SANDIA REPORT
SAND2007-4888
Unlimited Release
Printed August 2007

LDRD 102610 Final Report New Processes for Innovative Microsystems Engineering with Predictive Simulation

Scott A. Mitchell, Ann E. Mattsson, Stephen W. Thomas

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation,
a Lockheed Martin Company, for the United States Department of Energy's
National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: http://www.osti.gov/bridge

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online

SAND2007-4888
Unlimited Release
Printed August 2007

LDRD 102610 FINAL REPORT NEW PROCESSES FOR INNOVATIVE MICROSYSTEMS ENGINEERING WITH PREDICTIVE SIMULATION

Scott A. Mitchell, Ann E. Mattsson, and Stephen W. Thomas
Computation, Computers, Information and Mathematics
P.O. Box 5800, MS1316
Sandia National Laboratories
Albuquerque, NM 87185

ABSTRACT

This LDRD Final report describes work that Stephen W. Thomas performed in 2006. The initial problem was to develop a modeling, simulation, and optimization strategy for the design of a high speed microsystem switch. The challenge was to model the right phenomena at the right level of fidelity, and capture the right design parameters. This effort focused on the design context, in contrast to other Sandia efforts' focus on high-fidelity assessment. This report contains the initial proposal and the annual progress report. This report also describes exploratory work on micromaching using femtosecond lasers. Steve's time developing a proposal and collaboration on this topic was partly funded by this LDRD.

INTRODUCTION

This document describes the work that Stephen W. Thomas performed for the 2006 late-start LDRD 102610. In early 2007 Steve Thomas left Sandia. This LDRD final report was compiled by Scott Mitchell, the program manager for this LDRD and Steve Thomas's department manager, after Steve left.

Proposal

The following proposal was written by Steve Thomas around 14 April 2006. It was later selected for funding as a FY2006 late start LDRD.

Project Title:	**New Processes for Innovative Microsystems Engineering with Predictive Simulation**
Responsible Manager:	**MITCHELL,SCOTT A. Org.: 01411**
Principal Investigator:	**THOMAS,STEPHEN W. Org.: 01411**

Abstract:

What exploratory engineering process leads to best innovations when high performance predictive simulation is available? We propose to investigate the way in which innovation-centric engineering problem-solving responds to trade-offs among model fidelity and simulation run time available in a high performance parallel computing environment. Specifically, we propose to test the hypothesis: "The use of highly-responsive, moderate-fidelity simulation tools can substantially enhance the likelihood of creative engineering insights leading to successful new designs for an otherwise refractory Microsystems exploratory design problem (the RF Ohmic Switch)." We use the term moderate-fidelity here to mean any combination of models and simulation codes whose prediction accuracy may only be semi-quantitative, but whose simulation run time is on the order of several minutes, compared to approximately several hours for a full-fidelity simulation run using a model suitable for design certification. The RF Ohmic Switch design problem is an excellent test-bed for this hypothesis because the problem of creating a reliable Switch design has so far proven refractory to both traditional build-and-test exploratory design and to post-design analysis using high-fidelity simulation. We will thus be able to make a clear association between any discovery of new, reliable switch designs within this project and the introduction of an engineering process using moderate fidelity-simulation. This research project is high-risk because there can be no guarantee of a positive result with a single design-innovation problem (e.g. a new, highly reliable design for the Switch) even if the experimental hypothesis is true.

Tie to Mission:

Project success has the potential to enhance the effectiveness of the engineering innovation process in a wide range of microsystems projects for discovery of new technologies, and for product designs with DOE and other applications. For example, a new design that significantly increases the reliability of the RF Ohmic Switch would lead to new multi-sensor DP and NP capabilities.

Work Proposed:

We propose to investigate the effectiveness of understanding-based engineering (UBE) engineering processes for design of the Radio-Frequency (RF) Ohmic Switch as a function of simulation fidelity and flexibility. Current engineering process models for designing this switch are based on either low-fidelity, 1-dimensional models, or high-fidelity, very design-specific models. We plan to use moderate-fidelity simulation tools and assess: a) how can we use these tools to enhance our understanding of the designs we have already created? b) What new designs are suggested? c) How well are the predicted new understanding and/or performance of new designs validated by fabrication and test of existing and/or new device designs? The moderate- fidelity simulation tools we intend to use include Salinas (a high-performance parallel structural dynamics code produced under the auspices of the ASC program), with run times reduced by 10-100 times through simplified meshes using beam and shell models.

The metric for project success is how well we answer the question "How much does the addition of the availability of moderate-fidelity simulation enhance design innovation in the microsystems exploratory design context? In particular, does this experiment yield a successful new Switch design?"

2006 Annual Report

The following is the LDRD annual report that Steve Thomas submitted to the LDRD office.

Annual Report Summary
Status: Submitted
Web Final Submit Date: 10/17/2006

Project Number: 102610
Title: New Processes for Innovative Microsystems Engineering with Predictive Simulation

Project Manager:	MITCHELL,SCOTT A.
Project Investigator:	THOMAS,STEPHEN W.
Team Members:	MASSAD,JORDAN E.
	BAKER,MICHAEL S.
	KELLOGG,RICK A.
	DYCK,CHRISTOPHER W.

Annual Report Text

Project Purpose

The purpose of this small late-start project was to discover processes by which computational simulation might be used for creative design problem solving for an otherwise refractory multi-physics exploratory design problem. Can we use predictive simulation to help us make a nonlinear, creative leap from a design that does not work to a design that does? The particular testbed design problem we chose was the re-design of a high-speed electromechanical switch (HSEMS) which had been through several design-fabrication-test cycles, achieving promising levels of performance (switch frequency, power consumption), but failing to meet reliability requirements (average number of switch cycles before failure). Prior to starting this project, the measured performance of the latest HSEMS design had been successfully explained using large-scale, high performance modeling and simulation via the dynamics code Andante. Local design optimization and sensitivity analysis via Andante simulation also showed that no local, linear perturbation of the HSEMS design could produce the required reliability. The problem we address with this project is discovery of how computational engineering techniques (e.g. modeling, simulation, optimization) might be extended to support derivation of a successful design which must be a nonlinear (and perhaps "creative") leap from existing designs.

Current FY Accomplishments

As a result of experimentation with new design models and optimization algorithms, we found a qualitatively different new HSEMS design which simulation predicts will likely meet the objective of substantially improved reliability, while meeting performance constraints. We hope that fabrication and test of this new design in FY07 will validate these predictions.

The computational engineering process we used is based upon

a) embedding the existing design in a substantially larger design class, allowing for qualitatively new design approaches;
b) building a parameterized simulation model for this new design class;
c) applying a new, global, computational optimization algorithm to the simulated design parameters.

We found that global optimization revealed local optima corresponding to design approaches which we likely would not have found with standard optimization codes. At least one of these optima corresponded to a design that is substantially different from the existing design, in ways that are intuitively surprising. For example, electrostatic actuation replaces actuation via a spring retractor. Moreover, simulation predicts the new design will meet the goal of substantially improved reliability. We believe this technique, using global optimization to find large, counterintuitive design "leaps," is potentially generalizable to other challenging design problems.

Significance
For a single, focused problem, this project demonstrated a new computational engineering process which appears to provide significant support for creativity in complex engineering design. We find this result significant, because it runs counter to expectations of many design engineers to the effect that modeling and simulation are primarily (only) useful for analyzing existing designs, and perhaps, via optimization, for design refinement. To the contrary, we found here that global optimization could find a radically different design, which simulation-based analysis predicts solves a design problem which has been otherwise refractory over multiple design-fabrication-test cycles.

The computational engineering steps for the new process are in principle generalizable across a broad range of DOE mission scenarios involving complex design for which innovation is a critical component. These steps are:

1) Embed the (remotely) feasible class of designs in a parameterized design model;
2) Couple a suitable computational simulation code to this model to predict and analyze performance of an arbitrary design realization;
3) Apply global optimization on one or more performance metrics to find many or all local optima of the design parameters;
4) Scan the local optima and identify any which correspond to large improvements in performance and/or apparent changes in "design intent." Fully analyze the latter, with the aim of introducing new design(s) into fabrication and test.

The results of this project suggest that this process will support significant increases in design innovation and resulting design performance.

The results of this project suggest that algorithms for provably-convergent global optimization, over objective functions derived from engineering simulations, are worthy of further research, development and code implementation. The set of such algorithms (provably convergent for "egg-carton" functions that have, for example, known variograms) is very new and is to our knowledge not implemented anywhere in production codes at Sandia or DOE. The engineering process above would benefit from algorithms that go beyond even current theory, for example to provably find all the local optima with objective function values in a given range.

Project Metrics
Ashley Avery, a PhD candidate in Math/EE, was a Summer Intern during 2006 and had 100% of her time supported by this LDRD. This LDRD also supported her for a short time under contract after she returned to her university. She contributed to the work described above.

University Collaborations: UT Austin, Mech. Engr. Dept, Prof Bob Moser

Steve's contribution

In 31 July 2006, Steve described his contributions in design and modeling, simulation, and optimization (MSO) for the RF switch microsystem in the following way. This LDRD is not explicitly mentioned by name below, but is anticipated and implied.

MESA –RF Ohmic Switch Re-Design

- Background: Likely the highest consequence current MEMS project at Sandia, the RF Ohmic Switch is the result of about $12 M and 4 years of exploratory development sponsored by DARPA, NP, and DP. This device demonstrates high-speed switching performance superior to transistors in a range of potential applications from satellite sensors to cell phones. The project is in jeopardy because DARPA withheld CY06 funding based on failure to meet DARPA's escalating switch-lifetime requirements.
- Analysis and Optimization of FY05 Design: I helped to design and validate the extensions to Andante, and later to Salinas, needed to model electrostatic and dynamic contact forces essential to adequate simulation of this switch. Using simulation and lab results, I helped the team to recognize switch closure kinetic energy is an important optimization metric. I demonstrated via optimization (via OA's – metric is non-differentiable) that none of the suggested FY05 design perturbations could likely make an adequate improvement to the switch.

- Introduced, Optimized Electrostatic Vector (EV) Design: The introduction of electrostatic forces as an alternative to spring-retraction (EV) enables a design optimization "jump" to a much better-performing local optimum. An even better local optimum than design intuition expected was revealed in the OA optimization process. Simulation of these EV optima shows that they have good potential to increase switch lifetime to meet DARPA's requirements. At least EV design will be fabricated (expensive) before the next DARPA review.
- Tools for MLO Needed: The above experience strongly suggests that optimization tools capable of efficiently and systematically locating multiple local optima (MLO) would be of substantial value in exploratory design, where "jumps" from one design regime to another are likely to be important. To my knowledge such tools are nowhere available. See next.
- Theory Enabling MLO: Proved for the first time that a class of algorithms based on uncertainty-enhanced-surrogate functions will find a global optimum under mild assumptions about the objective function. Assumptions are for example much weaker than those of the DACE model, standard in V&V analysis. This can be a theoretical foundation for a new class of MLO optimizers, see above. Creating and testing algorithm prototypes this summer.

New research idea in femtosecond lasers

A portion of work done under this LDRD was devoted to developing a new microsystem research collaboration and idea. The idea was to do research on femtosecond lasers; such lasers show promise for microsystems, specifically micromachining. Thus this work fit the general charter of this LDRD, to develop strategies for innovative microsystems engineering. In this case, femtosecond lasers held a promise of being an innovative process, but a lack of fundamental scientific understanding of how they worked prevents the ability to predict their performance in engineering and manufacturing. One key challenge is the short timescale on which these lasers operate, which stymies direct observation. Hence work was needed to gain a fundamental understanding of the physics through predictive simulation.

Activity summary

Steve Thomas spent time gaining an understanding of the state of art of femtosecond lasers. Steve Thomas made trips to conferences and universities to develop a collaborative relationship with key university professors in the field: UT Professors Adela Ben-Yakar (http://www.me.utexas.edu/ben-yakar/) and Bob Moser (rmoser@ices.utexas.edu) and Harvard Professor Eric Mazur (http://mazur-www.harvard.edu/emdetails.php). UT Faculty visited Sandia's Computer Science Research Institute (CSRI) and gave the following CSRI Seminar. Sandian Ann Mattson wrote a proposal with Steve titled "Multidisciplinary Science Base for Nano-Scale Materials Engineering via Ultra-fast Laser." This proposal was submitted to Sandia's NINE LDRD Strategic Partnerships Investment Area, but not selected for funding. A long version of the proposal follows at the end of this report.

CSRI Seminar

Title: Ultrafast Laser Ablation for Micromachining, Nanosurgery, and LIBS

Speaker: Adela Ben-Yakar and Bob Moser, Mechanical Engineering Department, The University of Texas at Austin

Date/Time: Wednesday, August 2, 2006, 10:00 – 11:00 am (MT)

Location: Bldg. 980, Room 95 – Sandia NM, Bldg. 940, Aud. – Sandia C

Brief Abstract: Ultrashort, high peak-power lasers present a unique opportunity for precision micromachining. This novel micromachining technique benefits from the rapid interaction of femtosecond lasers with materials, which allows material removal before significant heating occurs. The result is extremely precise and controllable processing with minimal collateral damage. In this presentation, we will discuss our research efforts on femtosecond laser micromachining of glass substrates to generate fluidic microchannel geometries not possible through traditional microlithographic techniques. We will also discuss a theoretical analysis of the heat transfer and fluid dynamics of the ablation process. Characterizing the detailed flow and thermal processes associated with ultrafast laser ablation process is important in enabling precise and well-controlled microstructuring. Femtosecond lasers also have potential applications in biology and biomedical engineering, and in the non-destructive analysis of material composition using LIBS (Laser Induced Breakdown Spectroscopy), and these applications will also be discussed.

Femtosecond laser ablation of solid materials involves a number of processes, including non-linear absorption, plasmas, shock propagation, melt propagation and resolidification. While there is a growing interest in femtosecond lasers and an increasing number of experimental observations, there are no comprehensive computational models of the various complex processes involved. The multi-physics fluid simulation infrastructure (Rocfluid) developed at the Center for Simulation of Advanced Rockets is a good vehicle for the addressing this problem, and this planned application will be discussed.

CSRI POC: Scott Collis, (505) 284-1123
URL: http://www.cs.sandia.gov/CSRI/Seminars/2006/yakar_moser.htm

NINE Proposal Description

Steve Thomas described the project to his university collaborators in the following way:

The Idea is intended to be responsive to the programmatic desires of our NINE LDRD Strategic Partnerships Investment Area. They are addressing the President's American Competitiveness Initiative, with the intent of priming the project pump for a new DOE National Institute for Nano Engineering (NINE) at Sandia next year. This NINE LDRD funding, aside from the usual LDRD aim of scientific discovery, has some unusual objectives that work in favor of our pre-proposal:

1) Form strategic research and education partnerships with first rate research universities.

2) Contribute to attracting and educating tomorrow's nano-engineers, anywhere in the range K-12 to post graduate school. Capture the public imagination and generate excitement about nano science and engineering as careers.

3) Form strategic partnerships with industry, which will capitalize on the science and technology produced on 1) and participate in providing the education and careers in 2).

4) The grand goal is to boost American technological competitiveness, perhaps over a 1-3 decades time scale.

NINE the Institute will have similar objectives and significant funding for its programs at universities.

Long Proposal

The following is a long version of the proposal that Ann Mattson wrote with Steve Thomas.

1. Overview of the Problem and Idea

Femtosecond laser-material interactions can produce new and useful structural and surface property changes at nano- and larger scales, with a number of promising applications. Further evolution and engineering of this technology is limited by gaps in the basic predictive science, particularly at time scales less than 100 picoseconds, and at subnanometer (sub atomic) to nanometer length scales. The problem of understanding and predicting laser-material interactions in these gaps is difficult because a) direct experimental measurement at these time scales is limited, and b) first principles modeling and simulation at the needed multiple temporal and spatial scales has been computationally impossible. We propose to combine the unique experimental and computational science resources of this team to use experimental measurements to guide, calibrate and validate the modeling and simulation of the right subset of first principles for the photon-electron-ion- material lattice interactions, and to couple these particle interaction models into continuum-scale models via particle-in-a-box fluidics or other Monte Carlo simulation technique. We believe we have an exceptional opportunity to solve this difficult problem because of the unique fit to this problem of research expertise, theoretical, experimental, and computational, of the members of this team.

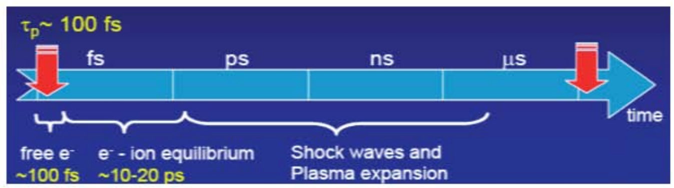
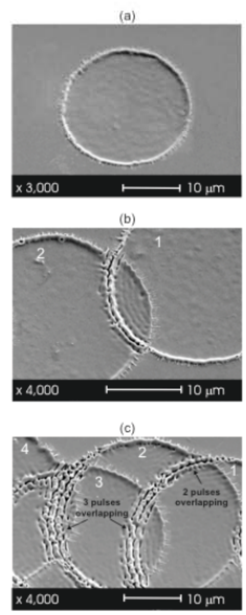


Figure 1: A schematic description of the ablation process of glass with a femtosecond laser pulse.

The fs-laser interaction with material can be schematically divided into time-domains as is shown in Fig. 1. We propose to fill a gap in the understanding of the laser-material interaction at ultra short time scales (less than a few ps) and ultra-small scales (nm scale). This understanding is an important missing piece of the foundation for the burgeoning scientific and engineering applications of femtosecond laser-material interaction. We aim at understanding the fundamental processes so that we can predict key phenomena that are not now predictable. One example of such phenomena is shown in Fig. 2. When borosilicate glass is exposed to a femtosecond laser pulse, an ablated crater with a rim is formed, Fig. 1(a). When multiple pulses are overlapped, Fig. 2(b-c), the rims 'interact' and form a rough surface. We call this phenomena <u>rim diffraction</u>. In order to improve the quality and precision of ultrafast laser micromachining and pulse-to-pulse repeatability of fs-laser micro-/nano-fabrication technique, it is important to understand, model and quantify the nature of this process and any material rearrangement that occurs.

Figure 2: SEM images of crater rims generated on glass by (a) one laser pulse, (b) two overlapping laser pulses, and (c) three overlapping fs laser pulses. The numbers correspond to the order of the incident laser pulses.



Understanding of the ultra-fast, ultra-small interactions has been limited because they have been too fast to measure directly (and still are) and too multi-scale (photon, electron, ion, plasma, molecular solid) to simulate from first principles. We propose to fill that gap in understanding through a three-year first-principles simulation based multiscale research program, guided and validated by laboratory measurements at UT and Harvard.

2. Proposed R&D

2.1. Technical Approach

To achieve our goal of predicting key phenomena in the laser ablation process that are not now predictable we propose to (1) identify and investigate fundamental processes at the very short time-scales and (2) use this understanding to connect to and improve continuum descriptions at larger spatial and temporal scales.

<u>*Theoretical Approach (Mattsson, Hoyt, Moser, Trucano):*</u> For a fundamental understanding of the non-thermal ablation process it is important to treat ions and electrons separately. Most importantly the ions and electrons have different temperatures over a large time domain. It is also possible that non-equilibrium distributions of kinetic energies of both ions and electrons are important factors in the understanding of basic processes. In addition quantum effects in the electron-electron and electron-ion interactions might need to be taken into account. Electrons can be moving freely or be bound to the ions in the crystalline material. We will design calculations to investigate the importance of all these factors for the later time evolution of the ablation process. Some tools are already available for performing these calculations, such as Density Functional Theory (DFT)

codes, and we will start out using these. However, there are new processes that need to be incorporated into such tools, for example, electron-phonon interactions between hot bound electrons and cold ions in a DFT code.

It would be preferable to validate the studied processes directly via experiment, but because of the very short timescales of these fundamental processes we most likely will need to validate out understanding indirectly by transferring small scale information to larger scale modeling and simulation efforts in a multiscale scheme. Results from the microscopic simulations will thus be used to inform the development and validation of continuum non-equilibrium models.

The challenges involved in modeling the early evolution of the ablation process in a continuum context include: 1) the lack of thermal equilibrium between electrons and ions at early time, 2) the lack of kinetic equilibrium of the ions at early time, and 3) the lack of electrical neutrality of the plasma at early times. Challenge (1) has been effectively treated in the past using two-temperature models, while techniques for continuum treatment of (3) require the coupling of Maxwell's equations, as in magneto-hydrodynamics (MHD). Finally, the kinetic non-equilibrium of (2) is most directly treated by solving for the particle distributions through the Boltzmann equations. One approach would be to treat the Boltzmann equations directly via Monte Carlo methods (e.g. Direct-Simulation Monte Carlo---DSMC), but we would like to explore the possibility of representing at least the approach to equilibration through the continuum evolution of a few distribution parameters.

Experimental Approach (Ben-Yakar, Mazur): The focus of the experimental work is to make detailed measurements that will improve the understanding of the fs-laser ablation mechanisms and help validate the numerical model that is being developed under this proposal. The experiments are designed to measure the non-equilibrium properties of the laser-induced plasma using various time-resolved optical pump-probe techniques. Using various experimental techniques Ben-Yakar group at UT Austin and Mazur group at Harvard will investigate the evolution of both the solid target and the ablation plume following femtosecond laser irradiation of different materials. We will probe the dynamics of femtosecond laser irradiation for different fluence regimes: below and above the ablation threshold and above the plasma formation threshold.

For fluences below the ablation threshold we will use a dual-angle-of-incidence pump-probe reflectometry technique[1, 2] to measure the dielectric function dynamics of the target with femtosecond time resolution. From the dielectric function response of the material we will be able to determine the kinetics of phase transformations within the material. Understanding the response of the material exposed to different background gases (including vacuum and ambient air) below and up to the ablation threshold will allow a more complete understanding of the dynamics of the ablation process.

For fluences above the ablation and plasma formation thresholds, the evolution of the target surface and ablated material will be investigated using time-resolved optical microscopy. We will obtain time-gated spatially resolved reflectivity snapshots of the target surface before, during, and after ablation occurs. These snapshots will allow us to monitor changes in the surface morphology as a function of laser fluence. In vacuum, the molten target surface and the expanding ablation front surface are known to act as interfering optical surfaces that produce Newton-ring interference fringes in the snapshots[3]. We will observe the temporal evolution of these fringes during ablation to determine the velocity of the ablation front as a function of laser fluence.

Finally, structural time evolution of plasma and the position of shock waves will be measured using time-resolved schlieren/shadowgraphy imaging.

[1] Downer MC, Fork RL, Shank CV, "Femtosecond imaging of melting and evaporation at a photoexcited silicon surface," *J. Opt. Soc. Am. B* **2**, 595 (1985). [2] Roeser CAD, Kim AMT, Callan JP, Huang L, Glezer EN, Siegal Y and Mazur E, "Femtosecond time-resolved dielectric function measurements by dual-angle reflectometry," *Rev. Sci. Instrum.* **74**, 3413 (2003). [3] D. von der Linde and K. Sokolowski-Tinten, Applied Surface Science 154, 1 (2000).

Industrial/Education Outreach (Thomas, Mazur, Ben-Yakar, Moser): The proposed project will carry out specific planned activities to engage potential industrial partners, and to excite and involve potential future nano scientists and engineers. We plan a three-pronged approach to these outreach activities:

1) Industrial outreach and partnership: We will invite potential industrial partners to participate in research exchange seminars and on-site research collaboration at each of our three institutions. One of us (Mazur) has had early success in engaging industrial follow-up development of a nanoscience application – with resulting industrial funding for a new nano project – using this approach. Our goals include engaging at least one industrial partner to make an in-kind contribution of research collaboration at Sandia during the third year of this project. Incentive for that participation will be the availability at Sandia of capabilities for computational fs-laser-material predictive simulation available nowhere else.

2) Education: This project will engage and support the research of at least two Ph.D. candidates at Harvard and UT Austin, and provide opportunities for undergraduate laboratory involvement throughout the year. In

addition, this project will engage undergraduates through identification, compilation, and deployment of course enrichment material from laboratory and computational results for use in such undergraduate classes as materials science and fluid mechanics. Our goal is to fill an educational pipeline producing both researchers and practitioners of future nano science and engineering.

3) Public outreach: The project contributors will give one or two presentations per year on the subject of our research or on nanoscience at public institutions of informal education. Examples of such institutions include: Boston: Museum of Science (http://www.mos.org), Albuquerque: Explora (http://www.explora.us), Dallas: Museum of Nature and Science (http://www.scienceplace.org). Our goal is to build the widest possible public awareness of and excitement about nano science and technology.

2.2. Key R&D Goals and Project Milestones

Goal/Milestone	Completion Date
Investigation of fundamental processes for relevance in the laser ablation process	
- hot bound electrons in cold lattice	Year 1-2
- free non-equilibrium classical electrons	Year 1-2
- free non-equilibrium quantum electrons	Year 1-2
- Calculation of relevant parameters for larger scale simulations	Year 3
Development of a multiscale scheme	
- Determining best way of coupling the different scales	Year 1
- Development and testing of continuum tools	Year 2-3
Multiscale simulations of laser ablation processes	
- Modeling rim diffraction	Year 3
- Modeling other macroscopic phenomena of interest	Year 3
Fs-time resolved measurements (first ps)	
- Equipment assembly & testing	Year 1
- Dielectric function dynamics & optical microscopy	Year 2-3
- First ps target material characterization	Year 2-3
Cross-cutting efforts	
- Integrated computational/experimental validation studies	Year 1-3

2.3. Risk and Likelihood of Success

The atomic and subatomic scale investigations of fundamental processes are partly done in uncharted territory. For this effort to be successful, we must discover and focus on at most several key processes, model them from first principles, and compute from them large numbers of particle interactions. Each of these challenges requires new discovery to be successful, and in this kind of uncharted territory there can be no guarantee of success. These risks are mitigated by the following factors: 1) the nature of the interaction between the different particle scales (photon-electron, electron-ion, and ion-lattice) are sequential which greatly facilitates scale decoupling; 2) this research team is purpose-built to include the necessary expertise in laser-material interaction theory, experiment, sub atomic particle interaction, atomic and nano scale particle interaction, Monte Carlo fluidic simulation, and inter-calibration and validation of experimental and computational results. Against this difficult research problem we bring a uniquely qualified team.

3. Relationship to Other Work

3.1. Previous Work

Although never in concert, several of the various types of investigations that we are proposing for obtaining understanding about the laser ablation processes at ultra-small and -short scales have been carried out before. For example, the effect of hot electrons on the crystal lattice ion potentials and corresponding phonon spectra has been carried out[4], but no electron-phonon coupling and subsequent equilibration has been included. Molecular Dynamics simulations of free electron/ion systems (plasmas) have been performed, but the large mass difference between electrons and ions is a challenge that has yet to be overcome. Laser induced material breakdown has been treated at the continuum level, but without quantitative input from shorter time scales.

[4] V. Recoules, J. Clérouin, G. Zérah, P.M. Anglade, and S. Mazevet, “Effect of Intense Las Irradiation on the Lattice Stability of Semiconductors and Metals”, Phys. Rev. Letters **96**, 055503 (2006).

3.2. Relationship to Other Ongoing Work

An unfunded task, “Response of a Solid Surface to a Femto-Second Laser Pulse”, has been added to an existing contract between Sandia and the Institute for High Energy Densities in Moscow, Russia. They have done previous work with a non-equilibrium classical Molecular Dynamics code investigating non-ideal plasmas. We are negotiating to have a copy of their code, which would be a good starting point for our own non-equilibrium investigations.

3.3 Appropriateness of Approach

To bring new understanding about fundamental processes into the nano-science field, it is crucial to treat electrons and ions separately. Only then can the fundamental non-equilibrium processes involved in the early stages of laser ablation be investigated. Further, to have this new understanding impact the understanding of larger scale phenomena, such as the rim diffraction, a multiscale scheme based on the use of first principle investigation tools is needed.

4. Resources

4.1. Key Research Team Members

Name	Org	Role
Ann Mattsson	01435	PI, Atomic Scale Theory
Steve Thomas	01411	Computer Science, Education
Jeff Hoyt	01814	Atomic Scale Theory
Tim Trucano	01411	Validation Theory
Adela Ben-Yakar	UT Austin	Fs-laser experiments
Eric Mazur	Harvard	Fs-laser experiment, Education
Bob Moser	UT Austin	Continuum Theory

4.2. Qualifications of the PI to Perform This Work

Our multidisciplinary research team incorporates scientists from Sandia, The University of Texas at Austin and Harvard University, and brings together faculty from Physics and Mechanical Engineering Departments. Our team brings several key ingredients that are essential for this project. 1) We must be able to model at the quantum level (photons-electrons-ions), an area covered by Ann Mattsson's DFT and quantum field theory expertise. 2) We must be able to deal with particle-particle interactions, where we will use Jeff Hoyts Molecular Dynamics expertise. 3) We must have deep theoretical knowledge of laser material interaction, brought to us by Eric Mazur of Harvard and Adela Ben-Yakar of UT, both world-recognized experts. 4) We must be able to couple into molecular lattice and continuum models, expertise brought to us by Bob Moser of UT, also a world-recognized expert. 5) We need expertise in the algorithms of parallel computation, where a number of us have expertise. Finally, we must couple experiment to simulation through validation theory, expertise brought to us by world-recognized expert Tim Trucano.

5. Importance

5.1. Relevance to Laboratory Missions

New scientific understanding created and embodied in predictive computational models within this project, if successful, will provide a foundation for new nano technologies relevant to DOE, DHS, and other missions over a broad range including nearly anything where nano-manipulation of materials surfaces can lead to a technical advantage. Applications technologies currently in early stages of development include: nano scale machining of fluidic sensors and actuators, engineered material surface properties on semiconductors, metals, and glasses for enhanced performance in energy conversion, and molecular surgery in both biologic and non-biologic nano systems. These applications include some of the most exciting nano technologies on the horizon, and all will benefit from scientific understanding and predictive models created in this project.

5.2. Programmatic benefit to IA, If Successful

This project provide a valuable scientific, industrial, and educational foundation for enhanced American competitiveness in nanotechnology. The project will:

- Produce a world class, and world recognized basic advance in understanding in one of the most exciting fields of nanotechnology;
- Deliver that advanced understanding to industrial application.
- Strengthen and build new strategic partnerships at UT Austin and Harvard.
- Create at least one new industrial partnership.
- Introduce a successful new paradigm for building industrial partnerships.
- Engage and educate future nano scientists and engineers.
- Inform and excite the public imagination about nano technology and its potential.

Distribution:

1	MS 1318	D. E. Womble, 01410
1	MS 1318	J. R. Stewart, 01411
1	MS 1316	S. A. Mitchell, 01412
2	MS 9018	Central Technical Files, 8944
2	MS 0899	Technical Library, 4536
1	MS 0188	D. Chavez, LDRD Office, 1011