Materials Science and Engineering Research Projects 2008-09

During 2008-2009, the Department of Materials Science and Engineering (MSE) faculty, students and staff conducted a large and diverse research program. The vitality of this research program is reflected by its breadth of research funding sources, including most major federal agencies and many corporations. MSE research ranged from theoretical and experimental studies of nanocrystalline materials to fabrication of advanced compound semiconductors to development of materials and processes for the mitigation of corrosion based failures of aircraft. All major materials classes are represented and much of the research is team-oriented and interdisciplinary. Collaborators in these research programs include the corporate sponsors and faculty and students from other engineering departments (Chemical, Mechanical, Electrical, and Nuclear) plus faculty and students from the departments of Chemistry, Physics, Mathematics, and Textiles. There are also active research collaborations with the College of Veterinary Medicine, Microbiology, and the College of Management.

Materials science and engineering research has become an enabling technology that spans science and engineering and is critical for development of new products from aerospace to automotive to microelectronics. This breadth of impact is accomplished through a broad interdisciplinary approach to research. MSE faculty and students reflect this diversity and breadth (e.g., see **www.mse.ncsu.edu**). Since the field of materials science and engineering is expanding in scope and impact, graduate education and research comprise a significant fraction of the department's activities. This is best demonstrated by the department's annual graduation numbers for PhD and MS degrees, which sometimes exceed the number of BS degrees.

Undergraduate MSE students are also significantly involved in research efforts within the department, which has been found to improve academic performance. The department continues the offer of part-time research employment to its MSE undergraduates. During this past year, the senior design course undertook projects with local and regional industry, with each project using research laboratory equipment under the advisement of MSE faculty and graduate students. MSE undergraduates also gain research experience through participation in the Undergraduate Research Symposium and the Technology Education and Commercialization (TEC) program. The TEC program is conducted jointly with the College of Management and provides student teams with experience developing promising NCSU research into commercial ventures.

Improving textiles with cyclodextrins

C.M. Balik, A. Tonelli
NTC
$12,000

We are currently synthesizing star polymers with a CD core and polystyrene (PS)arms. These novel star polymers are being used as compatibilizers for blends of PS and poly(dimethyl siloxane) (PDMS). The cyclodextrin core threads PDMS and the star arms provide compatibility with the PS matrix. In this unique method of blending, the star molecules effectively create physical "handcuffs" for individual PDMS molecules in the PS matrix. We have shown that addition of these star molecules to a cloudy solution of PS and PDMS causes the solution to become clear.

Atomic level modeling of energy transfer, friction, wear and microstructure evolution at the rail-projectile interface

D. W. Brenner
Office of Naval Research (MURI subcontract from Ga. Tech)
$425,000
05/11/2004 – 12/12/2009

One of the limiting phenomena for the development of electromagnetic launch technology is wear at the armature/rail interface. We are using a combination of atomic and continuum-level modeling techniques to characterize wear mechanisms at sliding metallic interfaces—in particular the interplay of frictional heating, heat conduction, plasma formation and electromagnetic migration—to explore coatings that potentially inhibit wear.

Atomic and multiscale modeling to predict the sensitivity of energetic materials

D. W. Brenner
Army Research Office (MURI)
$575,000
05/01/2005 – 04/30/2010

A novel combination of atomic and continuum modeling is used to simulate the shock dynamics of energetic materials, including hot spot formation and the resulting detonation initiation. The data from these studies are used to quantify the relationship between defects and shock sensitivity—vital knowledge in the Army's development of safer munitions.

Characterizing friction and wear properties of engineering materials from atomic simulations

D. W. Brenner
Office of Naval Research
$75,000
02/01/2008 – 01/31/2010

We are developing a variety of new modeling tools for linking friction and wear processes over the disparate time and length scales associated with molecular modeling and real-world engineering applications. The modeling tools, which focus on both metals and covalent solids, couple molecular dynamics simulations with grid-based coarse-grain models for surface chemical kinetics, heat transfer, wear and microstructure evolution at sliding interfaces.

Multifunctional extreme environment surfaces: Nanotribology for air and space

D. W. Brenner
Air Force Office of Scientific Research (MURI program)
$217,978
06/1/2004 – 0 6/30/2010

This project is part of a large experimental-modeling effort to develop the scientific basis for tribological properties in terms of scale-dependent thermal, chemical and mechanical processes. Understanding tribological properties is critical for the engineering of advanced materials and coatings with properties tailored for aerospace applications. A hierarchy of continuum and atomic modeling is used to explore fundamental friction and wear phenomena and to explore new materials with unique properties.

Materials World Network: Designer nanodiamonds for detoxification

D.W. Brenner, T-J M. Luo
National Science Foundation
$471,000
05/01/2006 – 04/30/2009

A multidisciplinary team of Russian and U.S. researchers are creating hydrosols of functionalized diamond nanoparticles that act as designer gastrointestinal enterosorbents for mycotoxins. Mycotoxins—the toxic byproducts of molds—are a major problem in developing countries where food shortages make disposing of potentially moldy feed impractical. The designer diamond nanoparticles, which are being developed through a combination of experiment and theory, are a completely new and novel set of enterosorbent materials that can be made in bulk and tuned to bind to specific toxins while minimizing harmful side effects.

Microstructurally engineered armor systems for enhanced survivability through optimum energy and momentum dissipation

D. W. Brenner, M. Zikry
Army Research Office
$400,000
10/01/2006 – 9/30/2009

First principles methods are used to determine the role of Ag and Mg impurities in promoting the formation of the gamma phase in Al-Cu alloys. The introduction of this phase strengthens these alloys, and has been shown to produce properties that are desirable for high strain-rate deformation. The results of these atomic-level calculations are used in larger-scale plasticity simulations, which aid in the interpretation of experimental studies on these important alloys.

Nanoengineered Reactive Materials for Tunable Ignition and Energy Release

D.W. Brenner, J-P Maria, D. Irving
Army Research Office
11/01/2008 – 07/31/2009
$50,000

We are exploring the structure-property relationships that regulate oxygen exchange in reactive multilayers of CuO (or other oxygen sources) and Cr (or other reactive metals) and are pioneering an exploration of how the properties of the terminal phases in a "thermite" couple control diffusion. These include anionic conductivity, relative covalency, and molar volume. These multilayers are of keen interest for energetic material applications that require tunable power output with in situ control.

Studies into the effect of an applied electric field on the processing and properties of materials

H. Conrad
Funding organization
$xxx
MM/DD/YYYY – MM/DD/YYYY

The objective of this project is to determine the extent, magnitude and governing physical mechanisms of the effect of an electric field on the properties of metals and ceramics, giving consideration to conserving energy and reducing costs in industrial practice.

Institute for Maintenance Science and Technology

J. Cuomo, R. Sanwald and J. Strenkowski
Naval Air Depot
$200,000/year for 5 years
04/01/2004 - 04/01/2009

This contract funds the solution of real-time engineering problems at the Naval Air Depot. The IMST has been setup to focus the resources of NC State University in solving these problems. Individual problems, funded through task orders, include evaluations of fatigue life issues for aging aircraft

Electrical inert crack monitoring gauge

J. Cuomo, R. Sanwald, E. Grant
DRS Technical Services, Inc., Elizabeth City, NC
$245,000
06/01/07 – 12/31/09

This is a project to design a compact system that can be fabricated on a printed circuit board to query up to 20 distinct locations in an aircraft. Work on this project includes determining the power requirements and identifying appropriate battery technology. A portable compact device (palm pilot) will be used for data collection. Differently configured crack detectors will be developed to meet physical constraints and provide redundancy.

Electron beam melting of aluminum

J. Cuomo, R. Sanwald, D. Cormier
DRS Technical Services, Inc., Elizabeth City, NC
$667,281
04/1/07 – 12/31/09

Research is ongoing to define the necessary processing parameters to achieve densities approaching 100%. Research includes developing procedures for proper chemistry to accommodate vaporization of base material alloying elements. Microstructures and mechanical properties will be characterized and relationships with processing developed.

Vertical lift center of excellence manufacturing improvement processes

J. Cuomo, R. Sanwald, D. Cormier, J. Strenkowski
Fleet Readiness Center – East, Cherry Point, NC
$875,000
10/1/07 – 12/20/08

The objective of this proposal is to further the pre-eminent world-class alliance between NC State University and the military bases and their industrial suppliers in North Carolina. The four current projects are: Cold Spray Metallic Processing, Workplace Chromium Mitigation Technologies, Non-Destructive Testing, Reverse Engineering and Agile Manufacturing Technology.

Utilization of recycled carbon fibers

J. Cuomo
Firebird Advanced Materials, Inc., Raleigh, NC
$108,183
01/01/2007 – 5/25/09

Provide support to Firebird Advanced Materials by completing a service of analytical and sample preparations tasks.

Tunable Narrow Band gap Absorbers for Ultra High Efficiency Multi-junction solar cells

N.A. El-Masry, S. Bedair
Department of Energy
$1,400,000
2008 – 2011

Our research team is developing a new sub-cell for a multi-junction solar cell to be integrated by Spectrolab (a Boeing subsidiary) into its four-junction cell structure. The success of the research effort will have a direct impact on the Boeing SAI program currently funded by DOE. The goal of this research is to integrate a 1.5 – 1 eV sub-cell into a four-junction cascade solar cell structure. It is expected to achieve a practical efficiency rating of 40 percent at one sun and a rating of 45 percent at high solar concentration.

Dilute Magnetic Semiconductor Devices Based on Fermi Level Engineering

N.A. El-Masry, S. Bedair
Army Research Office
$440,000
2007 – 2010

We have achieved the electric field control of ferromagnetism in [i(GaMnN)-p(GaN)-n(GaN)] by depleting and enhancing the hole concentration responsible for the ferromagnetic properties. Reverse bias depletes holes from the GaMnN layer and changes the magnetic state from ferromagnetic to paramagnetic (erase). Forward bias enhances hole concentration and the DMS changes from the paramagnetic to the ferromagnetic state (write). The objective of this project is development of a nonvolatile memory cell with very low power demands, large on/off ratio and logic devices that scale beyond CMOS in both density and power/operation.

LED on nonpolar substartes (ARO-STIR)

N.A. El-Masry, S. Bedair
Army Research Office
$50,000
2008 – 2009

We are investigating the stacking of several quantum wells emitting at different wavelengths in a GaN/InGaN LED structure. Emission wavelengths in the blue, green and red spectral regions can be achieved by adjusting the InN% in the wells. In a two-terminal device with the proper design, white light is produced. Results of experiments in growing LEDs of InGaN quantum wells on nonpolar surfaces indicate that this approach can yield multicolor emissions. This research can lead to more efficient and flexible approaches in the field of solid state lighting and compact display devices.

Visual + tactile instrumentation for high-throughput virtual design of insensitive munitions and blast-mitigating armor

D. Irving
Army Research Office
$81,000
05/01/2009 – 04/30/2010

This instrumentation will enable high-throughput virtual design of new materials through the integration of a semi-immersive visual display, a three-dimensional haptic for image manipulation and analysis and a dedicated minicomputing cluster. This unique instrumentation will allow multiscale materials simulations to be simultaneously run, manipulated and analyzed in real time, as opposed to traditional remote queuing and post-run analysis, hence providing a powerful tool for high throughput virtual design of materials with tailored properties.

NUE: Teaching Nanoscale Engineering Across Undergraduate Disciplines

M.A.L. Johnson, J.Lavelle, G. Jones
National Science Foundation (Nanoscience for Under-graduate
Education)
$200,000
9/06-9/08

A cross-disciplinary team of educators from the Colleges of Engineering and Education will translate emerging nanoscale research at the College of Engineering into meaningful undergraduate learning opportunities for students in multiple disciplines: specifically targeting increased understanding of structure, process and design considerations related to physical phenomena at the nanoscale. New curricular content based on nanoscience engineering principles will be developed and taught and assessed quantitatively to comparisons of learning outcomes between these groups in order to evaluate the perceptions and understanding of nanoscience principles by students in each of these undergraduatepopulations.

DURIP: Pulsed CL/EBIC Instrument Attachment

M.A.L Johnson
Army Research Office
$105,000

This grant was for the purchase of a cathodoluminesence / electron beam induced current attachment for a scanning electron microscope that will be used to analyze semiconductors developed for projects funded by the Army Research Office.

Integrated Thermoelectric Cooling Device

M.A.L Johnson
Carolinas Photonics Consortium
$10,000
12/01/2007 – 07/31/2008

The thermoelectric cooling device was purchased with this grant from the Carolina Photonics Consortium.

STTR Phase II; Bulk Non-Polar GaN Substrate Development

M.A.L. Johnson
US Army Research Office and Kyma Technologies
$300,000
08/07 – 07/09

Research and development of non-polar bulk GaN substrates based on the successful initial demonstration of non-polar growth by hydride vapor-phase epitaxy (HVPE). Investigation of processes leading to low extended defect formation (dislocations and stacking faults) in m-plane and a-plane substrates. Studies of homoepitaxial seeding and seed expansion in substrate synthesis will be coupled with detailed simulations of growth process kinetics, leading to controlled synthesis and scientific understanding of processes for in substrate growth. Collaborative university-industry project for competitive multi-phase STTR program.

Laser physical vapor deposition of boron carbide films

J. Kasichainula
Oak Ridge National Laboratories (ORNL)
HTML User Facility - Free Use of in House equipment at ORNL
7/1/02 – 07/1/09

Boron carbide films are developed for wear resistant applications in machining wood and wood products. Laser physical vapor deposition is used in the deposition of the coatings. Characterization is performed using X-ray, Raman spectroscopy, and FTIR spectroscopy.

Characterization of epitaxial growth, residual stresses and interfacial microstructure in lithium niobate on diamond layered structures with an AlN buffer layer

J. Kasichainula
HTML User Facility-Free Use of in House equipment at ORNL
5/1/04 – 8/1/09

Thermal stresses developed between lithium niobate and diamond are responsible for poor adhesion and cracking of the films. The interfacial phases formed are also responsible for poor acoustic coupling. X-ray diffraction, transmission electron microscopy, and Raman spectroscopy are used to characterize the residual stresses and interfacial phases.

IMR: Acquisition of a nanoindenter for research and education on novel complex materials

J. Kasichainula, W. Krause, R. Gorga, R. Scattergood, R. Spontak
NSF-DMR
$350,000
10/01/2005 – 10/01/2009

The objective of this project is to test tribological behavior of nanocrystalline films in an effort to understand and distinguish the differences from microcrystalline films. Nanoindentation testing and modulus mapping in conjunction with the atomic force microscope is used to determine hardness, adhesion, coefficient of friction and wear behavior.

Development of nitride and carbonitride coatings of titanium and chromium for hard wear resistant applications,

J. Kasichainula
ACME United
$11,000.
01/01/2008 – 06/06/09

The purpose of this project is to develop superior, wear-resistant coatings for scissors and other cutting implements.

Optimize bonding of a polymer to a PVD coating containing titanium for cutting products

J. Kasichainula
ACME United
$11,000.
06/01/2008 – 08/31/09

The purpose of this project is to develop a non-stick coating for cutting tools that doesn't affect the tool's hardness.

Analysis and characterization of surgical blades

J. Kasichainula
MYCO Medical
$5,000
12/01/2008 – 09/30/2009

The objective of this project is to test surgical blade materials to determine the best material for cutting tissue cleanly without tearing.

Grain size stability and consolidation of nanostructured particulates

C.C. Koch, R.O. Scattergood
National Science Foundation
$461,101
09/15/2005 – 05/31/2009

This project's objective is to develop strategies for stabilizing nanoscale microstructures during consolidation of powder particulates at elevated temperatures. The research centers on a systematic study of grain growth and kinetic or thermodynamic factors that influence it in selected metals and alloys prepared by mechanical attrition. The model systems based on bcc Fe and fcc Ni are selected since they exhibit different behavior for nanocrystalline grain growth. Alloy additions are used to reduce the grain-boundary energy (thermodynamic approach) or limit the grain-boundary mobility (kinetic approach).

Creep behavior as a function of grain size in high-fluidity Zn-Al die casting alloys

C.C. Koch, K.L. Murty
International Lead Zinc Research Organization
$154,698
01/01/2007 – 12/31/2009

This project centers on studies of the creep of selected Zn-Al die casting alloys as a function of grain size. The alloys under scrutiny are those with high fluidity that are readily cast into very thin sections. These alloys are Zn-4.5 wt. % Al with minor additions of Mg and Cu. For comparison with the die cast materials, fine grain structures of the same composition are prepared by ball milling to allow the grain size to be reduced to nanoscale proportions. Creep measurements are conducted by impression creep tests. The creep data are then analyzed to determine the mechanism responsible.

Novel bulk nanocrystalline thermoelectric materials by mechanical milling or mechanical alloying

C.C. Koch
DARPA/DOS, subcontract from RTI International
$193,757
05/15/2008 – 05/14/2013

The objective of this project is to develop strategies for preparation of bulk nanocrystalline thermoelectric materials with increased figures of merit. The methods of preparation involve high-energy ball milling followed by powder compaction—methods found to be very effective in the synthesis of nanostructured materials. Important research issues include materials selection, preparation methods and powder consolidation methods. Since all materials of interest can be processed in nanocrystalline form by the several ball-milling methods, the selection of materials is guided by the interests of the team.

Breaking the strength ceiling: A fundamental study to make ultra-strong bulk Mg alloys

C.C. Koch, Y.T. Zhu
Army Research Laboratory
$70,001
06/15/2008 – 06/14/2009

In this project, we are attempting to produce bulk nanostructured Mg alloys with ultrahigh strength and good ductility, and to study the mechanisms that gave them the superior properties. Our focus is on two Mg alloys: Mg97Zn1Y2 alloy and ZH60A alloy. This will involve the processing and fundamental study of the strength and ductility of three types of nanostructured Mg alloys: 1) Mg97Zn1Y2 alloy via ball milling + consolidation, 2) Mg-Zn-Zr Alloy (ZK60A) via cryogenic rolling + age hardening, 3) High-pressure torsion (HPT) + age hardening of ZK60A.

Engineering of band-edge VT and EOT minimization through Ti compositional profile control in TiN / high-K gate stacks

D. Lichtenwalner, V. Misra
Texas Instruments
$72,000
MM/DD/YYYY – MM/DD/YYYY

The objective of this project is to study the effects of TiN processing on threshold voltage of high-K metal MOS gate stacks, making use of our molecular beam epitaxy (MBE) system designed for growth over 8-inch Si wafers.

Dielectrics on SiC for work function and mobility control of nMOSFET devices

D. Lichtenwalner, V. Misra
CREE Inc.
$60,000
MM/DD/YYYY – MM/DD/YYYY

The objective of this project is to study alternative methods of dielectric growth on SiC and to increase channel mobility beyond the limits imposed by current high-temperature processing methods for SiO2 dielectrics.

Bio-nano composite electrodes for enzyme-based biofuel cell

T-J.M. Luo
Oak Ridge Associated Universities
$10,000
5/01/07-8/01/08

The goal of this project is to create nanoporous silica material that contains silver nanoparticles and enzyme for improved electrochemical applications. This material can allow effective electron transfer between encapsulated enzymes and electrodes. Efforts have focused on spontaneous metallization mechanism and its applications in creating bio-nanocomposite materials.

Survey of physical properties of biological spores

T-J.M. Luo
Clean Earth Technologies
$10,000
1/1/2008-12/31/2008

This project is a collaborative survey of physical properties of biological spores – such as density, charges and dimensions. Characterization methods were developed using microfluidic devices, micro-manipulators, scanning electron microscope and the atomic force microscope.

Developing GEMOSOL technology for new biomaterials

T-J.M. Luo
NC Biotechnology Center
$66,618
8/15/2008-8/14/2010

This project explores the use of aminosilane as an effective chemical binder for hydroxyapatite biomaterials. This method of synthesis allows biomaterials to be fabricated at room temperature, permitting the addition of celluar growth factors that would be destroyed in more extreme environments. The current effort is focused on developing a fabrication strategy and methodology for biocompatibility and properties characterization.

Epitaxial Multifunctional Materials and Applications: Revolutionary Epitaxial Solutions Creating a Platform for a New Generation of Military Applications

J-P Maria
ONR
$275,000
06/2004 – 05/2009

This program introduces the preparation and characterization of epitaxial oxides on wide bandgap semiconductors as an avenue for a new generation of multifunctional heteroepitaxial devices. It is part of a large MURI program contracted through Georgia Tech. and focuses on preparation of titanate films on GaN for the purpose of self-cleaning antiseptic surfaces. The scientific kernel of this program involves learning how high quality titanate films can be prepared directly in contact with nitride semiconductors.

Structure property relations in $BiFeO_3$: A defect chemistry investigation

J-P. Maria
National Science Foundation
$400,000
08-1-06 - 7-31-11

The BiFeO3 program explores fundamental relationships between controlled defect chemistry, crystalline structure, and the electrical properties of ferroelectric thin films. The cornerstone of this investigation involves developing a novel thin film processing methodology, offering control of both cation stoichiometry and point defects in a complex oxide through gas-phase equilibrium. This will be accomplished by designing a quantitative atmosphere-controlled furnace enabling independent and reproducible variation of temperature, BiOx overpressure and pO2 for the BiFeO3 system. This instrumentation and methodology represents a fundamental contribution to electroceramic processing science, and will result in several unique capabilities:

Transformational Methods for Front Face Metallization

J-P. Maria
DuPont Microcircuit Materials
$75,000
06-01-08 – 05-31-10

The aim of this research is to develop novel concepts for replacing existing silver-glass frit patterning technology for the metallization of mulitcrystalline and single crystalline Si solar cell front face. Technical issues to address include controlled reactions with the nitride antireflection coatings and making robust electrical contacts to the high sheet resistance cell emitters.

BST Thin Films

J-P Maria
Teledyne Scientific and Imaging
09/01/ 2008 – 08/31/2009
$120,000

This project involves preparing barium strontium titanate thin films and integrating them with acoustic reflector substrate stacks for the purpose of tunable acoustic resonator applications. Our focus is on how to prepare oxide thin films in a manner compatible with delicate oxide heterostructure stacks. We are also exploring the structure-property dependencies that link crystal quality, residual strain and the diffuseness of ferroelectric transitions in thin layer barium strontium titanate.

Cell-borne chip for controlled therapeutic protein production and delivery

A. Melechko
Oak Ridge National Laboratory UT-Battelle LLC, (Prime US DOE)
$22,967.00 (NCSU portion; Total $175,000 for one year)
01/30/2009 through 09/30/2009

This objective of this project is to design a chip small enough to fit on a single cell for delivery of genetic material that spurs production of therapeutic proteins. Vertically aligned carbon nanofibers coated with gold nanoparticles serve as vectors for delivering the material and controlling its function within the cell.

Design and synthesis of nanomaterials

A. Melechko
Oak Ridge National Laboratory UT-Battelle LLC, (Prime US DOE)
$65,288 NCSU portion via subcontract (Total $495,000 per year)
02/01/2009 to 01/31/2010

This project is focused on the synthesis of alloy nanoparticles on surfaces by destabilizing thin films. This self-organization and self-assembly technique enables the manufacture of nanoparticle arrays that provide specified functionality.

Wafer engineering of III-nitrides and ZnMgO alloys

J. Narayan
Kopin Corporation
$50,000
10/01/2007 – 09/31/2010

The purpose of this grant is to investigate thin film epitaxy, characteristics of epitaxial growth, defects and interfaces and nature of dislocations, Ohmic contact epitaxy, structure-property correlations and device performance.

NSF-NIRT on synthesis and characterization of self-assembled nano arrays for magnetic and superconducting applications

J. Narayan
National Science Foundation
$1,400,000(NCSU and NC A&T)
08/01/2004 – 07/31/2009

The focus of this research is to develop novel nanostructured magnetic materials where nanodots are assembled by controlling the kinetics of clustering, while overcoming thermodynamic forces leading to Ostwald ripening. These nanodots can be aligned epitaxially with respect to the substrate via domain matching epitaxy where dots are formed by matching of integral multiples of planes across the film-substrate interface. Thus, these dots have a fixed orientation relationship with respect to the substrate, which can be controlled to optimize the magnetic properties of nanodots. The nanodots in high-Tc superconductors provide effective flux pinning sites to enhance critical current density in the presence of a magnetic field. These nanostructured materials have novel applications ranging from information storage to single-electron transistors to high density superconductors.

III-nitride– and II-oxide-based heterostructures and devices

J. Narayan
Army Research Office
$420,000
07/01/2009 – 06/30/2014

This project will address two major issues related to the epitaxial growth of wide-bandgap III-nitrides (GaN, GaInN) and II-Oxides (ZnO based). First, the research will investigate the principles of domain matching epitaxy as it is applied to the epitaxial growth of GaN, GaInN, and ZnO films on commercially ubiquitious sapphire(0001), Si(111) and Si(100) substrates. The second thrust will center on the electrical and magnetic doping of these films. Ultimately, the findings will be applied to the fabrication of test structures.

NSF Center for Advanced Materials and Smart Structures (jointly with NC A&T)

J. Narayan
National Science Foundation
$3,000,000
07/01/97 – 06/30/2009

The center has four components: (1) advanced ceramics, (2) advanced composites, (3) High-Tc superconductors and perovskite materials and smart structures, and (4) III-V Nitrides and Devices. The primary focus of the center is on novel materials processing, nanoscale characterization, stricture-property correlations, device fabrication, and training of graduate and undergraduate students. The center was funded initially for five years and has been renewed for the next five years.

Energy Frontier Center for Defect Physics in Structural Materials (CDP) ORNL Lead

J. Narayan
Department of Energy
$18,500,000 (total grant)
06/01/2009 – 5/31/2014

The Energy Frontier Center for Defect Physics in Structural Materials is hosted by Oak Ridge National Laboratory

(ORNL) and brings together researchers from ORNL, six universities, and the Lawrence Livermore National Laboratory. The center will address the most basic research challenges in structural materials for energy. It will provide the fundamental scientific knowledge to allow atomistic control and manipulation of the defects, defect interactions, and defect dynamics that currently limit the performance and life span of materials, with the goal of charting new pathways to the development of improved materials – materials with potentially undreamed of strength, toughness, radiation damage tolerance, and self-recovery.

High Efficiency Organic Solar Cells with Novel Transparent Electrodes

J. Narayan
National Science Foundation
$352,000
04/15/2007 – 03/31/2010

This research focuses on transparent electrodes based upon gallium, aluminum and indium doped zinc oxide and molybdenum oxide materials to replace existing indium tin oxide based electrodes. The emphasis on novel microstructures, property measurements, structure-property correlations and modeling to optimize organic solar cell efficiencies. This project focuses on molybdenum oxide (MoOx doped with Mn) and zinc oxide (ZnO doped with Ga or Al) based materials as alternative to ITO as TCO layer on the glass substrate. These materials are less expensive with better chemical stability and diffusion barrier properties than ITO. Recently, we have carried out (in collaboration with Professor Forrest's group) investigations using gallium doped ZnO in the above cell (glass (substrate)/TCO/CuPc/C60/Ag or Al (electrode)) configuration, and obtained solar conversion efficiency, comparable to that from their ITO based organic solar cells. These results from ZnO:Ga films which were not optimized, are specially exciting, and show a great potential for replacing ITO. Another TCO system of interest is MoOx(2< x<3) which could be potentially better than ZnO-based materials in view of its work function being closer to 5.2 eV. In addition to these novel materials, we propose to investigate atomic structure and chemistry of various interfaces (namely glass/TCO, TCO/CuPc, CuPc/C60, C60/Ag) and correlate them with solar cell characteristics. The organic solar cells (OSCs) will be fabricated in our laboratory utilizing our optimized materials and structures. The proposed research has four components: (1) Synthesis and processing ZnO (doped with Ga or Al) and MoOx(2< x<3) films on glass, and sapphire (0001) where these films cab be grown as epitaxial single crystal via domain matching epitaxy. The grain size and the nature of grain boundaries will be varied systematically to establish microstructure-electrical property correlations; (2) Establish resistivity versus temperature correlations for various microstructures ranging from random poly, to textured poly, to single crystals; (3) Study the properties of defects and interfaces and correlate this information with solar cell efficiency; and (4) Fabricate high-efficiency solar cells utilizing TCO films of optimized microstructures and properties.

Ultrafast phase transition and critical issues in structure-property correlations of vanadium oxide

J. Narayan
National Science Foundation
$495,000
07/01/2008 – 06/30/2012

The objective of this project is to develop highly sensitive bolometer imaging arrays that can be integrated into silicon circuits and operated at or above room temperature in infrared cameras or smart sensors. Deployed on the battlefield, these imaging devices could potentially enable soldiers to "own the night" during maneuvers after dark. The project will address synthesis and processing of vanadium oxide thin films with increasing grain size all the way to high-quality single-crystal on sapphire and silicon substrates. These epitaxial films should exhibit a sharp transition, large amplitude and very small hysteresis.

Defects and Interfaces in Thin Film Heterostructures across the Misfit Scale

J. Narayan
Department of Energy, Office of Science, Division of Materials Sciences
$ 500,000
08/01/2008 – 07/31/2012

In this project, we address critical issues related to the formation of nonpolar III-nitride single-crystal thin films on r-plane (1-102) of sapphire and Si(100) substrates with lattice misfit ranging from about 1% to over 20%. Nonpolar directions lead to structures free of built-in electrostatic fields, resulting in improved quantum efficiency. These thin-film heterostructures on Si(100) will also lead to a successful integration of device functionality ranging from digital computing and signal processing to optical sources and smart sensors. However, there are fundamental issues related to thin film epitaxy, critical thickness, defects and interfaces, which need to be addressed systematically to realize such integrated systems.

Development of Nanocrystalline Cu-X Alloys (X = Mo and Nb)

J. M. Rigsbee and J. P. Chu
Cooperative Research with National Taiwan Ocean University

Biased magnetron sputtering techniques are being used to develop non-equilibrium Cu-Mo and Cu-Nb alloys. These alloys are useful in high temperature applications requiring high strength and thermal conductivity. The microstructures consist of nanocrystalline BCC and FCC Mo or Nb particles distributed in a Cu matrix. Preliminary results suggest that these microstructures do not coarsen and retain their high strength properties at temperatures up to 900C. Structure-property relationships are being developed for these materials as a function of alloy composition and thermal processing.

Characterization of the Microstructures of Nanophase Ceramic Particles Produced by Diamond Grinding

J. M. Rigsbee and P. F. Becher (ORNL)
Oak Ridge National Laboratory

Diamond grinding offers a low cost approach for the production of nanophase ceramic and metallic particulate suitable for the fabrication of novel high temperature nanocrystalline materials. Such materials would have applications for increased energy efficiency. The need exists to characterize the nano-scale microstructures of these particulate materials, using transmission electron microscopy, to determine the particle size distributions, chemistry and crystal structure.

Silicon Solar Consortium (SiSoC) Research Center (NSF operational grant)

G. Rozgonyi
National Science Foundation (IUCRC program)
$89,000
$89,000 per year, for 5 years

The Silicon Solar Consortium (SiSoC) Research Center involves faculty from four U.S. universities and personnel from 14 global PV manufacturers. The Center has scientific and technical components related to advanced silicon-based photovoltaic materials and a major educational component to assure an adequate supply of scientists and engineers is available to meet the future needs of the photovoltaic research and manufacturing communities.

Mechanical properties of mono– and multicrystalline silicon: correlation with impurities and defects

G. Rozgonyi, K. Youssef
SiSoC Research Project
$70,000 per year, for two years
10/01/2007 – 09/30/2009

This project deals with the application of four complementary experimental techniques for evaluating mechanical properties and crack initiation/propagation processes before and after mechanical failure of mono- and multi-crystalline silicon wafers. The objectives are to understand the complex roles of crystal growth history, extended defect/impurity interactions, and intragrain vs. grain boundary sources of mechanical failure as a function of wafer thickness.

Impurity capture/release/passivation at a "model/ideal" structural interface in single and multi-crystalline silicon

G. Rozgonyi, J. Lu
SiSoC Research Project
$70,000 per year, for two years
10/01/2007 – 09/30/2009

The objectives are: (1) To characterize the (110)/(100) interface following contamination with various metallic impurities. (2) To determine the effectiveness and stability of hydrogen passivation of the (110)/(100) interface. (3) To establish the kinetics associated with phosphor-diffusion gettering of metallic impurities from the intentionally contaminated (110)/(100) interface. (4) To determine the extent of hydrogen remaining at structural defects following SiNx deposition by examining the deuterium profile across the (110)/(100) interface following SiNx PECVD deposition and contact firing.

Influence of local residual stresses on mechanical properties and crack initiation/propagation of silicon photovoltaic wafers

G. Rozgonyi, K. Youssef
SiSoC Research Project
$65,000 per year, for two years
06/01/2008 – 05/31/2010

The primary objectives of this project are: 1) to understand the role of local residual stresses arising from crystal growth processes on the crack initiation/propagation process during loading of silicon wafers in the presence of various types of impurities, defects, and grain orientations, 2) to quantify stress values and types on mechanical properties (hardness, fracture strength, bending strength, and elastic modulus) of silicon wafers, and 3) to examine the deformation behavior using a novel conducting nano-indentation probe.

Impact of light element impurities (O, C, N) on the structure and electrical behavior of photovoltaic crystalline silicon

G. Rozgonyi, J. Lu
SiSoC Research Project
$65,000 per year, for two years
06/01/2008 – 05/31/2010

The expected deliverables are: (1) FTIR oxygen/carbon/nitrogen profiling of as-grown and processed wafers, (2) O/C/N defect distribution and morphology of precipitates and associated defects, as well as electrical activity profiles of defect/impurity interactions, (3) Deep level trap analysis of electrical property variations, (4) O/C/N precipitation: the influence of associated defects such as dislocations and grain boundaries, and aluminum/ phosphorous diffusion, (5) impact of growth modifications on carrier lifetime, (6) critical O/C/N concentrations impacting the crystal integrity and electrical properties.

Low-temperature proximity gettering in layered silicon wafers: A return to our SiWEDS roots

G. Rozgonyi, M. Wagener, J. Lu
SiWEDS Research Project
$55,000 per year, for two years
04/01/2007 – 03/31/2009

Work includes: (1) characterizing metal precipitates and decoration at a (110)/(100) boundary, Silicon/oxide interface, and misfit dislocations, following various degree of Fe and Cu contamination and thermal annealing; (2) characterizing and determining the effect of band bending on impurity gettering efficiency; (3) characterizing the retention stability of metal impurities at the proximity gettering sites after various degrees of Fe and Cu contamination; thermal release annealing/quenching and passivation; (4) determining the effect of band bending on the retention stability of metal impurities at the proximity gettering sites.

Nanoscale dielectrics for high energy density power conditioning

Z. Sitar, J-P Maria
ONR
$675,000
07/01/2005 – 06/30/2008

The aim of this multi-university research program is to produce inorganic dielectrics and processes compatible with elevated temperature, high energy density power conditioning/filtering applications and practical manufacturing. The dielectrics being developed and optimized include calcium copper titanate (CCT), nano-crystalline aluminum nitride (nALN), and high permittivity rare earth - transition metal oxide glasses.

Doping of AlGaN alloys with Al content larger than 50 percent

Z. Sitar
ARL/HexaTech
$177,000
07/01/2008 – 6/30/2011

The objective of this project is to control the electrical properties of AlGaN alloys with high Al concentration by incorporating point defects. Without point defects, these alloys would be insulating. Doping solutions used today provide adequate conductivity only in the lower half of the alloy range. In most efforts to achieve desired conductivity with AlGaN alloys, the electrical properties were controlled by the poor material quality rather than the thermodynamics of defect formation. Our aim is to isolate the behavior of intentionally incorporated dopants from that of the extended lattice defects and intrinsic point defects.

Investigation of stability of and control of stress in AlGaN alloys and heterostructures.

Z. Sitar
ARL/HexaTech
$184,000
07/01/2008 – 06/30/2011

This project involves a comprehensive plan to study growth of AlGaN alloys and superlattices for incorporation into future device layers. By exploiting and managing the elastic properties of materials, we can transition from AlN substrates to AlGaN device layers without introducing new defects. The lattice mismatch between the AlN substrate and the AlGaN device layers must be accommodated elastically. Through this research, we will study the stability of AlGaN alloys with high Al contgent and the elastic limits of AlGaN layered structures.

AlN substrates for UV avalanche photo-diodes

Z. Sitar
DARPA
$600,000
11/01/2006 – 10/31/2009

The overall objective of this project is to grow AlN crystals, and fabricate low defect density (<104 cm-2), UV-transparent AlN wafers thereof, for growth of high performance UV detectors not achievable on any other substrate. The research on AlN crystal growth focuses on (1) crystal and wafer expansion, (2) UV transparency, (3) further reduction of extended defects, and (4) fabrication of epi wafers.

Advanced Carbon Nanotechnology Program (ACNP)

Z. Sitar
US Army
$250,000
07/01/2004 – 05/19/2009

Our goal in this research is to initiate a comprehensive program on exploration of field emitted electrons from nanostructured carbon materials for e-beam pumping of optoelectronic devices. The focus is on efficient deep UV emission from AlN pumped with a nanotube-based electron emitter.

Catalytic synthesis of carbon nanotube arrays using alcohol

Y.T. Zhu
Los Alamos National Lab
$180,000
05/01/2008 – 09/30/2009

For this project, NC State scientists support the research conducted by the Los Alamos National Lab. This support includes investigation of new catalyst compositions and structures, such as nanocomposite catalysts that can be used to grow carbon nanotube arrays at high temperatures using alcohol (ethanol) as the carbon source gas. We are also growing carbon nanotube arrays through chemical vapor deposition.

Bulk nanostructured materials

Y.T. Zhu
Los Alamos National Lab
$70,000
07/01/2008 – 05/31/2009

For this project, we provided support for a Los Alamos National Lab program funded by the Department of Energy that aims to develop severe plastic deformation techniques to be used in the commercial production of bulk nanostructured materials. This support included monitoring the nanomaterial characterization work performed by Russian partners; assisting Metallicum, the U.S. industrial partner, with the commercialization effort; investigating fundamental deformation mechanisms/properties of the nanomaterials; and publishing technical papers and making presentations at conferences.

Ultrastrong, lightweight carbon nanotube fibers for space structures

Y.T. Zhu
NC Space Grant
$9,500
08/01/2008 – 08/31/2009

A wide variety of applications envisioned for the exploration of space will require significantly stronger, stiffer and lighter materials that those currently available. The objective of this project is to synthesize carbon nanotube fibers that are an order of magnitude stronger and stiffer per kilogram than the best existing engineered fibers. These newly developed fibers hold the potential to make space vehicles and structures stronger, lighter and safer, opening the door to further space exploration and new space technologies.

CONTACT INFORMATION

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www.mse.ncsu.edu