

**Faculty Profiles** 



Consortium for Innovation in Manufacturing & Materials

## Stephen Akwaboa

Contact

Assistant Professor, Mechanical Engineering Southern University, Baton Rouge +1-225-771-2709 stephen\_akwaboa@subr.edu



## Specialization

Computational Fluid Dynamics, Heat Transfer, Hypersonic flows and algorithm development.

#### Expertise

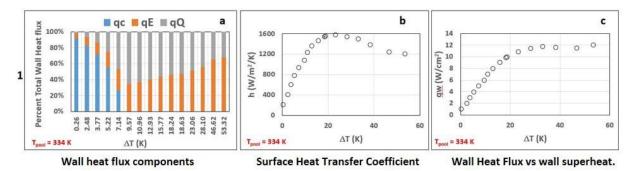
Modeling, processing, and thermo-mechanical property characterization of composite materials, high temperature superalloys and ceramic thermal barrier coatings.

## Education

Ph.D. in Mechanical Engineering from North Carolina A&T State University (2008).

#### Research

Ongoing research in our group, supported by CIMM, focuses on developing computational heat transfer models for analysis of multi-phase heat transfer in micro-scale heat sinks manufactured by metal forming. Numerical modeling and simulation approaches for analyzing additive manufacturing processes involving laser as input heat sources is under development. AM produce parts through the layer by layer addition of molten material generates large temperature gradients that cause plastic deformation. Thermo-mechanical models are developed to predict the thermal history and mechanical distortion. This enables the process to be studied and for distortion mitigation techniques to be developed. Such investigations require models that accurately capture the physics of the deposition process.





## Thomas C Bishop

Associate Professor Chemistry & Physics Hazel Stewart Garner Professor Louisiana Tech University

#### Contact

+1-318-257-5209 bishop@latech.edu



#### **Specialization**

ICME and data.

#### Expertise

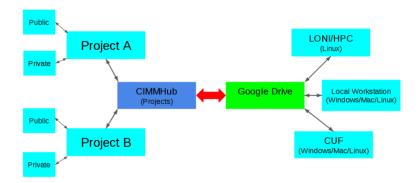
Workflows for High Performance – High Throughput all-atom and coarse grained modeling and simulation.

#### Education

PhD in Physical Chemistry University of Illinois at Urbana-Champaign (1996); M.S. Applied Math from NYU Courant Institute (1990); B.S. in Physics from LSU (1988).

#### Research

CIMM sponsored activities in our group focus on workflows for achieving integrated computational materials engineering and development of CIMMHub as a resource for research and collaboration support. Efforts are focused on exploiting Google Drive as a data management solution for CIMMHub that unifies experimental (CUF) and computational resources (LONI) and development of Workspace tools.





Uttam K. Chakravarty

Assistant Professor University of New Orleans Contact +1-504-280-6191 uchakrav@uno.edu



#### **Specialization**

Computational mechanics, finite element analysis, computational fluid dynamics, and additive manufacturing.

#### Expertise

We are working on the CFD analysis of Ti-6Al-4V melt pool in powder-bed electron beam additive manufacturing to characterize the process parameters associated with it including the melt pool geometry, beam power, beam speed, beam diameter, and temperature profile along the melt scan.

#### Education

Dr. Chakravarty received his B.S. in Mechanical Engineering from the Bangladesh University of Engineering and Technology in 1999, an M.S. in Mechanical Engineering from the Tuskegee University in 2003, another M.S. in Aerospace Engineering from the Georgia Institute of Technology in 2005, and his Ph.D. in Aerospace Engineering from the Georgia Institute of Technology in 2008.

#### Research

Dr. Chakravarty actively conducts research in the areas of solid mechanics, composite structures, vibrations and control, finite element analysis, computational fluid dynamics, fluid-structure interaction, additive manufacturing, and small-scaled unmanned aerial systems. His research has been published in the ASME Journal of Applied Mechanics, ASME Journal of Vibration and Acoustics, Journal of Aircraft, Journal of Intelligent Materials Systems and Structures, Mechanics Research Communications, International Journal of Micro Air Vehicles, Composite Structures, Composites Part B: Engineering, Composite Structures, Materials Science and Engineering A, and Acta Materialia. He has also published several peer-reviewed conference papers, and presented in many national and international conferences.



## Xiang (Shawn) Chen

Contact

Assistant Professor Institute for Micromanufacturing, Mechanical Engineering Louisiana Tech University +1-318-257-2616 shawnxc@latech.edu



## **Specialization**

Computational mechanics, multiscale modeling

#### Expertise

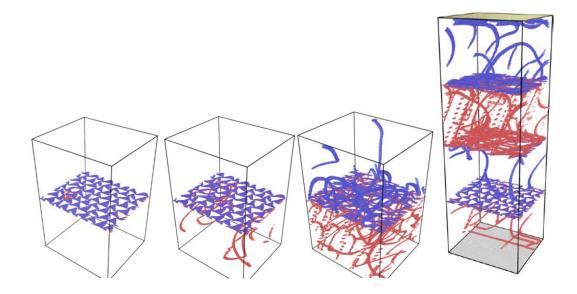
Concurrent atomistic and continuum modeling; phonon transport; dislocation-interface interaction.

## Education

PhD in Mechanical Engineering from the University of Florida (2016)

#### Research

Ongoing research in our group, supported by CIMM, focuses on the methodology development and application of a coarse-grained atomistic modeling for the study of dislocation dynamics and the associated size effect in multilayered materials from nano- to meso-scale.





## Pedro A Derosa

Professor of Physics Physics Program Chair Larson #1 Endowed Professorship Louisiana Tech University

# Contact

+1-318-257-5139 pderosa@latech.edu



## Specialization

Computational materials science; hybrid materials

## Expertise

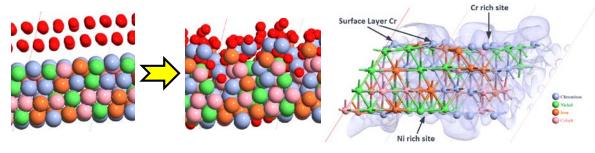
First principles and coarse grain studies of hybrid materials with emphasis on atomic level interactions and charge and particle transport phenomena.

## Education

PhD in Physics (1997) and *licenciado* (BS+MS) in Physics (1993) from University of Córdoba, Argentina; post-doctoral fellowship at University of South Carolina (1998-2003).

#### Research

A project in my group that relates to CIMM deals with surface oxidation of high entropy alloys (HEA). The objective is to study the formation of different oxides on the multicomponent surface, particularly the competition among the oxide groups of the different atomic elements. Density Functional Theory (DFT) and Molecular Dynamics (MD)/DFT is used for these calculations. Individual O atoms, groups of O atoms and O layers are added on top of a HEA surface. DFT is first used to find an equilibrium geometry. The study then continues with MD/DFT that allows for chemical reactions to occur and the formation of oxide groups been predicted. Electronics density and Density of States allows to characterize chemical reactions leading to oxidation.





Dentcho Genov

Associate Professor Louisiana Tech University Contact +1-318-257-4190 dgenov@latech.edu



## Specialization

Computational materials science; computational electromagnetism

#### Expertise

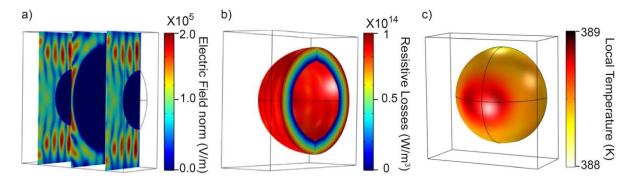
Electromagnetic theory of artificial electromagnetic materials; Nano-photonics and Plasmonics; Multi-physics self-consistent modeling of complex phenomenon pertaining to Selective Laser Melting.

#### Education

PhD in Electrical Engineering from Purdue University (2005); post-doctoral fellowship at University of California at Berkeley (2005-08).

#### Research

CIMM-supported research focuses on the development of a computational framework to self-consistently merge full-wave electromagnetic and heat transfer simulations, to gain a better understanding the complex multi-physics processes involved in Selective Laser Melting (SLM). We aim at technology optimization through understanding the effects of the metal powders microscopic structure and uniformity on laser absorptivity, increase in the SLM energy efficiency and printing rate, reduction of vaporization and improved material utilization.





#### Shengmin Guo

Holmes Endowed Professor of Mechanical Engineering Louisiana State University **Contact** +1-225-578-7619 sguo2@lsu.edu



#### **Specialization**

Thermal fluids, instrumentation, power generation, laser additive manufacturing, and high temperature materials.

#### Expertise

Plasma spray coating, Laser based additive manufacturing, metallic and ceramic material processing, Gas turbines.

#### Education

Ph.D. in Engineering Science from Oxford University, England (1998).

#### Research

Ongoing research in our group, supported by CIMM, focuses on laser based additive manufacturing, including alloy design, alloy powder synthesis, laser 3D printing hardware and software integration, and laser 3D printing process optimization.





#### Louis H. Haber

Assistant Professor of Chemistry Louisiana State University **Contact** +1-225-578-7965 Ihaber@lsu.edu



## **Specialization**

Experimental physical chemistry; ultrafast and nonlinear spectroscopy, nanomaterials

#### Expertise

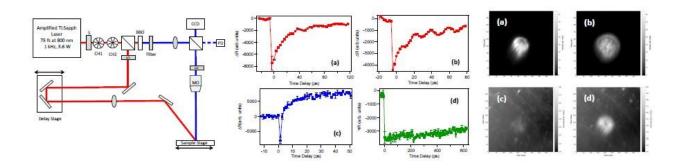
Transient absorption spectroscopy, second harmonic generation, pump-probe reflectivity and ultrafast microscopy; nanoparticle synthesis and characterization.

#### Education

Ph.D. in Chemistry from UC Berkeley (2009); post-doc at Columbia University (2009-2012).

#### Research

The research project in our group supported by CIMM investigates laser heating and melting dynamics in metal alloy and semiconductor surfaces and nanomaterials. We have constructed a new ultrafast laser setup that uses femtosecond laser pulses for pump-probe reflectivity and time-resolved microscopy measurements for studying fundamental wavelength-dependent and power-dependent solid-to-liquid phase transitions in selective laser melting. In addition to crystalline and polycrystalline surfaces, we are also preparing metal alloy nanoparticles deposited on substrates for future laser melting dynamics experiments.





#### Samuel Ibekwe

Professor Southern University, Baton Rouge, LA

## Contact

+1-225-771-2525 Samuel\_ibekwe@subr.edu



## **Specialization**

Solid Mechanics, Materials Engineering

#### Expertise

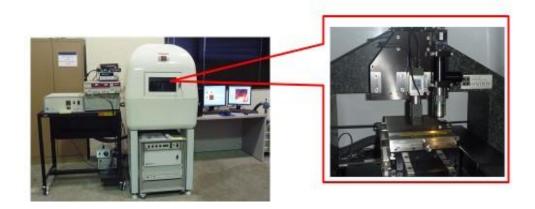
Impact Response of Composites; Fabrication, testing, analysis, and evaluation of advanced composite materials.

#### Education

Ph.D. Materials Engr. & Science, South Dakota School of Mines & Tech. (1991)

#### Research

One project in our group supported by CIMM is studying input parameters in Selective Laser Melting (SLM) of AISI 316L Stainless Steel that will result in optimal desired material properties. Nanoindentation analysis is being carried out to determine nanohardness, elastic modulus, in addition to fracture toughness, wear resistance and hardness uniformity of statistically varied input parameters. Coupled with microstructural characterization, the impact of these inputs on SLM manufactured components would be determined and predicted.





## H. Dwayne Jerro

Professor and Chair Southern University, Baton Rouge, LA Contact

+1-225-771-3580 Dwayne\_Jerro@subr.edu



## **Specialization**

Mechanics and Mechanical Design

#### Expertise

Composite materials design, testing, and characterization

#### Education

Ph.D. Mechanical Engineering, Louisiana State University (1998); Certificate - Institute for Mechanics & Materials Summer School, Univ. California, San Diego (1994).

#### Research

One project involves the design of radiation sensor(s) using Additive Manufacturing techniques. This design includes consideration of factors that have the potential of altering the performance of the sensor over its service life, such as moisture and humidity. Another project in our group supported by CIMM is studying input parameters in Selective Laser Melting (SLM) of AISI 316L Stainless Steel that will result in optimal desired material properties. Nanoindentation analysis is being conducted to determine nanohardness, elastic modulus, in addition to fracture toughness, wear resistance and hardness uniformity of statistically varied input parameters. Coupled with microstructural characterization, the impact of these inputs on SLM manufactured components would be determined and predicted.



## Ghanashyam Joshi

Contact

Professor Southern University, Baton Rouge, LA +1-225-771-5917 Ghanashyam\_Joshi@subr.edu



## **Specialization**

Manufacturing and Design, Materials Engineering

## Expertise

Materials processing and characterization, Fatigue and fracture prognostics

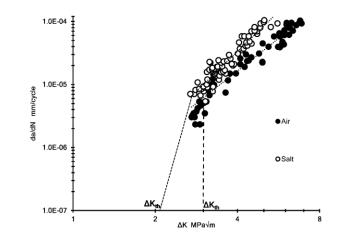
## Education

Ph.D. Mechanical Engineering, Michigan Technological University. (1993); Post-doc at National Institute of Standards and Technology (1993-95); Faculty Fellowships at AFRL, NASA, DoE/ORNL, NIST, DoD/ARL, Boeing.

## Research

One project in our group supported by CIMM is studying fatigue crack initiation and growth in metals and composites. Thermomechanical fatigue including entropy and plastic strain accumulation are being investigated. Damage mechanics as well as fracture mechanics software simulations are carried out. The experimental fatigue tests for multi-sensor data based fatigue crack prognostics are carried out using servo- hydraulic MTS mechanical test machine. Failed specimens are further investigated using optical microscopy and SEM, for confirmation of marker bands, phases and grain structure. Prognostics system for fatigue crack growth/life tracking will be developed.







#### Michael Khonsari

# Contact

Dow Chemical Endowed Chair Professor of Mechanical Engineering Louisiana State University +1-225-578-9192 khonsari@lsu.edu



## **Specialization**

Tribology, Mechanical Fatigue, Rotating Machinery

## Expertise

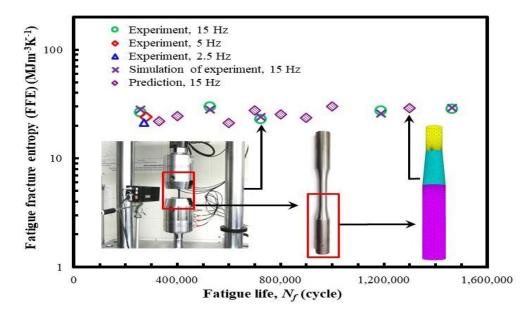
Surface characterization, interfacial phenomena, non-destructive testing, fatigue

#### Education

Ph.D. in Mechanical Engineering, The University of Texas at Austin (1983)

#### Research

Our group at LSU Center for Rotating Machinery has developed new techniques for measuring, predicting, analyzing components experiencing cyclic fatigue and damage due to degradation. The patented technologies enable one to reliability determine fatigue life in a non-destructive fashion, capable of monitoring structural health, predicting the reaming life of a specimen, and performing accelerated testing for new materials. These technologies are particularly useful for evaluation of the performance of 3D printed components.





#### **Richard L. Kurtz**

Director of CAMD Professor of Physics Louisiana State University Contact +1-225-772-4029 rlkurtz@lsu.edu



#### **Specialization**

Synchrotron based materials analysis; X-ray and electron spectroscopies

#### Expertise

Experimental surface science applying multiple analytical techniques to materials characterization focusing on oxides, thin films and supported nanoclusters on oxide surfaces.

#### Education

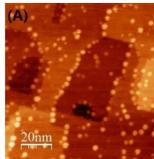
PhD in Applied Physics from Yale University (1983); National Research Council Ppostdoctoral fellowship at NIST (1983-85).

#### Research

One project that our group carries out with CIMM support is the characterization of the electronic structure of high-entropy alloy CoCrFeNi using photoelectron spectroscopy. This work involves both characterization of the electronic band structure with UPS as well as the chemical valence state using XPS. The stability of the surfaces of these materials are studied by carrying out oxidation measurements and the results show preferential oxidation of Cr and Fe while Co and Ni remain essentially metallic. These results can be compared directly to DFT studies carried out by other CIMM groups.



LSU's CAMD synchrotron



Cu nanoparticles on ZnO

CO Adsorption on 0.5ML Cu/ZnO T=85K 0.5ML Cu/ZnO T=



Consortium for Innovation in Manufacturing & Materials

# Guoqiang Li

# Contact

LSU Alumni Professor of Mechanical Engineering Louisiana State University/Southern University +1-225-578-5302 Iguoqi1@lsu.edu



## **Specialization**

Engineering mechanics; experimental mechanics;

## Expertise

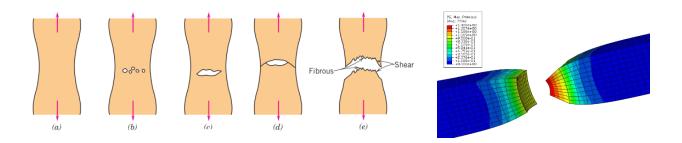
Structural analysis; composite joint; interfacial fracture.

## Education

Ph.D. in Civil Engineering from Southeast University (1997); postdoc at LSU (1997-2000).

## Research

Ongoing research in our group, supported by CIMM, focuses on interfacial fracture of 3D printed structures using selective laser melting (SLM). Major scientific issues addressed include: 1) interfacial fracture under Mode I, Mode II, and mixed Mode I&II loading; 2) finite element modeling of fracture of SLM printed dogbone specimen under uniaxial tensile loading. We are developing analytical modeling of the interfacial fracture of 3D printed metallic specimens, which have periodic zig-zag fracture path. We are also using commercially available software package such as ANSYS, to model the "cup and cone" fracture of printed specimens under uniaxial tension. Our research may help better understand fracture of printed metallic specimens under uniaxial tension of printed metallic specimens under uniaxial tension.





## Don Liu

## Contact

Contractor's Trust Professor Mathematics & Statistics, Mech. Engineering, Molecular Science, & Nanotechnology Louisiana Tech University +1 318 257 4670 donliu@latech.edu



## Specialization

Computational fluid dynamics; Numerical heat transfer; Computational mathematics.

## Expertise

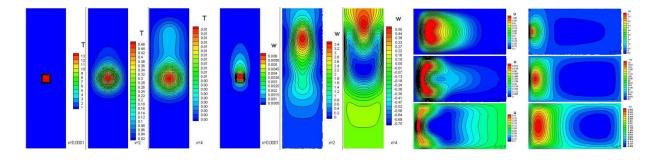
Spectral (high order finite) element method for numerical solutions to Navier-Stokes equations, energy equation, concentration equation, etc. partial differential equations describing conservation laws in three dimensional irregular spaces.

## Education

PhD in Applied Mathematics from Brown University (2004); PhD in Thermophysics from Chinese Academy of Sciences (1998); Post-doctoral fellow and research associate at NASA Goddard Space Flight Center, also at University of Maryland Baltimore County (2004-2006).

## Research

The project in my group supported by CIMM is to promote the better knowledge of phase change heat transfer phenomena via numerical simulations of laser-heating induced latent heat input and sensible heat transfer between melt, mushy and solid metal materials. These simulations involve tracking solid-liquid interfaces that are forming and disappearing in time and three dimensional finite spaces. The challenges include seeking numerical solutions to nonlinearly coupled partial differential equations about vector and temperature fields, predicting and tracking moving liquid-solid interfaces, and reconstructing interfacial surfaces, under various initial and boundary conditions. Governing equations involve six variables -- three velocities, pressure, temperature, and volume fraction, which is an indication of phase status: liquid, solid, or mushy zone. Self-developed parallel C++ codes were used to acquire modeling data.





#### Daniela S. Mainardi

Contact

Interim Director for Chemical and Nanosystems Engineering Thomas C. & Nelda Jeffery Professor Louisiana Tech University

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#### **Specialization**

Computational materials science and engineering; computational chemistry

#### Expertise

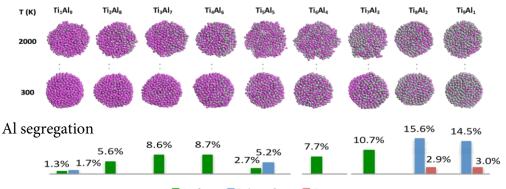
Molecular modeling of systems at the nano-scale with applications to catalysis and Materials Science.

## Education

PhD in Chemical Engineering - University of South Carolina (2003); MS in Materials Science and Technology – University of San Martin, Argentina (1998); BS in Physics – University of Buenos Aires, Argentina (1997).

#### Research

Our computational modeling approach developed for this CIMM project is helping elucidate the atomic ordering and distribution in Ti-Al alloys as temperature is reduced from 2000 K (where the metallic alloy is in the liquid phase) to 300K (where the alloy has solidified). A Python code created in the Mainardi group starts with a random initial configuration of the model system representing the alloy, then a Classical Monte Carlo algorithm is used to find the most probable atomic configuration, and finally the system is heat-treated at the temperature of interest according to a Molecular Dynamics simulation in this final step.



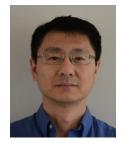
Surface Sub-surface Core



## Wen Jin Meng

Contact

Williams Professor of Mechanical Engineering Louisiana State University +1-225-578-5832 wmeng1@lsu.edu



## Specialization

Experimental materials science: micro/nano fabrication, surface engineering, plasma processing

#### Expertise

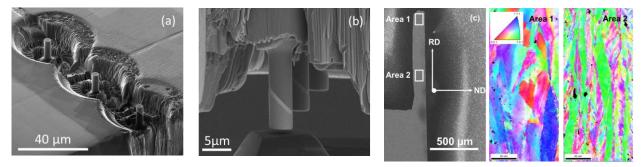
Plasma assisted vapor phase deposition; materials characterization; micro mechanical testing; micro/nano fabrication.

## Education

Ph.D. in Applied Physics from Caltech (1988); post-doc at Argonne National Laboratory (1988-89).

#### Research

Ongoing research in our group, supported by CIMM, focuses on small scale metal forming and pattern replication. Major scientific issues addressed include: 1) intrinsic and extrinsic materials' size effects relevant to sub-mm to micron scale forming and replication; 2) solid/solid interfacial mechanical integrity relevant to coating based surface engineering and mechanical performance of layered solids, including those made by additive manufacturing (AM). We are developing microscale, in-situ, mechanical testing capabilities, and applying them in combination with micro/nano scale materials characterization techniques to generate new understanding and new insights regarding mechanical size effects, interfacial mechanical response, and new materials for AM.





Consortium for Innovation in Manufacturing & Materials

#### Patrick F Mensah

Contact

Formosa Endowed Professor Associate Dean For Research Southern University +1-225-771-2975 patrick\_mensah@subr.edu



## Specialization

Experimental and computational fluid and heat transfer

#### Expertise

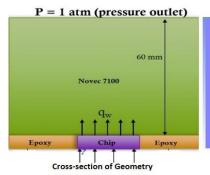
Modeling, processing, and thermo-mechanical property characterization of composite materials, high temperature superalloys and ceramic thermal barrier coatings

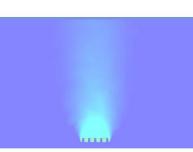
#### Education

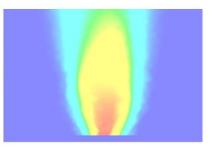
Ph.D. in Engineering Science from Louisiana State University (1998).

#### Research

Ongoing research in our group, supported by CIMM, focuses on developing computational heat transfer models for analysis of multi-phase heat transfer in microscale heat sinks manufactured by metal forming. Numerical modeling and simulation approaches for analyzing additive manufacturing (AM) processes of metal powders involving laser as input heat sources is also under development. AM produce parts through the layer-by-layer addition of molten material that generates large temperature gradients that cause plastic deformation. Thermo-mechanical models predict the thermal history, mechanical distortion due interfacial thermal stresses. This enables the process to be studied and for distortion mitigation techniques to be developed. Such investigations required models that accurately capture the physics of the deposition process.







Patterned: Vapor contour @ q" = 50 W/cm<sup>2</sup>

Unpatterned: Vapor contour @ q" = 50 W/cm<sup>2</sup>



## Dorel Moldovan

Fruehan Family Professor of Mechanical Engineering Mechanical & Industrial Engineering Dept., Louisiana State University

#### Contact

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#### **Specialization**

Atomistic and mesoscale modeling and simulation of materials.

#### Expertise

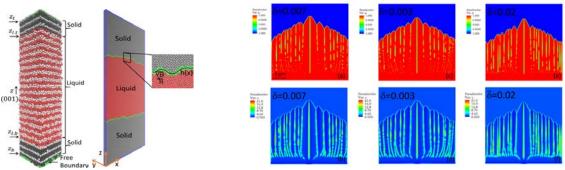
Molecular dynamics and free energy calculation methodologies; simulation of interfacial phenomena/properties and microstructure formation and evolution.

#### Education

PhD in Physics from West Virginia University (1999); post-doc at Argonne National Laboratory (1999-2002)

#### Research

The CIMM supported ongoing research in our group focuses on the development of atomistic level understanding of the mechanism and parameters controlling the kinetics and microstructure development during rapid solidification of metals and metallic alloys. Major scientific achievements include: i) the development of new interatomic MEAM potentials suitable for high temperature molecular dynamics (MD) and Monte Carlo (MC) simulations of crystal-melt interfaces in metallic alloys ii) using Ti-Ni as alloy model system, we developed, validated, and used a set of methodologies for MD and MC simulations used to determine crystal-melt (CM) anisotropic interfacial properties such as: CM interfacial energy, interfacial mobility, and kinetic coefficient and the corresponding anisotropy parameters; properties which are difficult or even impossible to measure in experiments iii) developed an hierarchical atomistic - phase field simulation approach for investigation of microstructure formation during rapid solidification. Our research has the potential to impact technologies with great relevance to additive manufacturing by providing accurate quantification of the role of various external and material parameters such as temperature field, cooling rates, alloy composition, crystal-melt anisotropic properties, etc., on the formation of dendritic structure and solute segregation pattern during rapid solidification.





#### Arden Moore

Assistant Professor Mechanical Engineering Institute for Micromanufacturing Louisiana Tech University

## Contact

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#### **Specialization**

Heat transfer; nanomaterials

#### Expertise

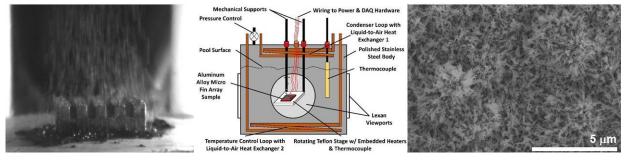
Experimental thermal transport investigations at macro-, micro-, and nanoscales; Conduction and phase change processes; Thermal and electrical characterization of materials.

#### Education

PhD in Mechanical Engineering from The University of Texas at Austin (2010); postdoctoral fellowship at University of Texas at Austin (2010-11); previously a Thermal Advisory Engineer at IBM (2011-2013).

#### Research

Our group is focused on investigating technologically relevant applications of the fundamental manufacturing science being developed through CIMM. One project focuses on optimizing low profile heat sinks made via scalable microforming for use in direct immersion two-phase cooling environments. Another utilizes the design flexibility of additive manufacturing to realize non-traditional heat sink designs inspired by nature. For both of these works, we are also looking at multiscale surface features such as nanowires that can be formed via scalable methods to enhance heat transfer at the macroscale.





#### Juana Moreno

Associate Professor Physics & Astronomy and Center Computation & Technology Louisiana State University Contact

+1-225-578-7586 moreno@lsu.edu



## **Specialization**

Computational materials science, strongly correlated systems.

#### Expertise

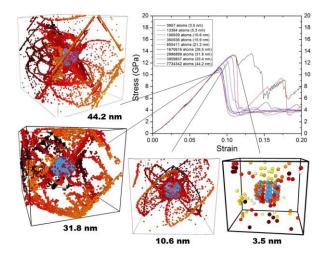
Dynamical mean-field theory and its extensions to explore the experimentally relevant transport and magnetic properties of correlated electron systems.

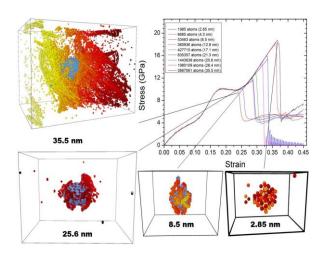
## Education

PhD in Physics from Rutgers, The State University of New Jersey (1997); post-doctoral positions at the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy (1996-1998) and Northwestern University, Evaston, US (1998-2001).

## Research

One project in our group supported by CIMM is aimed at understanding the role of voids on metallic alloys. We study the failure mechanisms at the atomistic scale when subjected to loading. This work requires extensive computations of the stress-strain curves, yield stress, elastic constants, etc at different loading rates, cell sizes and void volume fraction. This year we have focused on Ni<sub>3</sub>Al and NiAl.







#### Yang Mu

Research Assistant Prof. Mechanical Engineering Louisiana State University **Contact** 225-578-5947 ymu1@lsu.edu



#### **Specialization**

Vacuum technology, Physical vapor deposition, thin film preparation, material characterization, mechanical testing in micro-scale

#### Expertise

Vapor phase deposition; materials characterization; micro mechanical testing; micro/nano fabrication.

#### Education

PhD in Engineering from LSU (2016); post-doctoral research associate at LSU (2016-18).

## Research

We design and build ultra-high vacuum system to deposit metal/ceramic thin films. And carry out characterization on thin films prepared. Method of in-situ and ex-situ mechanical testing on thin film interfacial region has been developed to test its integrity.



Contact

Adarsh D. Radadia

Assistant Professor Chemical Engineering Louisiana Tech University +1-318-257-5112 radadia@latech.edu



#### **Specialization**

Surface chemistry and characterization; Micro-analytical instrumentation

#### Expertise

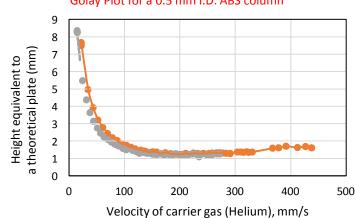
Surface modification chemistry of metal oxides for gas chromatography column development; System-level integration of a micro gas chromatograph

#### Education

PhD in Chemical Engineering from University of Illinois (2009); post-doctoral research associate at University of Illinois (2009-11).

#### Research

One project in our group supported by CIMM is aimed at understanding the passivation chemistry needed at the interface of a metal column and the required polymer coating for separation of volatiles with different organic functional groups. This work requires extensive gas chromatography-mass spectrometry experiments. To address the need to develop cost-effective micro gas chromatographs, we are also exploring the use of fused filament extrusion to build a preconcentrator, a column and a detector.



#### Golay Plot for a 0.5 mm I.D. ABS column



#### B. Ramu Ramachandran

#### Contact

Associate VP for Research Dean of Graduate School T. L. James Eminent Scholar Chair Professor Louisiana Tech University +1-318-257-4304 ramu@latech.edu



## **Specialization**

Computational materials science; computational chemistry

#### Expertise

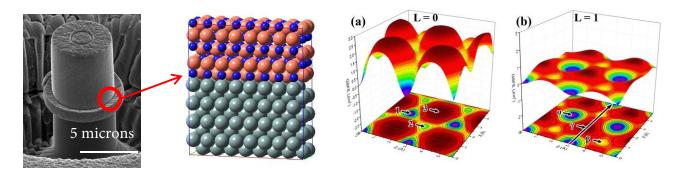
First principles simulations of structures and properties of solids and surfaces; Density functional theory applied to metal/ceramic interfaces and oxidation of metals and alloys.

#### Education

PhD in Chemistry from Kansas State University (1987); post-doctoral fellowship at University of Texas at Austin (1987-89).

#### Research

One project in our group supported by CIMM is aimed at understanding the properties of metal/ceramic interfaces and their failure mechanisms at the atomistic scale when subjected to shear loading. This work requires extensive first principles Density Functional Theory (DFT) calculations. To address the shear failure mechanism at larger length scales, we are also developing new Modified Embedded Atom Method (MEAM) potentials using DFT calculations. Another CIMM-supported effort involves the study of oxidation of metals and alloys, again using DFT calculations.





## **Paul Schilling**

Professor University of New Orleans **Contact** +1-504-280-6632 pschilli@uno.edu



## **Specialization**

Materials Characterization

#### Expertise

Materials characterization including mechanical properties and microstructural characterization; metastable alloys; spark plasma alloying.

#### Education

Ph.D. in Mechanical Engineering, Louisiana State University, 1992.

#### Research

Dr. Schilling directs an applied research program in the development and characterization of materials. He has worked extensively in novel metallurgical techniques including mechanical alloying for the development of nanocrystalline alloys; and metal surface modification by electro-plasma processing and electro-spark alloying for improved corrosion and wear resistance. Studies have included the application of mechanical alloying in the production of nanostructured half-Heusler alloys for thermoelectric power generation, and the characterization of processing effects on the stir zone in friction stir welded aluminum alloys. In addition, Dr. Schilling is the co-author of the computer-aided design text, Parametric Modeling with SolidWorks.



## Dr. Naidu V. Seetala

## Contact

Edward Bouchet Endowed Professor in Physics Grambling State University +1-318-274-2574 naidusv@gram.edu



## **Specialization**

Material Science and Nano-technology: Ultra high temperature ceramic nanocomposites, Polymer composites - nanoporosity using positron annihilation lifetime spectrometer, Nanocatalysts using sol-gel/oil-drop methods for syn-gas conversion for higher alkanes, and hydrogen production using WGS reactions for fuel cell applications, and Magnetic nanoparticles for storage media applications.

#### Expertise

Established state of the art research facilities at GSU including Positron Annihilation Lifetime Spectroscopy, Magneto-sputter thin film coater, Vibrating Sample Magnetometer, SQUID magnetometer, Environmental SEM with EDXS, X-ray Diffraction (XRD), and Mossbauer spectroscopy.

#### Education

Obtained Post-Doctoral Research training at the University of Texas at Arlington for about 3 years after completing Ph.D. in Physics from the Saha Institute of Nuclear Physics, Calcutta, India.

#### Research

Obtained research experience as visiting scientist at Argonne National Laboratory, NASA Glenn Research Center, and Wright Patterson Air Force Base, the MINT center, University of Alabama at Tuscaloosa, and as an adjunct professor at Louisiana Tech University. Received funding as a PI for several research grants supported by NASA, DOE, NSF, ONR, and AFOSR. He has over 70 research publications in refereed journals. His NASA research has been highlighted on CBS KNOE TV8 Evening/Night News, and his Ultra High Temperature Ceramics research has been highlighted in "The News Star", Special Issue, Monroe. As per the "Research Gate Spotlight", his publications reached 200 citations and 400 reads just in last year.



## Shuai Shao

**Contact** +1-225-578-1

Assistant Professor of Mechanical Engineering Louisiana State University +1-225-578-1711 sshao@lsu.edu



## **Specialization**

Computational materials science with interests in solid-solid interfaces.

## Expertise

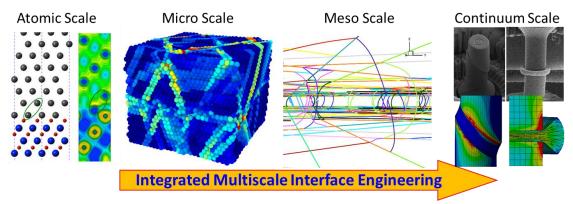
Materials modeling across length and time scales: first principal density functional theory, molecular dynamics, dislocation dynamics, continuum plasticity modeling.

## Education

Ph.D. in Mechanical Engineering from Washington State University (2012); post-doc at Los Alamos National Laboratory (2012-2016).

#### Research

The main focus of my group, supported by CIMM, is to realize the multiscale interface engineering of metal/ceramic material systems. We first attempt to understand the structure and properties of the metal/ceramic interfaces through an integrated multiscale modeling approach. We start from the atomic scale and micro scale: where the intrinsic properties of the interfaces, such as their energetics and dislocation structures, are probed using first principles and atomistic modeling tools. Such findings are then analyzed and incorporated into a meso scale dislocation dynamics model. The output from the meso scale model is then used to inform the continuum scale plasticity models, which, in turn, enable the accelerated design of metal/ceramic materials.





#### Name

#### Contact

Damon Smith Assistant Professor of Mechanical Engineering University of New Orleans +1-504-280-6167 dsmith3@uno.edu



#### **Specialization**

Nanoparticles, Nanocomposites, Advanced Materials for Additive Manufacturing

#### Expertise

Enhancement of mechanical and physical properties of additive manufacturing materials through incorporation of multifunctional nanoparticle additives.

#### Education

University of New Orleans, New Orleans, LA, Physics, B.S. 2003 University of New Orleans, New Orleans, LA, Applied Physics, M.S. 2005 University of Texas at Austin, Austin, TX, Materials Science and Engineering, Ph.D. 2009

## Research

Research in our group is concerned with the scalable, high-yield synthesis of nanoparticles and their assembly into new classes of fabrics, composites, and other macroscale materials. We are currently exploring the inclusion of metal and semiconductor nanoparticles within thermoplastic matrices to produce multifunctional nanocomposites compatible with extrusion, injection molding, and 3D printing processes. The understanding of how these manufacturing processes influence material structure at the nano-, micro-, and mesoscale and the characterization of the associated structure-property relationships is key to optimizing their performance. Applications of interest include biomedical devices and 3D electronics and optoelectronics.



Phillip T. Sprunger

Scientific Director of CAMD Professor of Physics Louisiana State University **Contact** +1-225-328-3943 phils@lsu.edu



#### **Specialization**

Experimental condensed matter physics; surface/interfacial electronic, structural, and chemical phenomena

#### Expertise

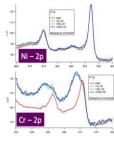
Electron- and photon-based spectroscopies and scattering; synchrotron-based X-ray and VUV absorption/photoemission; thin-film, surface, nano metal alloys and oxides.

#### Education

PhD in Physics from University of Pennsylvania (1993); postdoc in nanomaterial at University of Aarhus, Denmark (1993-1995)

#### Research

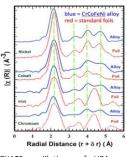
One research thrust of our group supported by CIMM focuses on the synthesis and characterization of high-entropy alloys (HEA) such as CrCoFeNi and CrCoFeNiCu. Specifically, we have used a number of experimental probes to elucidate the microstructural, electronic, and chemical bulk and surface properties. We have found the although the surface atomic composition is equivalent to the bulk, Ni (and Co) are relatively inert to oxidation. This yields insight into corrosion resistance of HEAs. In addition, we are currently installing an *in-situ* x-ray scattering system to monitor details of laser-melt/solidification processes of alloy powders used in advanced manufacturing.



XPS of CrCoFeNi surface upon adsorption of oxygen



EBSD image showing large grain growth of CrCoFeNi



EXAFS oscillations of HEA and standards revealing local structure



## George Z. Voyiadjis

Boyd Professor Department of Civil and Environmental Engineering Louisiana State University Contact

+1-225-578-8668 voyiadjis@eng.lsu.edu



#### **Specialization**

Computational solid mechanics; Computational materials science

#### Expertise

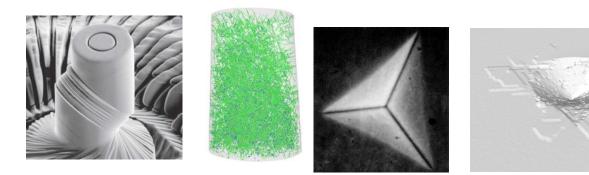
Voyiadjis' primary expertise is in plasticity and damage mechanics of metals, metal matrix composites, polymers and ceramics with emphasis on the theoretical modeling, numerical simulation of material behavior, and experimental correlation.

## Education

D.Eng.Sc. (Engineering Mechanics), May 1973, Columbia University. M.Sc. (Civil Engineering), May 1970, California Institute of Technology.

#### Research

The current research in our group, supported by CIMM, focuses on nonlocal continuum modelling and atomistic simulation of small scale metal forming and pattern replication. Major scientific issues addressed include intrinsic and extrinsic materials' size effects relevant to sub-mm to micron scale forming and replication. The size effects in metallic samples of confined volumes are addressed during the nanoindentation and micropillar compression experiments. We are developing continuum models in metallic samples of confined volumes to capture the size effects observed during the atomistic simulations and microscale, in-situ, mechanical experiments.





#### **Leland Weiss**

Contact

Interim Director of Civil & Mechanical Engineering & Construction Engineering Technology Thurman Lauret Professor Louisiana Tech University +1-318-257-5113 lweiss@latech.edu



#### **Specialization**

Small-scale thermal management and materials for device applications

#### Expertise

Micro and Meso-scale fabrication techniques and device design and characterization. Microfluidics and small-scale energy generation and thermal control.

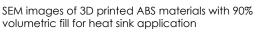
#### Education

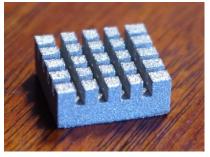
PhD in Mechanical Engineering from Washington State University (2007); B.S. in Mechanical Engineering from Carnegie Mellon University (1999)

#### Research

CIMM sponsored activities in our group focus on manufacturability and materials research applied to fused deposition modeling techniques (3D printing) and stainless steel 3D printed structures through CIMM cross-campus collaborations. Additives that include metallic and nanoscale powders are incorporated with more traditional, non conductive plastics like ABS using high shear techniques. This enhances thermal and electrical conductivities of these materials. Using microscale features, these heat sinks and heat exchangers are under investigation and comparison with metal based counterparts. This work fundamentally enhances on-site repair and design flexibility for a wide range of heat transfer applications through advanced manufacturing approaches.







Metal 3D printed Heat Sink using Stainless Steel and high surface area finish



Contact

## Collin D. Wick

Assoc. Dean of Grad. Studies College of Eng. and Science Louisiana Tech University +1-318-257-2345 cwick@latech.edu



## **Specialization**

Computational materials science; computational chemistry

#### Expertise

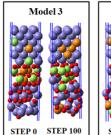
Development of efficient algorithms for first principles and large scale simulations. Molecular model parameterization for metals and ceramics. First principles calculations of material properties and the impact of doping and oxidation on metals, ceramics, and their interfaces.

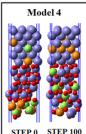
## Education

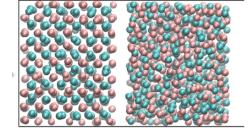
PhD in Physical Chemistry from University of Minnesota (2003); post-doctoral fellowships at National Technical University Athens (2004) and Pacific Northwest National Laboratory, Richland, WA (2004-2007).

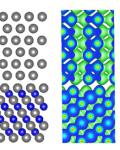
## Research

We primarily use DFT calculations to investigate the doping and oxidation of metals, metal surfaces, and metal-ceramic interfaces. To expand the scale of potential systems that can be investigated, we also developed a methodology to efficiently parameterize modified embedded atom models (MEAM). The parameterization methodology utilizes Monte Carlo minimization along with a genetic algorithm to rapidly search the multidimensional parameter space necessary for MEAM. We also developed a Monte Carlo minimization procedure to rapidly determine the distribution of oxides and dopants at metal surfaces and metal/ceramic interfaces.











**Chester Wilson** Associate Professor Louisiana Tech University Contact +1-318-497-0659 chester@latech.edu



#### **Specialization**

Microfabrication, MEMS/NEMS/Integrated Circuit Design, Nanotechnology

#### Expertise

Fabrication of complex alloy nanochemistry dervived particles, Microfabrication of metalic alloy parts, Development of 2D carbon-metalic bonding.

#### Education

PhD in Electrical Engineering from University of Wisconsin-Madison (1987); post-doctoral fellowship at University of Michigan-Ann Arbor (1987-89).

#### Research

One project in our group supported by CIMM is aimed at electrochemical methods to manufacture metal micro- and nanoparticles. Molten spray methods, which are the most widely used method for larger particles to be used in 3D manufacturing, are produced using a spray atomizer of one form or another. Some sprays use gas, flames, or water. Electrochemistry is well understood and has been in used for many processes for a long time. However, electrochemistry has not been widely studied for the purpose of manufacturing micro- and nanoparticles.

