



# 2019 Joint AFOSR & NSF Program Review: Quantitative Representation of Microstructure and Aerospace Materials for Extreme Environments

Dr. Alexis Lewis and Dr. Ali Sayir | May 20-24, 2019 | Alexandria, VA



DAY 1 – 20 MAY 2019		
7:30-8:00	REGISTRATION	
8:00-8:10	WELCOMING REMARKS	A. Lewis & A. Sayir
8:10-8:50	William Colglazier / AAAS & Previous Science Advisor of Secretary of State & NAS	
8:50-9:00	BREAK	
PREDICTIVE MATERIAL SCIENCE		
9:00-9:40	(QRM 18) Microstructural Quantification and Virtual Reconstruction	M. Maiaru U MASS LOWELL
9:40-10:20	(QRM 18) Visual Info to Quantify Microstructure-Processing Relationship	E. Holm & B. Webler CMU
10:20-10:40	BREAK	
10:40-11:20	(QRM 18) Cellular Materials via a Multiscale Quantitative Representation	Y. Zhu & L. Li VIRGINIA TECH
11:20-12:00	(QRM 18) Hybrid Adversarial-Training Methods for 3D Microstructures	S. Niezgoda & D. Dimiduk OHIO STATE UNIVERSITY
12:00-13:00	Linda Sapochak / NSF	WORKING LUNCH
13:00-13:30	LEGOMAT: Locally Extracted Globally Organized Microstructure Models	V. Sundararaghavan U. MICHIGAN
13:30-14:00	A Machine Learning for Quantitative Structure-Property Relationship	S. Patala NCSU
14:00-14:30	BREAK	
14:30-15:00	Atom Probe Tomography Imaging to Microstructural Quantification	E. Marquis & W. Windl U. MICHIGAN / OSU
15:00-15:30	Computationally Guided Discovery of Shape Memory Alloys	J. Vlassak and R. Arroyave HARVARD U. & TEXAS A&M
15:30-16:00	Scientific Understanding of Interfaces	H. Sehitoglu UIUC
POSTER INTRODUCTIONS		
Students & Unfunded projects & New starts (underlined)		
16:00-17:30	<ul style="list-style-type: none"><li>• C. Woodward. / AFRL:</li><li>• R. Kukreja / UC DAVIS:</li><li>• S. Yang / SU A&amp;M:</li><li>• M. Berg / KANSAS STATE:</li><li>• R. M. Modibedi / CNR:</li><li>• B. Yildiz / MIT:</li><li>• M. Shakiba / VT:</li><li>• Y. Ren / CUNY:</li><li>• J. Lebeau / MIT:</li><li>• L. Piper / BINGHAMTON:</li><li>• M. Raschke / COLORADO:</li><li>• I. Javaheri / MICHIGAN:</li><li>• E. Wang / MIT:</li><li>• Z. Zhang / PURDUE:</li><li>• K. Pachuta / CWRU:</li><li>• R. Santos / CWRU:</li><li>• P. Acar / VT:</li></ul>	<p>Window Development Tools for Hypersonic Applications, Speed Limit of Magnetization Dynamics in Magnetic Heterostructure, High Temperature and Pressure Multicomponent Alloy Design Field Enhanced Optical Transmission in Metal Crystalline Films using Electrochemical Atomic Layer Deposition Mechanisms of Surface Chemical and Electrochemical Stability on Perovskites Multiphysics Modeling and Sensitivity Analysis of Fiber-Reinforced Composites Chemical Engineering of Nanoscale Polarization at the SrTiO<sub>3</sub>/Ge Interface. Connecting Chemical Order and Nanoscale Polarization Electronic and Thermal Properties of Niobium Oxide Nonlinear Nano-Optics: A new regime of nonlinear optics in confined geometries Polycrystalline Microstructure Reconstruction Using Markov Random Fields Area-Enhanced Hierarchical Evaporator for Extreme Thermal Management Electrical Conductivity Relaxation in NiO thin Film Crystals Salt Precipitation of 2D Cobalt Oxide Nanosheets Surface State 2DEG on Li-covered CoO<sub>2</sub> Mono- and few-layer Films Multi-Scale Uncertainty Quantification in Computational Modeling of Materials</p>



# 2019 Joint AFOSR & NSF Program Review: Quantitative Representation of Microstructure and Aerospace Materials for Extreme Environments

Dr. Alexis Lewis and Dr. Ali Sayir | May 20-24, 2019 | Alexandria, VA



**DAY 2 – 21 MAY 2019**

## **SYNTHESIS SCIENCE**

7:30-8:00	Registration	
8:00-8:30	Density Functional Theory Studies of Hydrogen/Nitrogen	D. A. Gómez-Gualdrón&J. Wilcox CSM
8:30-9:00	Electronic structure basis for solubility and phase stability in metal alloys	M. Ghazisaeidi OSU
9:00-9:30	The Local Structure and Chemistry in Marginal Glass Forming Alloys	E. Kalay and I. Kalay ODTU
<b>9:30-10:00</b>	<b>BREAK</b>	
10:00-10:30	The Nature of Quasi-periodic Avalanche Bursts Fatigue Cracks	J. El-Awady JHU
10:30-11:00	Theory and Experimentation of High Temperature Shape Memory Alloys	I. Karaman TEXAS A & M
11:00-11:30	Computational-Experimental Reactive Wetting of Hf-Ti-Me Alloy Melts	V. Kumar and A. Bronson UTEP
11:30-12:00	Phenomenological Theory of Transport Phenomena in Molten Sulfide system	A. Allanore MIT
<b>12:00-13:00</b>	<b>William Carter / DARPA DSO</b>	<b>WORKING LUNCH</b>
13:00-13:30	Role of Carbon Vacancies on Properties of Transition-Metal Carbides	S. Kodambaka UCLA
13:30-14:00	Scalable, Solution-Phase Routes towards Metal Carbides	J. Goldberger OSU
14:00-14:30	Creep Deformation and Durability of Ultra High Temperature Materials	M. Ruggles-Wrenn AFIT
<b>14:30-15:00</b>	<b>BREAK</b>	
15:00-15:30	High-Temperature Ceramic Grain Boundaries with Electric Fields	J. Luo UCSD
15:30-16:00	(YIP 17) Far-from-Equilibrium Structures and Processes	R. Jayan CMU
16:00-16:30	Computationally-Guided Discovery of Semiconductors & Conduction Polarity	J. Goldberger & W. Windl OSU



# 2019 Joint AFOSR & NSF Program Review: Quantitative Representation of Microstructure and Aerospace Materials for Extreme Environments

Dr. Alexis Lewis and Dr. Ali Sayir | May 20-24, 2019 | Alexandria, VA



DAY 3 – 22 MAY 2019

## PREDICTIVE MATERIAL SCIENCE AND SYNTHESIS SCIENCE

7:30-8:00	Registration	
8:00-9:00	Atomically thin 2D oxides	A. Sehirlioglu, W. Lambrecht, and X. Gao, M.-H. Berger CWRU & PARISTECH
9:00-9:30	Prediction of Diffusionless Phase Transformations in Complex Materials	R. Hay AFRL
<b>9:30-10:00</b>	<b>BREAK</b>	
10:00-10:30	Feasibility Investigation to the Interfacial Understanding of Dissolution	C. Randall PSU
10:30-11:00	Advances In Green Processing to form Transparent Ceramics	R. Speyer GIT
11:00-11:30	Optical Ceramics Science for High-Power Lasers	R. Gaume UCF
11:30-12:00	Study of Heavy Metal Oxide Glasses for High Power Lasers	K. Lipinska UNM
<b>12:00-13:00</b>	<b>Isik C. Kizilyalli / ARPA-E</b>	<b>WORKING LUNCH</b>
13:00-13:30	Metal/Dielectric Interface in Dielectric Degradation and Breakdown	D. Irving NCSSU
13:30-14:00	Controlling resistance degradation of high-permittivity dielectrics	A. Klein DARMSTADT
14:00-14:30	Nonlinear optical imaging of coupled breakdown dynamics in dielectrics	S. Greenbaum and Y. Ren HUNTER COLLEGE
14:30-15:00	Anisotropy and Defects on the Electrocaloric Relaxor Ferroelectrics	E. M. Alkoy GEBZE
15:00-15:30	Nanoscale Pyroelectric Hybrid Materials	J. Shi RPI
15:30-16:00	(DURIP) Field-induced Evolution of Dielectric Materials	E. Dickey & D. Vashaee NCSSU
<b>POSTER SESSION</b>  Students & Unfunded projects & New starts ( <u>underlined</u> )  <b>16:00-19:00</b>  <b>NO HOST SOCIAL</b>	<ul style="list-style-type: none"> <li>• <u>C. Woodward / AFRL:</u></li> <li>• <u>R. Kukreja / UC DAVIS:</u></li> <li>• <u>S. Yang / SU A&amp;M:</u></li> <li>• <u>M. Berg / KANSAS STATE:</u></li> <li>• R. M. Modibedi / CNR:</li> <li>• B. Yildiz / MIT:</li> <li>• M. Shakiba / VT:</li> <li>• Y. Ren / CUNY:</li> <li>• J. Lebeau / MIT:</li> <li>• L. Piper / BINGHAMTON:</li> <li>• M. Raschke / COLORADO:</li> <li>• I. Javaheri / MICHIGAN:</li> <li>• E. Wang / MIT:</li> <li>• Z. Zhang / PURDUE:</li> <li>• K. Pachuta / CWRU:</li> <li>• R. Santos / CWRU:</li> <li>• P. Acar / VT:</li> </ul>	Window Development Tools for Hypersonic Applications, Speed Limit of Magnetization Dynamics in Magnetic Heterostructure, High Temperature and Pressure Multicomponent Alloy Design Field Enhanced Optical Transmission in Metal Crystalline Films using Electrochemical Atomic Layer Deposition Mechanisms of Surface Chemical and Electrochemical Stability on Perovskites Multiphysics Modeling and Sensitivity Analysis of Fiber-Reinforced Composites Chemical Engineering of Nanoscale Polarization at the SrTiO <sub>3</sub> /Ge Interface. Connecting Chemical Order and Nanoscale Polarization Electronic and Thermal Properties of Niobium Oxide Nonlinear Nano-Optics: A new regime of nonlinear optics in confined geometries Polycrystalline Microstructure Reconstruction Using Markov Random Fields Area-Enhanced Hierarchical Evaporator for Extreme Thermal Management Electrical Conductivity Relaxation in NiO thin Film Crystals Salt Precipitation of 2D Cobalt Oxide Nanosheets Surface State 2DEG on Li-covered CoO <sub>2</sub> Mono- and few-layer Films Multi-Scale Uncertainty Quantification in Computational Modeling of Materials



# 2019 Joint AFOSR & NSF Program Review: Quantitative Representation of Microstructure and Aerospace Materials for Extreme Environments

Dr. Alexis Lewis and Dr. Ali Sayir | May 20-24, 2019 | Alexandria, VA



## DAY 4 – 23 MAY 2019

7:30-8:00	Registration	
8:00-8:30	Computational Investigation of Quantum Thermal and Electric Transport	T. Haugan AFRL
8:30-9:00	PT-Symmetric Programmable Materials	S. K. Ozdemir & M. Demirel PSU
9:00-9:30	Defect Equilibration Studies in Binary Metal-Oxides	S. Ramanathan PURDUE
<b>9:30-10:00</b>	<b>BREAK</b>	
10:00-10:30	Soft Chemical Approaches to the Synthesis of Metastable Materials	D. Freedman NORTHWESTERN
10:30-11:30	Extreme Nonlinearity in Transition Metal Oxides	A. Demkov and J. Ekerdt UT AUSTIN
11:00-11:30	Directionally-Solidified Spiral Eutectics: Towards Chiral Materials	A. J. Shahani MICHIGAN
<b>12:00-13:00</b>	<b>TBD / ONR</b>	<b>WORKING LUNCH</b>
13:00-14:00	Nonlinear Studies of Electro-Optic and Magneto-Electric Materials	G. Khodaparast, S. Priya, M. B. Raschke, A. Belyanin and C. Stanton VT / COLORADO/ FLORIDA
14:00-14:30	Ceramic Nanolaminates for Electromagnetic Shielding for the RF	J. Kennedy, D. Nepal, R. Pachter, and R. Vaia AFRL
<b>14:30-15:00</b>	<b>BREAK</b>	
15:00-15:30	Surface Roughness Effects in Reflection and Emission of IR Radiation	K. Sendur SABANCI
15:30-16:00	Permittivity, Polarization, and Gas Dynamics in Electroceramics	B. Tilley WPI
16:00-16:30	Millimeter Wave Interactions with High Temperature Materials	B. Hoff AFRL
16:30-17:00	Nonreciprocal Metal-Dielectric Structures for Electromagnetic Isolation	A. Chabanov UTSA





# 2019 Joint AFOSR & NSF Program Review: Quantitative Representation of Microstructure and Aerospace Materials for Extreme Environments

Dr. Alexis Lewis and Dr. Ali Sayir | May 20-24, 2019 | Alexandria, VA



DAY 5 – 24 MAY 2018		
7:30-8:00	Registration	
8:00-9:00	(MURI 18) Gallium Oxide Materials Science and Engineering (GAME )	J. Speck UCSB
9:00-10:00	(MURI 18) Doping and Defects in Ga <sub>2</sub> O <sub>3</sub> for High Breakdown Field	M. Scarpulla U UTAH
<b>10:00-10:30</b>	<b>BREAK</b>	
10:30-11:00	Material Properties of $\beta$ -Ga <sub>2</sub> O <sub>3</sub> for Electronic and Electric Applications	S. Badescu, D. Thomson, and S. Ganguli AFRL
11:00-11:30	Growth Mechanism and Defect Formation in $\beta$ - (Al <sub>x</sub> Ga <sub>1-x</sub> ) <sub>2</sub> O <sub>3</sub> /Ga <sub>2</sub> O <sub>3</sub>	A. Popp and G. Wagner IKZ
11:30-12:00	Extreme Environment Stability of Wide Band Gap $\beta$ -Ga <sub>2</sub> O <sub>3</sub>	N. Alem PSU
<b>12:00-13:00</b>	<b>Alexis Lewis / NSF</b>	<b>WORKING LUNCH</b>
13:00-13:30	The Strain-stress Relations for Bandgap, Phonon and Plasmon Energy's	M. Schubert U. NEBRASKA –LINCOLN
13:30-14:00	Mechanisms and Control of Dielectric Breakdown in Electronic Materials	L. Brillson OSU
14:00-14:30	Mechanisms of Electrical Contact Resistance	M. Baykara & A. Martini UC MERCED
14:30-15:00	Fabrication, Processing and Characterization of Contacts to $\beta$ -Ga <sub>2</sub> O <sub>3</sub>	R. V. Chintalapalle & L. Porter UTEP & CMU
15:00-15:30	Toward Bio-Inspired Smart Thermal Spreaders (BSTS)	H. Ghasemi U. HOUSTON