plasma Accelerators (PPA) that are variants of the Marshall Gun. These devices operate in different magnetic interaction regimes. The MPD operates at relatively small magnetic Reynolds number (Rm) and the PPA operates at large R_m. We are concentrating on the PPA. There is particular interest in the pulsed systems since they can be operated over a wide range of available power by varying the pulse duty cycle to retain efficient high-power operation while controlling average power.

Our approach is to evaluate simulations results from the advanced computational code GEMS with data collected from a laboratory prototype thruster that is designed for accurate diagnostics. MACH2 simulations were utilized to guide the design of this prototype. The thruster consists of a cylindrical centerbody 2-inches in diameter inside of a coaxial 4-inch tube (Figure 1). This tube is divided into a 2-inch upstream section and a 5-inch downstream section by a quartz insulating ring. The ring has sputtered metal strips connecting the two sections of the tube which, when vaporized by the ignition power supply, provides the plasma propellant that triggers and then is driven by the main power supply. The main power source, a 17.5 µF 40 kV capacitor charged with a 30 kv power supply, provides a maximum energy storage of almost 8 kJ and, with the calculated discharge time of 10 µsec, an average power of nearly 800 megawatts.

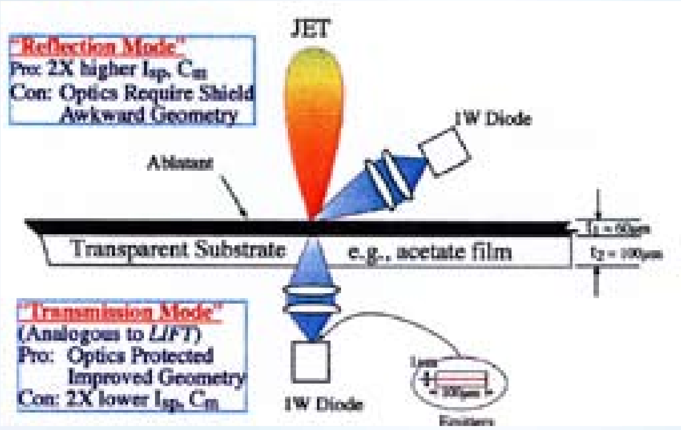
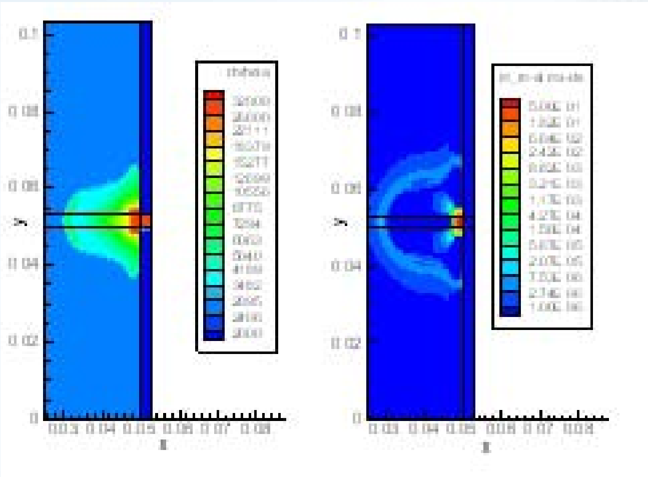


Figure 1. Schematic diagram of the µ-LPT illustrating the "reflection" and "transmission" modes.

The thruster has been fabricated and installed in a vacuum chamber fabricated from stainless steel tubing and plate. The plasma discharges through a section of vacuum chamber with flat quartz windows that are used for interferometric, photographic, and spectroscopic measurements. Initial high-speed photography has documented successful firing of the thruster. Diagnostics to obtain electron number density downstream of the exit plane and estimates of exhaust velocity have been installed. Rogowski coils have been installed to monitor the current in the trigger and main capacitor circuits. Tests with B-dot probes are planned to help characterize the development of the current sheet inside of the thruster. B-dot probes have been fabricated, assembled, and installed in the thruster. The b-dot probes will be connected to high-speed, 20 MHz data acquisition channels. After obtaining B-dot data, spectroscopic measurements are planned. Results from these tests are expected to be available in the near future for comparison with computer simulation results.

Recent MACH2 simulations have focused on the evolution of the fuse plasma utilized to trigger the main thruster capacitor (Figure 2). The main body of the foil expands slightly from the initial pressure during the first microsecond. A puff of plasma with a velocity of 20 to 30 km/sec crosses the annulus in less than a microsecond and has the potential to trigger the main discharge. High-speed photography and Rogowski coil data from the experiment indicate that the main capacitor is discharging roughly 200 nanoseconds to 300 nanoseconds after initiation of the trigger capacitor. This suggests relatively good agreement between the simulations and preliminary experimental data. MACH2 simulations of the complete thruster configuration are now underway and comparisons with experimental results are expected to be ready for the Joint Propulsion Conference.

Figure 2



MACH2 is an ALE code, based on CFD methods two decades old. Its architecture does not lend itself to modern gridding methods or parallel computation. Therefore, we are extending the electromagnetics capability of the MHD version of the three-dimensional General Equations Mesh Solver (GEMS) code that has been previously used to simulate a steady-state MHD generator to provide a time-accurate simulation capability that incorporates modern computational methods. To date, this extension has focused on identifying methods for solving coupled electromagnetic/fluid dynamic problems in regions where the MHD approximation fails, most specifically, in vacuum regions where the displacement current is significant. We have formulated a solution algorithm that does not depend upon the MHD approximation, but solves the complete Maxwell equations at resource levels that appear to be similar to those associated with the magnetic induction equation. Testing of the method will begin after completion of some major changes in GEMS, including improved data structures and parallel distribution procedures for problems like the present that involve multiple types of physics. These changes should be complete in the near future. Numerical solutions of the present formulation will then be implemented to verify the methods

UTSI is participating with AEDC in a Trilateral Alliance (AEDC, MSFC, ORNL) project to develop optimization tools for NEP systems. For example, UTSI is developing a computer code that predicts electric propulsion performance that will be incorporated into the optimization tools.

Principles Investigators: Dr. Trevor Moeller
Sponsor: Arnold Engineering Development Center

Vertical EP Thrust Stand for 12V Vacuum Chamber, AEDC TASK 03-01

A vertical Electric Propulsion thrust stand development effort was added to AEDC Task Order 03-01 this year. The primary objective of this research and development effort is to develop a vertical thrust stand for use in the AEDC 12V chamber. This new thrust stand will provide AEDC customers with thrust measurements on various electric propulsion thrusters ranging in size from 1 kW to 50 kW. To address the significant research and development issues associated with this program, a two-year effort at UTSI is planned. Specific objectives for the first year are: 1) evaluate existing thrust stand designs to determine the features/techniques that provide the most promise for a vertical thrust stand for the 12V chamber; 2) develop a vertical thrust stand design; and 3) prepare engineering drawings. Specific objectives for the second year include: 4) fabricate and assemble the vertical thrust stand; 5) perform preliminary tests; and 6) provide AEDC with a detailed plan to incorporate a vertical thrust stand installation into the AEDC 12V.

Principal Investigator: Dr. Trevor Moeller
Sponsor: Arnold Engineering Development Center

MACH2 Simulations of a Laser Ablation Thruster

Introduction

Electric propulsion (EP) systems are known to have specific impulses that far exceed those of conventional chemical rockets. The reduced propellant expenditure associated with EP has driven the development of commercially available EP devices for satellites. Several, including resistojets, arcjets, Hall thrusters, and ion engines, have reached flight-ready status. These EP systems are predominately used for drag make up and/or orbit correction.

In recent years, interest in the reduction of satellite size has grown. The main benefit of low-mass satellites (1-20 kg) is reduced launch costs. As satellite mass is reduced, the mass and power budgets for the propulsion systems is lowered accordingly. The kilowatt power level available on large satellites is being reduced to less than 100 Watts for low-mass satellites. Since the mass and power requirements of flight-ready satellite propulsion systems have precluded their use on small satellites, microsatellite propulsion systems must be developed.

Reduction of propulsion system size is not trivial. As physical size is reduced, the thrust efficiency of electric propulsion devices tends to drop off significantly. Miniature electric propulsion devices have been studied, including Hall thrusters, microwave heated thermal thrusters [4], and pulsed power thrusters. Most of these EP devices operate in the 40 to 100 Watt power range.

Computer simulations are widely used, along with experimental test results, to gain a better understanding of the physical mechanisms that take place in electric propulsion thrusters. EP thrusters involve highly coupled interactions between electromagnetics, fluid and plasma dynamics, and radiation. The proposed multi-year research effort will address research issues associated with the physical mechanisms that occur in the micro-Laser Ablation Plasma Thruster (μ-LPT) being developed by Photonic Associates. This will be accomplished via computer simulations using the magnetohydrodynamic (MHD) code, MACH2.

Description of μ-LPT

The microthruster, developed by Phipps and Luke, operates by focusing fiber-coupled semiconductor diode lasers on a target to produce a small jet of ablated material. The μ-LPT has two modes of operation, a "Transmission Mode" and a "Reflection Mode." In the transmission mode, the laser beam passes through a transparent substrate film from the back side. A layer of absorbing material on the front surface ablates away from the laser. In the reflection mode, the laser impinges incident on the target material, and ablated material reflects from the surface. In the reflection mode the optics can become coated with material; operation in the transmission mode alleviates this problem. In both the reflection and transmission modes, the material ablated by the laser pulse leaves a crater in the surface of the solid propellant and thermally expands out from the crater to form thrust. It is interesting to note that when a continuous laser beam is utilized, the ablated material forms a channel in the surface of the solid propellant that produces thrust that is vectored in the direction of the channel.

Experimental data for the μ-LPT operating in both modes is available in the literature. A summary of the performance goals for the μ-LPT can be seen in Table 1. Of particular interest for comparison with computer simulations are thrust, the laser momentum coupling coefficient (defined as the impulse produced per unit energy of laser light), and specific ablation energy (defined as the energy of the laser light required to ablate unit mass of the target material).

Table 1. μ-LPT Performance Goals

Laser Wavelength	920 nm	[Demonstrated]
Laser Average Power (max)	2 W	[Demonstrated]
Coupling Coefficient Cm	60 micronewton/W	[Demonstrated]
Spec. Ablation Energy Q*	100 kJ/g	[Demonstrated]
Specific Impulse Isp	550 seconds	[Demonstrated]
Target Spot Size	70 micrometers	[Demonstrated]
Pulsewidth	2 ms typical	[Demonstrated]
Minimum Impulse Bit	50 micro dyn-s	[Demonstrated- see Gage]
Design Thrust	75 micronewton	[Demonstrated]
Lifetime Impulse	1000 newton-s	[Projected]
Ablation Mass	0.3 kg	[Projected]
Thruster Mass	0.8 kg	[Projected]

Plasma Simulation Codes

Plasma simulation codes can be broken into two general categories: particle simulation codes, such as Direct Simulation Monte Carlo (DSMC), and magnetohydrodynamic (MHD) codes. In the former, the heavy particles are tracked individually and the electrons are typically treated as a fluid. Monte Carlo reaction models are typically utilized to describe particle interactions, and all individual particles are moved based on the electric and magnetic fields that act upon them. Particle simulation codes are inherently very numerically intensive.

MHD codes treat the plasma as a fluid and adopt the assumptions that displacement current is small compared to conduction current, and the former is neglected. MHD codes are typically less numerically intensive than their particle-simulation counterparts. However, the assumptions associated with MHD codes make it difficult for them to be utilized for low-density plasmas and systems that contain vacuum/plasma interfaces. Therefore, particle simulations tend to be utilized to simulate problems with low-density plasmas, and MHD simulations tend to be used for higher density applications. In some situations, high-density regions are accompanied by vacuum regions that also must be modeled. The vacuum region precludes the use of most MHD codes and forces the use of particle simulation codes that require extensive computational resources to properly model the high-density regions of the problem.

Approach

MACH2 is a time-dependent MHD computer code that can be run in the axisymmetric mode. We have used the AFRL developed MACH2 code for nearly a decade to simulate a variety of plasma devices, including plasma opening switches, cableguns, ablative pulsed plasma thrusters, electrothermal chemical (ETC) guns, explosively formed fuses, MHD generators and plasma radiation sources. During these studies MACH2 was modified to account for some of the shortcomings of conventional MHD codes. The μ-LPT has plasma densities similar to that realized in the cablegun simulations mentioned above. Therefore, we believe that MACH2 will provide reliable simulations of the μ-LPT.

The objective of this work is to utilize MACH2 to simulate the laser ablation process in the μ-LPT and gain a better understanding of the detailed physical processes occurring in the high density plasma that is blown out of the solid propellant surface to generate thrust. Relatively extensive experimental performance data, available in the open literature, will be utilized for comparison with simulation results. It is of interest to note that extensive modeling of this thruster has been performed using the DSMC code MONACO. This DSMC modeling focused on the lower density plasma in the expansion of the plume. The proposed MACH2 simulations may provide a means of verifying the upstream boundary conditions utilized in these particle simulations.

To properly model the μ-LPT, a laser ablation model must be incorporated into MACH2. MACH2 has built-in laser absorption models that have been used to model successfully laser/materials interactions. For example, the laser absorption models were successfully utilized to study the plasma expansion that results when a laser pulse is focused on an aluminum surface. The proposed μ-LPT simulations will incorporate ablation models similar to those used and will be concentrated on the propellant ablation process, the evolution of the resulting crater, and the expansion of the ablated material from the propellant surface. This modeling effort will require the development of a property set for PVC, utilized as the propellant in the μ-LPT experiments. A hydrogenic approximation that is expressed in terms of partition functions will be utilized to establish thermodynamic properties. Ultimately, calculated values for thrust and the specific ablation energy will be compared with experimental test results in the open literature.

The upgraded MACH2 model will be developed and utilized to perform preliminary simulations of the μ-LPT during the first year of the proposed work. Comparisons with experimental results will also be made. During the second year of the proposed effort, the laser ablation model will be refined, as needed, based on the results of simulation performed in the first year's effort. With the insight gained, it is anticipated that system improvements will be proposed and modeled during the second year of the proposed work. The effort in subsequent years will highly depend on the results of the first two years, and on the possibility of expanded funding through the leveraging of funds.

Principal Investigator: Dr. Trevor Moeller
Sponsor: Hankuk Aviation University, South Korea

Hypersonic Vehicle Electric Power System (HVEPS)

In 2002-2003, CLA led the UTSI research program to help develop MHD generators for a new generation of high-speed Air Force vehicles. The generator would provide short bursts of high power electrical energy to supply laser or other beamed-energy weapon systems. UTSI was part of a team led by General Atomics. UTSI's effort focused on computational modeling of the MHD generator and sub-scale tests of MHD generators to validate design codes. A gap in funding during the second half of FY03 and the first half of FY04 resulted in decreased activities during this time. However, FY04 funding has been received and FY05 funding has been confirmed. During the last year, efforts to increase flow rates in the UTSI combustion test facility commenced. In the following year, efforts will be made to increase electrical conductivity of the flow and prepare for the receipt of an MHD generator channel for testing.

The HVEPS effort planned for the fiscal year includes completing facility upgrades to allow for (1) increased flow rates and higher electrical conductivities required for future MHD generator testing, (2) combustion facility flow field characterization, (3) and facility preparation for the installation of a subscale MHD generator with superconducting magnet. In addition to this experimental effort, the MHD version of the GEMS code will be further developed to allow the modeling of MHD generators.

Principal Investigator: Dr. Trevor Moeller
Sponsor: US Air Force

Focus Area

Laser Ignition

Laser-Induced Ignition of Rocket Engines

CFD Research Corporation (CFDRC) and UTSI/CLA were awarded a Small Business Innovative Research (SBIR) contract by the Air Force Research Laboratory to perform laser-induced ignition studies of a rocket engine. This collaboration that was initiated in the past year resulted in a proposal and contract award in this reporting period. The objectives of the Phase I award are to perform both laser-induced ignition of a methane/ gaseous oxygen engine and laser-induced breakdown spectroscopy (LIBS) of the fuel/oxidizer mixture. LIBS was proposed as a method to satisfy the need for situ measurements of the equivalence or fuel/oxidizer ratios of the mixing regions of the methane and oxygen. Additionally, LIBS detection of trace quantities of metallic elements will be evaluated as an indicator of rocket engine erosion or failure.

Shown in Figure 1 is the research rocket engine that has been provided to CLA by CFDRC. The Nd: YAG laser will be used as the LIBS excitation source, and fiber-optical coupling with spectrometric detection will be used for spectral observation. Calibrations and verification measurements will be performed using the flat-flame burner shown in Figure 2.

Principal Investigators: Dr. James W. L. Lewis, Dr. Ying Ling Chen, and Mr. Jim Hornkohl
Sponsor: Air Force Research Laboratory

Figure 1

Figure 2

Laser-Initiated High Energy Explosives

CLA, in collaboration with a Huntsville, AL company, MPG, Inc., has submitted to British Aerospace Systems a revised proposal and several presentations for the demonstration and development of laser-initiated explosives. The concept and proposed revised program was presented to British Aerospace Systems (BAE)/ Huntsville and the ordnance organization BAE/Kingsport. Based on the results of these efforts, a start date of October-November 2005 is anticipated.

Both the inadvertent and intentional replacement of electric igniters of explosives with radiation sources is common. The objective of this proposed research is to achieve laser-initiated detonation of high-energy explosives at locations and times that are determined by laser irradiation. Essentially, optically shape-charges can be achieved. The proposed program is to demonstrate and verify predictions of small charges of novel explosive materials at UTSI prior to performing larger-scale detonations.

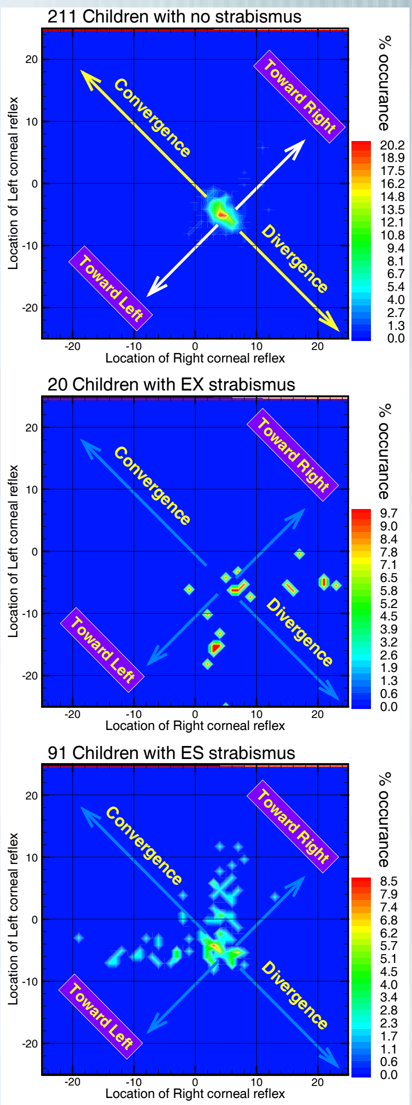
Principal Investigators: Dr. James W. L. Lewis and Dr. Ying Ling Chen
Sponsor: British Aerospace Systems

Focus Area

Biomedical Applications

Ophthalmic Instrumentation in CLA

In the past several years, the CLA vision science team has performed human eye modeling and computer simulations to observe and predict photoscreening images under various instrumentation and eye conditions. The simulation studies have shown that vision screening examinations of ocular health can be performed with dramatically improved accuracy and enhanced information content by using a combination of time-sequence of light sources of various spectral signatures and digital camera detection at two angular locations of the returning spectral radiance. With the emphasis on pediatric vision screening using telemedicine, target ocular measurements and instrumentation in CLA includes:



Analysis of ocular alignment from 300+ patients' photoscreening data. The upper plot shows results of 211 normal cases. The middle and lower plots show the results of the 111 abnormal ocular alignment cases. The 25% intermittent type of strabismus appears to be normal and is missed with this conventional technique.

A. <u>Binocular measurement of refractive status</u>: Based on photorefraction theory, an infrared system has been assembled and is being tested in CLA. A patent application for the system design and analysis algorithm has been prepared for submission by UT Research Foundation.

B. <u>Ocular orientation and convergence</u>: The orientation and convergence of the eyes are determined using the binocular Purkinje reflections and the Hirschberg method. This method was tested using an existing database of over 300 patients with and without strabismus. The figures show the loci of the binocular corneal reflex for normal and strabismic eyes. Using these results, a strabismus detection accuracy of 85% is achieved. To improve the capability of detection of both normal and intermittent strabismus, a dynamic measurement using this method will be employed in the new system.

C. Optical opacities detection: The coaxial red-reflex of retina (Bruckner image) will be used to analyze uniformity and both spectral and spatial radiance distributions of ocular elements.
D. Retinal tumor: An abnormal spectral, or color, distribution in the retinal reflex will be investigated for the detectivity of retinal tumors.
E. Irregular cornea surface: Eccentric infrared illumination in a dark environment is to be used for the detection of this condition. The analysis will use the distortion and the shape of the reflected irradiance distribution of the incident light beam similar to the red-reflex observation through the retinoscope and ophthalmoscope.

This innovative photoscreening system is designed to adapt to examinee's pupil response and retinal reflectance. An STTR proposal of this adaptive photoscreening system that includes all the described functions has been submitted to NIH in collaboration with a Nashville-based company eVision Technologies, and Dr. Sean Donahue, Chief of Pediatric Ophthalmology of Vanderbilt University in Nashville.

Principal Investigators: Dr. Ying Ling Chen and Dr. James W. L. Lewis
Sponsor: Center for Laser Applications

Simulation of Ophthalmic Measurement Using Eye Modeling

In 2003, CLA had performed the first computer simulation of photoscreening images for refractive-error eyes. These results, together with the investigation of the conventional photoscreening technique, were published in a leading optics journal, Optics Express, and caught attention in the vision screening community. During the last year, the research effort in simulating ophthalmic measurement using eye modeling continued. The most significant results include the investigations of ametropic, astigmatic, and keratoconus eyes with retinoscopy and photorefraction techniques. Figure 1 shows a nearsighted eye as viewed by optometrists with a commonly used ophthalmic device, the strip retinoscope (Figure 2). A strip retinoscope projects a bright slit beam onto the examined eye, and when the light sweeps across the pupil of a near-sighted eye, "against motion retinal reflex" is observed (Figure 1). For a far-sighted eye "following motion" would be seen. Until now, the theoretical derivation of retinoscopy in all the optometry and vision science text books use geometric optics to analyze the observation. This analysis and its representation are far too simple because of the complex ocular system of humans. To manage the use of this device, an optometrist needs a sufficient training period and experience in observing human patients. The CLA simulation reveals certain pupil appearances that are observed but have never been mentioned or explained in the text books. Alcon, a company making contact lenses, cataract replacement lenses, and laser surgery instruments, has expressed interested in our simulation work and consultation services of Dr. Chen. In the recent Optical Society of America (OSA) Vision meeting, the ophthalmology department in the University of Arizona indicated interest in utilizing our research work for medical training. The application of this work is promising.

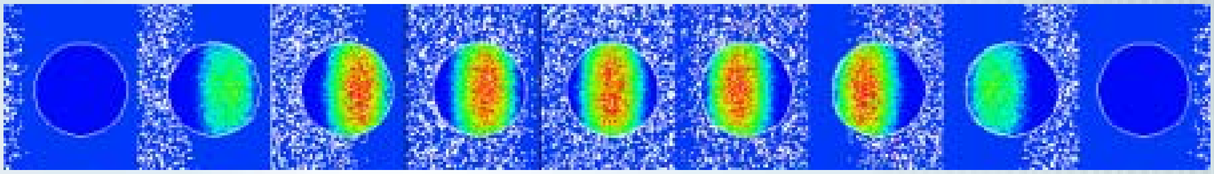


Figure 1. Visualization (computer simulation) of the pupil of a nearsighted eye in front of a strip retinoscope. A sheet beam of light is projected from the hand-held device onto the examinee's eye. When the light sweeps across the pupil (the white shadow in the images), "Against motion retinal reflex" is observed for a nearsighted eye as "Following motion" would be seen in a farsighted eye

Figure 2. Strip retinoscope is a hand-held device commonly used by ophthalmologists and optometrists

Principal Investigators: Dr. Ying Ling Chen and Dr. James W. L. Lewis
Sponsor: Center for Laser Applications

Cornea and Keratoconus (KC) Analysis

Last year, CLA reported our initial research on the abnormal condition of a protruding cornea, or keratoconus (KC) (as shown in Figure 1). These thinned corneal conditions increase the refractive power asymmetrically and result in near-sighted and astigmatic conditions that are very difficult to be corrected with spectacles or regular contact lenses. However, because expensive clinical instruments are required to provide a definite diagnosis, KC cases are often misdiagnosed by examiners as regular refractive errors and suffer poor visual qualities through their lifetimes. It is estimated that more than one per two- thousand suffer from this abnormality, and the prevalence is typically concentrated in young adults. In the past, the treatment was limited primarily to the use of rigid contact lens' to smooth the irregularity and ultimately corneal transplant to achieve near-normal vision. Within the past few years, the use of the insertion of segmented intra-corneal rings has shown promise as a method for achieving vision improvements. Since a treatment method exists to restore visual function, the early detection of KC is desirable, and the incorporation of KC screening in pediatric populations is indicated. It is noted that refractive laser surgery, such as LASIK, on a thinning cornea can result in a bad outcome (and possibly corneal replacement). Therefore, the importance of screening and early detection of KC is desired.

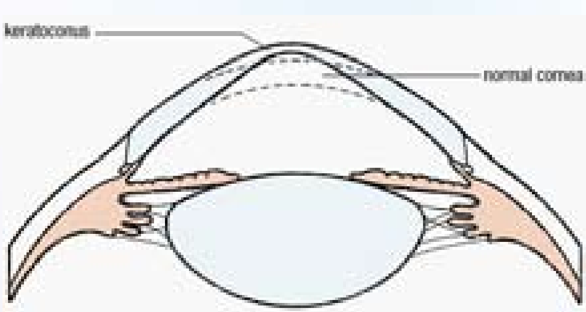
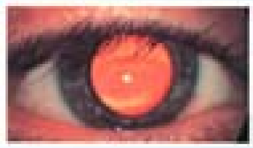


Figure 1. Illustration of keratoconus

To evaluate KC visual impacts, the CLA vision science team has performed theoretical KC eye modeling (as shown in Figure 2). For the first time, the KC cone shape, dimension, and location factors are able to be examined on computer and their impacts on visual performance can be evaluated. A pioneer corneal specialist, Dr. Ming Wang of Wang Vision Institute in Nashville has described this research as "revolutionary".

KC Patient Image



UTSI Computer Simulation

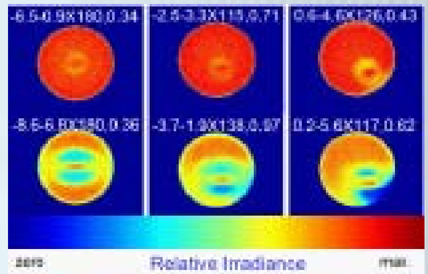


Figure 2. Co-axial retinal-reflex images of a KC patient (left) and simulation of 6 cases of KC eyes (right). The numbers in each image indicate the clinical prescriptions and spectacle-uncorrectable index of each model eye

The CLA KC eye modeling is further applied to the evaluation of KC screening work. The simulation work demonstrates the possibility of using a low-cost infrared device to differentiate KC cases from regular refractive-error eyes (Figure 3). Shown in Fig. 4 are the computed appearances of KC and astigmatic eyes as seen using a common retinoscope. These simulation results were published in 2004 October APS (American Physics Society) and OSA (Optical Society of America) conferences, and they indicate the potential of these computations for medical training purposes. An UK optometrist, Dr. Lynn White, who has been working in public health and KC clinic work in UK and the Caribbean, is greatly interested in the presented research work. Through frequent communication, Dr. White urges the development of a screening prototype in CLA while she actively establishes funding/support for KC screening project in Trinidad/Tobago. The initial clinic trial of the prototype device may be performed in Wang Vision Institute next year.

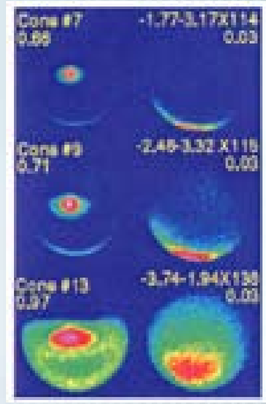
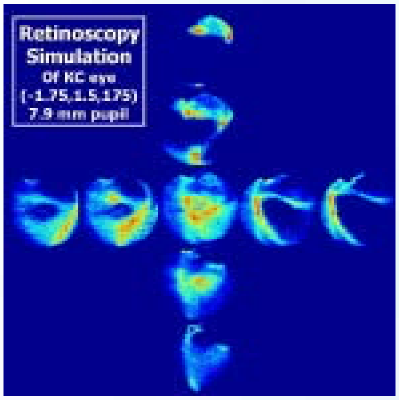


Figure 3. Protorefraction simulation of KC eyes (left) and astigmatic eyes (right)



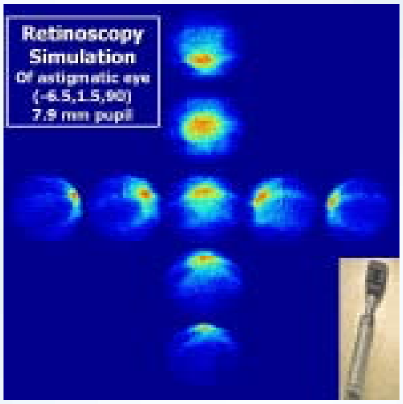


Figure 4. Retinoscope simulation of a KC (left) and a LASIK (right) patients

Principal Investigators: Dr. Ying Ling Chen and Dr. James W. L. Lewis
Sponsor: Center for Laser Applications

Computer Eye Modeling

Computer eye models are used in the design of ophthalmic or visual optics to simulate experiments, to predict the effects of refractive surgery or implants, or to understand quantitatively the role of optical components for various applications. Although many successful eye models are available today, all of these models are constructed for the healthy emmetropic (refractive-error free) adult condition, and average measured dimensions and optical parameters are adopted for all ocular elements. No specific gender, age, or race characteristics associated with any of these published models, even though such differences exist. Further, there is no eye model established to describe parameter variations in the population. The CLA vision science group has studied numerous eye models as well as the statistical distribution regarding the ocular parameter variations in large populations. Such information is particularly important in applications related to public health. In this past year, computer eye modeling efforts in CLA were directed in two innovative directions: 1). the individual tailored (customized) modeling, and 2). the modeling that describes statistical variations of large populations according to geographic / ethnic factors, gender, and age.

1). Efforts have been made in obtaining measured ocular data of human subjects including corneal topography, wavefront aberration, ultrasound A-Scan, and the de-coding of these data exported from medical instruments. The Wang Vision Institute of Nashville has supported this effort by providing data and clinical consulting. The customized model eye is constructed using a) the individual's corneal elevation map, b) the wavefront aberration map of the eye, c) the manifest refractive error measurement result, and d) the ultrasound A-Scan data that provide distances between surfaces of all ocular elements. Abnormalities such as cataract, corneal scars, and floaters, and physical changes such as tear layer changes, pupil size change, cataract surgery, and corneal surgery for refractive error or implant can be simulated with the eye model and therefore, can predict the impact on the vision of the individual. Currently, we have obtained three complete sets of individual data from the Wang Vision Institute. At least 4 levels of customized eye models, from less to most complicated, will be constructed in CLA this coming year and tested in the Vision Institute. Some potential applications of this work are:

a) Application in Customized Laser Corneal Surgery: with collaboration with Wang Vision Institute
b) Application in the instrumentation for keratoconus detection: CLA is currently modeling customized eyes for various degrees of keratoconus patients and LASIK patients with near-sightedness, far-sightedness, and astigmatism. Simulation results for KC screening are most promising. CLA has been contacted by an ocular professional in the United Kingdom regarding keratoconus screening. CLA has been invited to perform screening tests in the comparatively closed genetic population of Trinidad/Tobago where this ocular abnormality is anticipated to be an order of magnitude more frequent than the U.S. A prototype of a kerataconus screening device is expected to be assembled by the end of 2005, and tests on human subjects will be performed in the Wang Vision Institute.
c) Cyber Eye Bank for computer clinical trials: CLA has been preparing for an international, multi-center program that makes use of customized eye modeling. This project will collect data of individual eyes from various corneal institutions where most required data for customized eye modeling are routinely acquired. These data will be sent through internet to CLA for constructing model eyes and then form a computer optical eye bank. This eye bank could be used to test the optical design of ophthalmic and visual devices on computer without risk of testing on real human eyes. The collaboration will include:

- Wang Vision Institute, Nashville, TN
- Loma Linda University, Dept. Ophthalmology, San Bernardino, CA
- Universal Vision Biotechnology Co., LTD Taiwan

  Phase I, the feasibility evaluation, will be performed with Wang Vision Institute by the end of 2005.

2). The statistical distribution of ocular parameters of various geographic / ethic factors, gender, age, and refractive error has been collected and analyzed from published literature in the past year. The attempt of constructing model eyes with consideration of refractive errors, the most prevalent vision defect in population, continues. The correlation between refractive errors of the eyes and ocular parameters (the ocular axial lengths, cornea curvatures, and intraocular powers in particular) has been investigating. The correlations and the distribution of these variables have been adopted into the modeling for the first time. As an example, the following figures show the distribution of one of these ocular parameters, ocular axial length, in a collection of thousands measured data from seventeen published journal papers that were used in CLA eye modeling. The gray area in the figure describes the most probable distribution of ocular length in adults throughout the world. Females tend to have a distribution with shorter ocular length (not shown in this figure) that is slightly shifted toward lower left of this gray band. There is no strong evidence of race dependence of ocular length. The correlation of ocular length with refractive error is universally strong. The consideration of population distributions is easily incorporated into the analysis method to enable evaluation of the dependence of two arbitrary ocular parameters. Instrument measurement errors that result from population variations can be evaluated, and this ability provides the novel opportunity for virtual clinical trails.

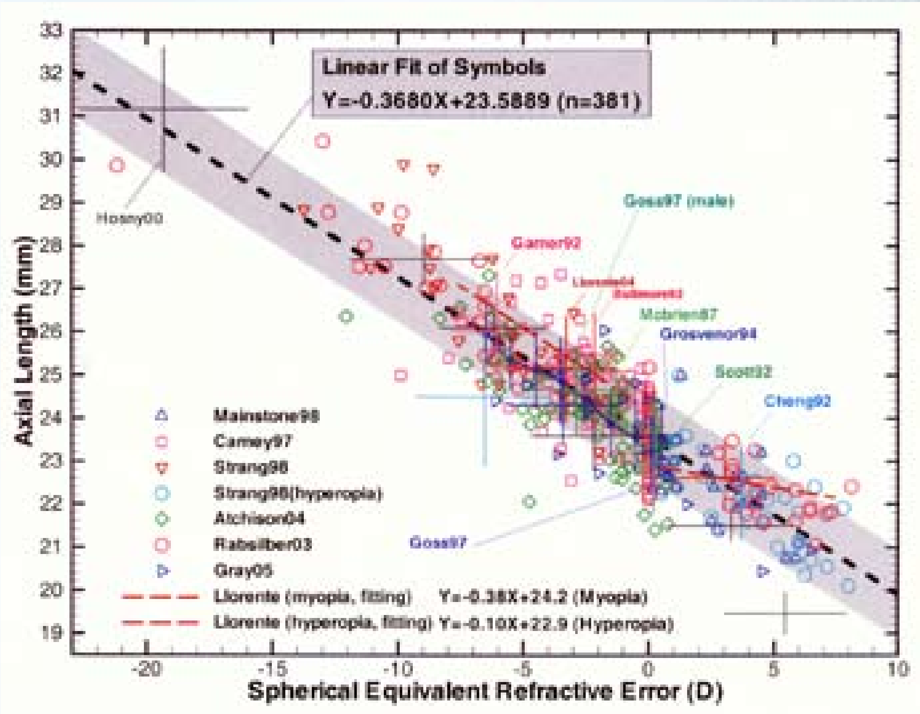


Figure 1. Measured data from 17 papers around the world shows the correlation between ocular length (Y-axis) and refractive error (X-axis)

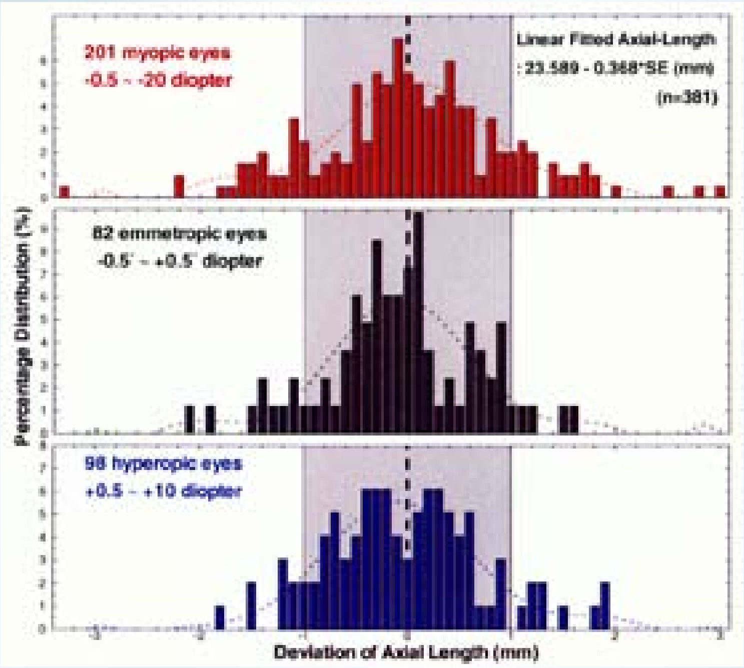


Figure 2. Distribution functions of eye length for near-sighted eyes (upper), normal eyes (middle), and far-sighted eyes (lower) alone the CLA predicted line (gray band in figure above)

Principal Investigators: Dr. Ying Ling Chen and Dr. James W. L. Lewis
Sponsor: Center for Laser Applications

Imaging Blood Flow in Dental Pulp Tissue

During the past year, the work continued on biomedical applications of laser-material interactions to image the blood distribution inside teeth. This work included successful completion of Pavlina Pike's dissertation on the subject matter. And it further included collaboration with Carolinas Medical Center, Erythema Diagnostics, and The University of North Carolina at Charlotte. The interaction of the ultra-short laser pulses with the material is thermally confined, i.e. the thermal diffusion takes place within the irradiated area. Therefore, the femto-second laser pulses create minimal thermal and mechanical damage to the surrounding area during laser imaging, drilling and/or ablation. This is important, because generation of micro-cracks of several tens of microns in the enamel would result in new carious attacks and thus defeat the treatment process. The non-destructive pressure wave generated inside the tissue when the optical absorption induces a resonance will overcome the limitations of conventional ultrasonic imaging inside teeth. Furthermore, there are currently no diagnostic tools available that may image soft tissue health inside teeth. The focus of the presented work is the calculation of the temperature rise due to the interaction of ultra-short laser pulses with dental tissue. Efforts are also reported of experimental investigations of the temperature.

The heat source is modeled as a Gaussian distribution in space. Since femto-second pulses are much shorter than the time to reach thermal equilibrium (approx 1ps), it is reasonable to approximate the time component of the source function can be approximated with a Dirac delta distribution. The solution of the heat equation is of the kind:

$$T = T_0 + \frac{4J}{\rho c \sqrt{\pi}\ (1+\tau)} \exp\left[-\frac{2r^2}{\omega^2 (1+\tau)}\right] \qquad \text{Equ 1}$$

where J is the laser fluence [J/cm2], ρ is the mass density, ω is the beam waist [cm], c is the heat capacity [J/g.K] and τ is the scaled time [s]. Presented on Fig. 1 is the numerical calculation of the temperature rise from 40 ms pulse train of 70 fs pulses. The experimental measurement of the temperature as a result of the same pulse train is shown on Fig. 2.

Analytical solution to the heat equation along with experimental result for the temperature increase in dental porcelain was presented. The calculated temperature rise can be used to predict the pressure amplitudes of the generated sound waves in the tooth based on the absorption of the laser light. These sound waves are then used to create the image of the tissue of interest.

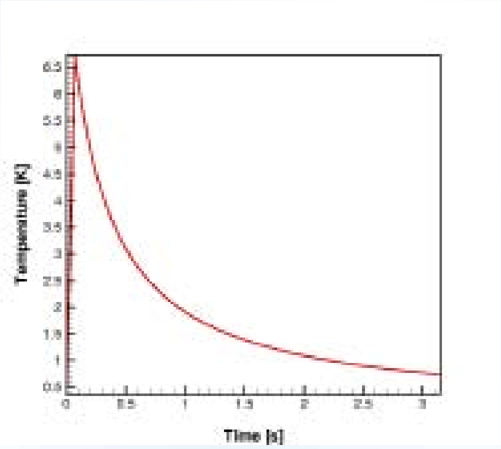


Figure 1

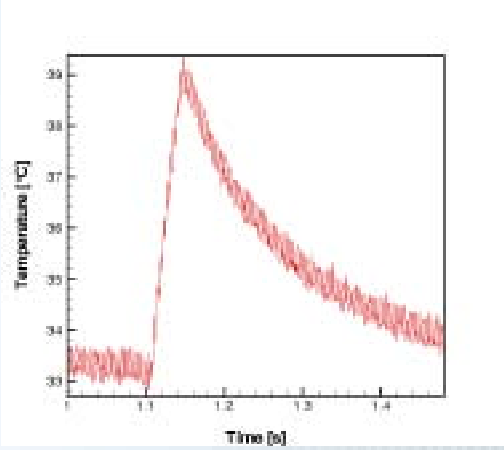


Figure 2

Principal Investigator: Dr. Chris Parigger
Sponsor: Center for Laser Applications

Future Directions for the Center for Laser Applications

Since the hire of Professor Hofmeister as Director, the Center for Laser Applications is reviewing research directions to determine the most fruitful path to increase funded research and education for the center. While it would be desirable to lay out a detailed plan and particular path, the necessities of external funding dictate that CLA be flexible in its approach to research. Any sizable research effort will depend on the talents of the principals involved, and we must build on our areas of expertise with existing staff. Within each area there are numerous paths that an investigator can follow. In order to build a sustained research program these paths must be carefully chosen to coincide with the needs of sponsors. Particularly, the national investment in nanotechnology has accelerated the pace of discovery. Trends that were clear a few years ago have evaporated, replaced by the latest-and-greatest challenges. Our goal is a nationally recognized research program where our research leads to significant discovery. Because of our size, these areas will necessarily be "niche" areas.

The structure of funded research programs has also changed. Sponsors now realize the need for multidisciplinary teams on research projects in the nano and bio areas. The breadth of knowledge require to accomplish a particular goal necessitates this approach. Additionally, funding decisions for large grants are increasingly focused on politics. Like it or not, there is a shift to "congressional interest" funding, emphasizing geography and influence over science. For these two reasons, teaming must play a major role in future research directions.

John Peterson, President of the University of Tennessee since 2004, delivered a plan for UTSI to the Chairs of the Senate and House Education Committees of the Tennessee General Assembly on December 31, 2004. This report stated that UTSI should focus on mission-oriented applied research and development in two areas: materials science, including laser applications, and aerospace science, including propulsion. The report also stated that this research and education effort should be "closely linked with efforts at regional centers and universities such as Arnold Engineering and Development Center, Oak Ridge National Laboratory, NASA Marshall Space Flight Center, UT Knoxville, UT Chattanooga, Tennessee Tech and Vanderbilt University." Given the stated directions of the legislature and the UT administration, the strong national emphasis on nanotechnology and the investment of the Department of Energy in ORNL's Center for Nanomaterials Science (CNMS), it is natural that UTSI pursue regional collaborations in areas of current strength: single-molecule detection and photonic processing of materials.

In the later arena we have submitted plans for the Joint Center for Advanced Photonic Processing of Materials which will involve UTSI, ORNL and University of Tennessee Knoxville. This effort will encompass the work with Laser Induced Surface Improvement and laser surface modification. New initiatives in this area will include three dimensional laser additive fabrication, Prof. Hofmeister's area of expertise. For example, there is a real need for fabrication strategies for high temperature nozzles for hypersonic work at AEDC and MSFC. Laser based fabrication of refractory materials is a targeted future area for CLA. In addition, the Joint Center for Advanced Photonic Processing of Materials will examine areas of nanotechnology that can be implemented with laser processing.

Emphasis in the former area, single-molecule detection, will be increased. This area combines Dr. Davis' national expertise in single-molecule fluorescence with the use of active nanostructures. A recent (November 29, 2005) NIRT submission to NSF underlines this commitment. The team for that proposal included investigators from UTK, ORNL and Vanderbilt University. CLA plans to invest in multiphoton, femtosecond materials processing for nanofluidic devices to support this effort, and will install clean space in the laboratory to facilitate this work.

The Center for Laser Applications is well positioned to continue with success in the coming years. The infusion of new faculty, post doctoral fellows and graduate students will increase our visibility and success in the coming years.

Visitors to the Laboratory FY 04-05

Small Business Leaders
UTSI's Low Cost Carbon Fiber Technology R&D

Dick Austin - Former USTI student

Ray Capp -
President of the Nashville Technology Council

Paula Roberts - Administrator,
Tennessee Small Business Development Center

Dean Peterson - Nashville Export Assistance Center,
U.S. Department of Commerce

Zlatica Ferreire -
International Trade Center and Tennessee Small Business Development

Brad Herker -
U.S. Department of Commerce, Nashville

Congressional Staff Visit
Mr. David Burns, Military Legislative Assistant (MLA), CM Tanner (TN-8)
Mr. Derek Horne, Legislative Correspondent, Sen Alexander(TN)
Mr. Richard (Dick) Tracey, MLA, CM Jim Cooper (TN-5)
Lt Col Jill Stiglich, SAF/LL
Lt Col Linda Richardson, SAF/LL
Col Vince Albert, AEDC/CV
Mr. Andy Roake, AEDC/PA
1Lt J.T. Stamm, AEDC/PA
Ms. Lori McKee, Field Representative, CM Davis (TN-4)
Mr. Kerry Steelman, Field Representative, CM Wamp (TN-3)

<u>Tennessee Department of Tourist Development</u>
Mona Swann, Citizens Community Branch
Ava Lynch, Southern Tennessee Medical Center
John Payne, Tennessee Economics & Community Development Agency
Carol Fulmer, Interlocal Solid Waste Authority

Robert J. Connor - Executive Director,
Air Force Material Command, Wright-Patterson AFB, Ohio

Dr. Jack Britt
Dr. Bob Levy
Dr. Dan Stewart

<u>Coffee Educators Visit UTSI</u>
Dan Brigman, Director of Coffee County Schools
Kenny Casteel, Assistant Director
Charlotte Philpott, Director of Technology
Lana Ray, Technology Integration and Technology Specialist

<u>Marshall Space Flight Center's Propulsion Research Center</u>
NASA:
Claude Irvine
Thomas Markusic
Kurt Polzin
Michael Lapointe
Accompanied by:
Albert Dawbarn, AEDC
Hunter Vaughn, AEDC

<u>Franklin County Leadership</u>
30 high school students and adults from different areas such as Nissan, AEDC, and the county.

Dr. Way Kuo
Dr. Luther Wilhelm
Dr. Wayne Davis

<u>National Space and Science Technology Center</u>
Bill Hicks, Chief Operating Officer
Gerald Smith, Executive Director
Accompanied by: Alex Money and Dr. Caruthers

<u>AEDC</u>
Brigadier General David Stringer,
Commander, AEDC
Dr. David Elrod

Dr. Arlene Garrison, UTK
Dr. Frank Harris, Oak Ridge Liason

Awarded Grants and Contracts

Grants and Contracts in Fiscal Year 2004-2005

R02-4007010
The Center for Laser Applications
State of Tennessee, Dr. J.W.L. Lewis
$849,500
July 2004 - June 2005

R02-4318029
"Maximum-Likelihood Multi-Channel Fluorescence Microscopy"
National Institutes of Health grant 1R03EB004586-01A1, Dr. L.M. Davis
$150,300
August 05 - Jully 07

R02-4325022
"Nuclear Fission Electrical Power and Propulsion"
AEDC, Dr. Moeller
$150,000
February 2005 - April 2006

Continued Grants and Contracts in Fiscal Year 2003-2004

R02-4007009
The Center for Laser Applications
State of Tennessee, Dr. J.W.L. Lewis
$833,800
July 2004 - June 2005

R02-4317021
"High Energy Density Coating of High Temperature Advanced Materials"
DOE, Dr. Dahotre
$150,000
September 2001 - December 2004

R02-4357067
Research Grant with Ford Motor, Dr. Dahotre
$150,000
May 1999 - December 2004

R02-4317022
"Evaluations of Erosive Response of Ceramic Coated Steel Substrates"
Caterpillar, Inc." Dr. Dahotre
$14,230
December 2002 - December 2004

R02-4317023 and R02-4317024
"High Speed Laser Synthesis of Amorphous Surface Structures"
National Science Foundation: U.S. – India Cooperative Research
$41,593, Dr. Dahotre
April 2004 - March 2007

R02-4331005
"LISI Phase I: Prototype Production Facility Development"
AEDC, Dr. Keefer and Dr. Dahotre
$2,568,000
August 2002 - February 2006

R02-4348020
"Hypersonic Vehicle Electric Power System Technology Program"
General Atomics, Dr. Moeller
$750,000
March 2004 - September 2006

R02-4348021
Hankuk Aviation University
Microthruster Project
$10,000, Dr. Moeller
February 2005 - February 2007

R02-4318024
"Polarization Multiplexer for Confocal Time-Resolved Fluorescence Polarization Measurements"
Abbott Laboratories
$7,907, Dr. Davis
May 2003 - August 2004

R02-4318023
"Model and Simulation of Single-Molecule Forster Resonance Energy Transfer (sm-FRET)"
Abbott Laboratories
$15,433, Dr. Davis
May 2003 - October 2004

R02-4318022
"Comparison of Data Analysis Methods for 2-Color Experiments for Pharmaceutical Drug Binding"
Abbott Laboratories
$15,433, Dr. Davis
May 2003 - October 2004

R02-4318025
"Single-Molecule Imaging"
Abbott Laboratories
$5,000, Dr. Davis
December 2003 - December 2004

R02-4318026
"Capillary System for Fluorescence Fluctuation Spectroscopy Applications to Pharmaceutical Drug Discovery Research"
Abbott Laboratories, Dr. L.M. Davis
$33,000
November 2004 - November 2005

R02-4318027
"Scanning Fluorescence Fluctuation Spectroscopy"
Abbott Laboratories, Dr. L.M. Davis
$24,600
November 04 - November 05

R02-4318028
"Scanning Fluorescence Fluctuation Spectroscopy Data Acquisition"
Abbott Laboratories, Dr. L.M. Davis
$8,000
October 04 - October 05

"Small Center in Chemical Physics"
UT Knoxville, Dr. L.M. Davis is a faculty collaborator
$70,000
July 04 - June 05
In FY2004-5, the center provided travel funds for Drs. L.M. Davis and G. Shen and CLA student Mr. D.A. Ball to attend a 3-day symposium in Knoxville, and also a $500 travel grant to support the sabbatical appointment of CLA visiting professor K.H. Lee.

Students

Student Thesis/Dissertation

Pavlina Jeleva, Ph.D., Physics, May 2005
"Photo-Acoustic Analysis of Dental Materials and Tissue"

Graduate Students in FY 2004-2005

Sandip Harimkar, Ph.D.	Materials Science	Dr. Dahotre
Nikki Brown, M.S.,	Materials Science	Dr. Dahotre
Greg Ingleman, Ph.D.	Materials Science	Dr. Dahotre
Daniel Rooney, M.S.	Engineering Science	Dr. Moeller
Karen Norton, M.S.	Physics	Dr. Davis
David Ball, M.S.	Physics	Dr. Davis
Kevin Baker, M.S.	Physics	Dr. Lewis
Konstantin Kolokolnikov, M.S.	Engineering Science	Dr. Keefer
Bo Tan, M.S.	Physics	Dr. J. Lewis
Anil Kumar Kurella	Materials Science	Dr. Dahotre
Pavlina Jeleva, Ph.D.	Physics	Dr. Parigger

Post Doctoral Fellows

S. Nayak, Summer-Fall 2004
R. Singh, Spring 2004 – Fall 2005
Paul Shen, Fall 2004 – present

New Students Recruited

Sonya Nelsen, M.S.	Engineering Science	Dr. Moeller
Matt Dackman, M.S.	Physics	Dr. Moeller
Lei Shi, M.S.	Physics	Dr. Chen
Anoop Samant, Ph.D.	Materials Science	Dr. Dahotre

Awards, Honors and Invitations

Trevor Moeller

Dr. Moeller served as a guest editor of a special issue of the IEEE Transactions on Plasma Science. This special issue will include selected oral contributed papers from ICOPS 2004.

Nominated to serve on the Plasma Science Application Committee of the IEEE Nuclear and Plasma Science Society. This committee is responsible for publication of the IEEE Transactions on Plasma Science and organization of the International Conference on Plasma Science. Elections for this committee are scheduled for the fall of 2005.

Narendra B. Dahotre

• Elected to the Class of 2004 Follows of ASM International

• Member of the Editorial Board, International Journal of Microstructure and Materials Properties, a quarterly technical refereed journal by Interscience, 2004-Present.

• Member of the International Advisory Board, Journal of Nanoscience and Nanotechnology, a monthly technical refereed journal by American Scientific Publishers, 2002-Present.

• Member of the International Advisory Board, Advanced Engineering Materials, a monthly technical refereed journal by Wiley-VCH, January 2001-Present.

• Member of the Editorial Board, Materials and Manufacturing Processes, a monthly technical refereed journal by Marcel Dekker, 2000-Present.

• Visited Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur (IIT-KGP), India, December 1-31, 2004 under the joint project, "High Speed Laser Synthesis of Amorphous Surface Structures", funded by NSF and DST, 2004-2007.

• Co-Chairman (2003 - 2005), Surface Engineering Committee, under Materials Processing and Manufacturing Division (MPMD) at the Minerals, Metals and Materials Society (TMS) of AIME.

• Guest Editor to the Journal of Materials Engineering and Performance, Vol. 13, No. August 2004, for the topic of Surface Engineering.

• Special Topic Advisor/Editor to the Journal of Mineral, Metals and Materials Society (JOM), on Nanomaterials and Surfaces, issue of October 2004.

• Special Topic Advisor/Editor to the Journal of Mineral, Metals and Materials Society (JOM), on Surface Science at the Nanometer Scale, issue of January 2004.

• Technical Reviewer to the Following Journals

* Materials & Manufacturing Processes, Marcel Dekker, Inc.
* Metallurgical and Material Transactions A, The Metallurgical Society (TMS) of AIME and American Society for Materials (ASM) International.
* Surface Coatings and Technology, Elsevier Science Publishing Co., Inc.
* Journal of Materials Engineering and Performance, American Society for Materials (ASM) International.
* Journal of Manufacturing Science and Engineering, the American Society of Mechanical Engineers
* The Journal of Vacuum Science and Technology, American Vacuum Society
* Journal of Materials Science, Kluwer Academic Publishers, Norwell, MA.
* Thin Solid Films, Elsevier Sciences S.A. Lausanne.
* Advanced Engineering Materials, Wiley-VCH, Germany
* Nano Letters, American Chemical Society
* Journal of Physical Chemistry, American Chemical Society
* Acta Materialia, Elsevier
* Journal of Mechanical Engineering Science, Professional Engineering Publishing Limited
* Materials Characterization, Elsevier
* Materials Science and Engineering: A, Elsevier
* Microscopy Research and Technique, Wiley InterScience
* Scripta Materialia, Elsevier

Publications and Presentations

Journal Publications

"Saturation Effects in Fluorescence Correlation Spectroscopy," L.M. Davis, G. Shen, and D.A. Ball, Proc. SPIE, Vol. 5700, pp. 128-137, 2005.

Paul K. Chu, Simon J. Cooke, Christine A. Coverdale, Adrian W. Cross, and Trevor Moeller, Guest Editors, Special Issue on Selected Oral Contributed Papers from ICOPS 2004, IEEE Transactions on Plasma Science, Vol. 33, No. 2, April 2005.

"Surface Modification for Bioimplants: The Role of Laser Surface Engineering," Anil Kurella and Narendra B. Dahotre, Journal of Biomedical Applications, Vol. 20, No.1, pp. 5-50, 2005.

"Thermal Transitions in Fe-Ti-Cr-C Quaternary System used as Precursor During Laser In-Situ Carbide Coating," A. Singh, Wallace D. Porter, and Narendra B. Dahotre, Materials Science and Engineering: A, Vol. 399, pp. 318-325, 2005.

"A Comparative Study to Estimate Effective Elastic Modulus of Laser Engineered Composite Boride Coating," T. Laha, A. Agarwal, and Narendra B. Dahotre, Advanced Engineering Materials, Vol.7, No. 7, pp.326-328, 2005.

"Laser Induced Multi-scale Textured Zirconia Coating on Ti-6Al-4V," Anil Kurella and Narendra B. Dahotre, Journal of Materials Science: Materials in Medicine, March 17, 2005.

"Influence of Laser Surface Modification on Corrosion Behavior of Stainless Steel 316L and Ti6Al4V in Simulated Body Fluid," Raghuvir Singh, Madhavi Martin and Narendra B. Dahotre, Surface Engineering, Vol. 21, No. 4, pp. 1-10, 2005.

"Microstructure and Microtexture," in Laser-dressed Alumina Grinding Wheel Material" by Abhijeet Khangar, Edward A. Kenik, and Narendra B. Dahotre, Ceramics International, Vol. 31, pp. 621-629, 2005

"Nanocoating for Engine Application," S. Nayak and Narendra B. Dahotre, Surface and Coatings Technology, Vol. 194, pp. 58-67, 2005.

"Observation of Exothermic Reaction During Laser Assisted Iron Oxide Coating on Aluminum Alloy" by S. Nayak, Hsin Wang, Edward A. Kenik, Ian M. Anderson and Narendra B. Dahotre, Materials Science and Engineering: A, Vol. 390, Issues 1-2, pp. 404-413, 2005

"Phase Evolution during Laser In-Situ Carbide Coating," Anshul Singh and Narendra B. Dahotre, Metallurgical and Materials Transactions-A, Vol. 36A, pp. 1-7, 2005.

"Thermography During Laser Surface Melting of Cast Aluminum Alloy," by S. Nayak, H. Wang, and Narendra B. Dahotre, Materials Science and Technology, Vol. 20, pp. 1609-1614, 2004.

"Auger Microscopy of Laser Induced Fe-oxide/Al Reaction Composite Coating," S. Nayak, H.M. Meyers, III, and Narendra B. Dahotre, Surface Engineering, Vol. 20, No.1, pp. 48-52, 2004.

"Laser In-Situ Synthesis of Combinatorial Coating on Steel," Anshul Singh and Narendra B. Dahotre, Journal of Materials Science, Vol. 39, pp. 4553-4560, 2004.

"In-situ Formation of Ni-alumina Nanocomposite During Laser Processing," S.C. Kuiry, S. Wannaparhum, Narendra B. Dahotre, and S. Seal, Scripta Materialia, Vol. 50, pp. 1237-1240, 2004.

"Infrared Thermography During Laser Surface Engineering of Ceramic Coating on Metal," Puja Kadolkar, H. Wang, T. R. Watkins, and Narendra B. Dahotre, Int. J. Advanced Manufacturing Technology, Vol. 23, No. 7, pp. 350-357, 2004.

"Nanosurfacing for Engine Application," S. Nayak and Narendra B. Dahotre, Journal of Minerals, Metals and Materials Society (JOM), Vol. 56, No. 1, pp. 46-48, 2004.

"Instrumented Indentation Characterization of Laser-Remelted A319Al Alloy," S. Nayak, L. Reister and Narendra B. Dahotre, Journal of Materials Research, Vol. 19, No 1, pp. 202-207, 2004.

"OH Two-Line Laser-Induced Fluorescence (LIF) Thermometry in Laser Ignition," Wenhong Qin, Ying-Ling Chen and J. W. L. Lewis, International Flame Research Foundation Combustion Journal, Article number 200508, 2005. http://www.journal.ifrf.net/200508chen.html

"Diatomic Honl-London Factor Computer Program," J.O.Hornkohl, C.G. Parigger, and L. Nemes, Appl. Opt., Vol. 44, pp. 3686-3695, 2005.

"Laser-Induced Carbon Plasma Measurements," L. Nemes, A.M. Keszler, J.O.Hornkohl, and C.G. Parigger, Appl. Opt., Vol. 44, pp. 3661-3667, 2005.

Other Publications

"MACH2 Simulations of the DECADE Plasma Opening Switch using a Teflon Plasma," D. Keefer and R. Rhodes, Megagauss Magnetic Field Generation, Its Application to Science and Ultra-High Pulsed-Power Technology, pp. 589-592, 2004.

"Opening Mechanisms in an Explosively Formed Fuse Opening Switch," D. Keefer, M.H. Frese, L.D. Merkle, R. E. Peterkin, Jr., N.F. Roderick, K. F. Stephens II, Megagauss Magnetic Field Generation, Its Application to Science and Ultra-High Pulsed-Power Technology, pp. 614-618, 2004.

"Experiments on Stark Widths and Shifts of Hydrogen Balmer Lines in Laser-Induced Plasma," C.G. Parigger, Post-Conference Proceeding of 17th ICSLS Spectral Line Shapes, edited by E. Dalimier, ISBN 2-914601-14-X, pp 97-104 (2004).

Accepted Publications

"Tribology of Laser Modified Surface of Stainless Steel in Physiological Solution," R. Singh and Narendra B. Dahotre, accepted for publication in the Journal of Materials Science, Vol. 40, 5619-5626, November 2005.

"Surface Modification for Bioimplants: The Role of Laser Surface Engineering," A. Kurella and N. B. Dahotre, accepted for publication in the Journal of Biomaterials Applications, Vol. 20, 5-50, November 2005,

"Morphological Modification in Laser Dressed Alumina Grinding Material for Microscale Grinding," A. Khangar and Narendra B. Dahotre, accepted for publication in Journal of Materials Processing Technology, Vol. 33, 1-10, December 2005.

"Synthesis of Platinum-Loaded Zirconia on Fecralloy Using Composite Plasma-Polymerized Films," P.D. Pedrow, R. Dhar, T.M. Moeller, Q. Ming, K.C. Lidell, and M.A. Osman, accepted for publication in the IEEE Transactions on Plasma Science, Vol. 33, 2035-2045, December 2005.

Submitted Publications

"Computer Real-Time Analysis in Mobile Ocular Screening," Ying-Ling Chen, Ph.D., J. W. L. Lewis, Ph.D. , Natalie Kerr, MD, and Ross A. Kennedy, MDCM. FRCS(C), accepted for publication subject to revisions. Journal of Telemedicine and eHealth.

"Keratoconus Eye Modeling," Y.-L. Chen, K. Baker, B. Tan, J. W. L. Lewis, and M. Wang, J. of Vision, accepted for publication subject to revisions.

Presentations

"4-Channel Single-Photon Avalanche Diode and TimeHarp-200 for sm-FRET and Drug-Binding Measurements," L.M. Davis, D.A. Ball, G. Shen, E.D. Matayoshi and K.M. Swift, 10th International Workshop on "Single Molecule Detection and Ultrasensitive Analysis in Life Sciences," Berlin, Germany, September 22-24, 2004.

"Single-Molecule Detection in Micron-sized Capillaries," D.A. Ball, G. Shen and L.M. Davis, 71st Annual Meeting of the Southeastern Section of the American Physical Society, Oak Ridge, TN, November 11-13, 2004.

"Photophysical and Instrumental Effects in Fluorescence Correlation Spectroscopy," G. Shen, D.A. Ball and L.M. Davis, 71st Annual Meeting of the Southeastern Section of the American Physical Society, Oak Ridge, TN, November 11-13, 2004.

"Confocal Fluorescence Microscopy for the Detection of Single Molecules in Biology," G. Shen, D.A. Ball and Lloyd M. Davis, Tennessee Mouse Genome Consortium Meeting, Fall Creek Falls, TN, November 18-20, 2004.

"Multi-Channel Imaging Capabilities at Low Signal Levels," L.M. Davis, and G. Shen, Frontiers in Optics/Laser Science, Optical Society of America, Tucson, AZ, October 16-20, 2005.

"Dynamic Properties of Photoluminescence from Porous Silicon," K.H. Lee, K.S. Jeon, D.A. Ball, G. Shen, and L.M. Davis, 96th Annual Meeting of the Korean Chemical Society, Wonju, Korea, Oct. 21-22, 2005.

"Saturation Effects in Fluorescence Correlation Spectroscopy," L.M. Davis, G. Shen and D.A. Ball, SPIE Photonics West 2005, San Jose, CA, January 22-27, 2005.

"Single-Molecule Detection and Imaging," D.A. Ball, L.M. Davis, and G. Shen, Annual UT/ORNL Chemical Physics Workshop, Knoxville, TN, February 10-12, 2005.

"Scanning Fluorescence Fluctuation Spectroscopy for Molecular Brightness Assays," L.M. Davis, G. Shen and D.A. Ball, Biophysical Society annual meeting, Long Beach, CA, February 12-15, 2005.

"Monte Carlo Simulations for Single-Molecule Fluorescence Applications," L.M. Davis, Presentation at special symposium on "15 years of Single-Molecule Detection," Pittcon 2005, Orlando, FL, February 27-March 4, 2005.

"Accounting for Saturation and Triplet effects In FCS Measurements," L.M. Davis, G. Shen, D.A. Ball, K.M. Swift and E.D. Matayoshi, 6th International Weber Symposium on Innovative Fluorescence Methodologies in Biochemistry and Medicine, Lihue, HI, July 22-28, 2005.

“Surface Engineering: In Materials Science-III,” Narendra B. Dahotre, Co-Organizer for the symposium, held during TMS Annual Meeting in San Francisco, CA, February13-17, 2005.

3rd International Surface Engineering Congress, Narendra B. Dahotre, Co-Organizer, ASM International, Orlando, Florida, August 2-4, 2004.

“Surfaces and Interfaces in Nanostructured Materials,” Narendra B. Dahotre, Co-Organizer, symposium, TMS Annual Meeting, Charlotte, North Carolina, March 14-18, 2004),

“Laser Processing for Surface Modification,” Narendra B. Dahotre, Session Chair, Surface Engineering: In Materials Science-III held during TMS Annual Meeting, San Francisco, CA, February 13-17, 2005,

“Diatomic H¨onl-London Factors Computations,” J.O.Hornkohl, C. Parigger, L. Nemes, in Laser Applications to Chemical and Environmental Analysis, LACEA 2004.

“Measurement of Laser-Induced Carbon Plasma,” L. Nemes, A.M. Keszler, J.O.Hornkohl, C. Parigger, in Laser Applications to Chemical and Environmental Analysis, 2004 OSA Technical Digest Series, Optical Society of America, Washington, DC 2004.

“Modeling of the Temperature Distribution in Dental Pulp Subsequent to Interaction with Ultrashort Laser Pulses,” P. Pike, C. Parigger, R.Splinter, and P.Lockhartm Optics in the Southeast (OISE), OSA Annual Meeting and Exhibit, Charlotte, North Carolina, Nov 4-5, 2004.

“The Effect of Developmental Delay and Type of Strabismus on the Reliability of Photorefractive Screening in Young Children,” Natalie C. Kerr, Ying-Ling Chen, Grant Somes, and J. W. L. Lewis, 2005 AAPOS Annual Meeting.

“Simulation of Ametropic Human Eyes” Bo Tan, Ying-Ling Chen, and J. W. L. Lewis, 71st Annual Meeting of the Southeastern Section, Oak Ridge, TN, November 11-13, 2004.

“Simulating Photo-Refraction Images of Keratoconus and Near-Sightedness Eyes,” Kevin Baker, Ying-Ling Chen, and J. W. L. Lewis, 71st Annual Meeting of the Southeastern Section, Oak Ridge, TN, November 11-13, 2004.

“Theoretical Considerations of Photorefraction Using Model Eyes,” Bo Tan, Ying-Ling Chen, and J. W. L. Lewis, Optics in the Southeast (OISE), OSA Annual meeting and Exhibit, Charlotte, North Carolina, November 4-5, 2004.

“Detecting Keratoconus Using Photo-Refraction Technique,” Kevin Baker, Ying-Ling Chen, and J. W. L. Lewis, Optics in the Southeast (OISE), OSA Annual meeting and Exhibit, Charlotte, North Carolina, November 4-5, 2004.

Invited Presentations

"Single-Molecule Detection and Drug-Binding Experiments at UTSI," L.M. Davis, Abbott Laboratories, North Chicago, IL, August 2, 2004.

"Fluorescence Fluctuation Spectroscopy for Bioscience Applications," L.M. Davis, Vanderbilt University, Nashville, September 7, 2004.

"Single-Molecule Detection and Fluorescence Fluctuation Spectroscopy," L.M. Davis, Tennessee Technological University, Department of Chemistry, Cookeville, November 19, 2004.

"Laser Surface Engineering: Laser Induced Reaction Coating for Automotive Application," Narendra B. Dahotre, Department of Metallurgy, Pune Institute of Engineering and Technology, University of Pune, India, December, 18, 2004.

"Laser Surface Engineering: Laser Coating of Ceramic on Aluminum," Narendra B. Dahotre, Department of Metallurgical and Materials Engineering, Indian Institute of Technology (IIT), Kharagpur, India, December 22, 2004.

Book and Book Chapters Published

"Nanocrystalline Diamond," Narendra B. Dahotre and P. D. Kichambare, Encyclopedia of Nanoscience and Nanotechnology, Editor: H.S. Nalwa, American Scientific Publishers, Stevenson Ranch, CA, 2004, 30 pp.

"Surface Engineering in Materials Science III," Narendra B. Dahotre, Co-Editor, The Metallurgical Society (TMS) of AIME, Warrendale, PA, 2005, 358 pp., ISBN:0-87339-590-5.

"Surfaces and Interfaces in Nanostructured Materials," Narendra B. Dahotre, Co-editor, The Metallurgical Society (TMS) of AIME, Warrendale, PA, 2004, pp. 398, ISBN:0-87339-566-2.

"Laser Induced Breakdown of Gases: Theory and Simulation," C. Parigger, submitted chapter for Book.