4\textsuperscript{TH} Southwest Energy Science and Engineering Symposium

March 22, 2014
Double Tree Hotel
600 North El Paso Street
El Paso, TX 79901

Department of Mechanical Engineering
College of Engineering
University of Texas El Paso
500 W. University Ave.
El Paso, Texas 79968
Phone: (915)-747-5450 Fax: (915)-747-5019
seses@utep.edu

Web Link: http://engineering.utep.edu/seses/
Welcome to the Southwest Energy Science and Engineering Symposium sponsored by Shell. The purpose of the symposium is to encourage communication among the engineers and scientists in and around the El Paso area’s universities and industries.

The following individuals and organizations are acknowledged for their assistance with the symposium.

**Conference Chair:**
Dr. Ahsan Choudhuri  
University of Texas El Paso

**Technical Chair:**
Dr. Yirong Lin  
University of Texas El Paso

**Logistics Committee:**
Carmen Medellin, University of Texas El Paso  
Laura Orozco, University of Texas El Paso  
Gloria Salas, University of Texas El Paso

**Hosted By:**
College of Engineering  
Department of Mechanical Engineering &  
Center for Space Exploration and Technology Research (cSETR)  
University of Texas El Paso

**Welcome and Introduction:**
Dr. Richard Schoephoerster  
Dean, College of Engineering  
University of Texas El Paso

**Session Chairs:**
Dr. Shaolin Mao, University of Texas El Paso  
Dr. Paras Mandal, University of Texas El Paso  
Dr. Calvin Stewart, University of Texas El Paso  
Dr. Eric Petersen, TAMU  
Dr. Vinod Kumar, University of Texas El Paso  
Dr. Evgeny Shafirovich, University of Texas El Paso  
Dr. Jack Chessa, University of Texas El Paso  
Dr. Norman Love, University of Texas El Paso  
Dr. C.V. Ramana, University of Texas El Paso  
Dr. Pavana Prabhakar, University of Texas El Paso  
Dr. Yirong Lin, University of Texas El Paso  
Dr. Sara Gaytan, University of Texas El Paso

**Keynote Address:**
Theva Thevuthasan, Ph.D.  
Staff Scientist and Manager  
Environmental Molecular Sciences Laboratory  
U.S. Department of Energy

Vijay Murugesan, Ph.D.  
Senior Materials Scientist  
Pacific Northwest National Laboratory  
U.S. Department of Energy
Southwest Energy Science and Engineering Symposium
UNIVERSITY OF TEXAS EL PASO
March 22, 2014

7:00 am
REGISTRATION
Double Tree Hotel
Main Lobby

8:00 am
BREAKFAST
Double Tree Hotel
Sky Lounge

8:05 am
OPENING NOTES
Dr. Ahsan Choudhuri
Professor and Chair,
Department of Mechanical Engineering
University of Texas El Paso

8:10 am
WELCOME
Dr. Richard Schoephoerster
Dean, College of Engineering
University of Texas El Paso

8:30 am
PARALLEL TECHNICAL SESSIONS I
Session 1-A Turbulent Combustion and Propulsion
Room: Salon I
Session 1-B Wind Power, Energy & Cyber Security
Room: Salon II
Session 1-C Solid Mechanics: Creep, Stress & Noise Control
Room: Salon III
Session 1-D Nano-materials and Solar Cells
Room: Discovery

9:50 am
BREAK

10:10 am
PARALLEL TECHNICAL SESSIONS II
Session 2-A Heterogeneous Combustion
Room: Salon I
Session 2-B Materials, Modeling & Metamaterial Sensor
Room: Salon II
Session 2-C Modeling, Fuel Injector, Heat Exchanger & Sensors
Room: Salon III
Session 2-D Coatings and Modeling
Room: Discovery

11:45 am
KEYNOTE SPEAKER
Theva Thevuthasan, Ph.D.
Environmental Molecular Sciences Laboratory
U.S. Department of Energy
“Molecular-scale, Multimodal Imaging to Accelerate Scientific Discovery”

1:00 pm
PARALLEL TECHNICAL SESSIONS III
Session 3-A Solid Propellants and Laminar Flames
Room: Salon I
Session 3-B Numerical Analysis & Modeling
Room: Salon II
Session 3-C Propulsion & Cyber Security
Room: Salon III
Session 3-D Design & Numerical Analysis
Room: Discovery

2:20 pm
BREAK

2:40 pm
PARALLEL TECHNICAL SESSIONS IV
Session 4-A Energy Storage & Composites
Room: Salon I
Session 4-B Materials Synthesis & Experimentation
Room: Salon II
Session 4-C Additive Manufacturing Design & Analysis
Room: Salon III
Session 4-D NSF REU
Room: Discovery

3:50 pm
KEYNOTE SPEAKER
Vijay Murugesan, Ph.D.
Pacific Northwest National Laboratory
U.S. Department of Energy
“Addressing Grand Challenges in Designing Energy Storage Devices”

5:00 pm
RECEPTION & ADJOURN
ABOUT THE SPEAKERS

Dr. Suntharampillai Thevuthasan is a Staff Scientist and Manager of the Interfacial Spectroscopy and Diffraction group at the Environmental Molecular Sciences Molecular Sciences Laboratory (EMSL), a Department of Energy national scientific user facility located at Pacific Northwest National Laboratory (PNNL). He received a B.Sc. (Honors) in Physics from the University of Peradeniya, Sri Lanka, and M.Sc. in Energy Technology from the Asian Institute of Technology, Thailand. He received his Ph.D. in Physics (Surface Science) from the University of Maine in 1989 and started his postdoctoral research at the University of Florida. Before joining PNNL in 1993, he was a postgraduate researcher at University of California-Davis and a guest scientist at Lawrence Berkeley National Laboratory for three years.

At PNNL, Dr. Thevuthasan has been developing experimental capabilities associated with research in surface science, materials synthesis and characterization of nanomaterials, and buried interface analysis in thin films. He made significant contributions to the study of surface structures of pure and adsorbate-covered single crystal surfaces, thin film and interfacial characterizations using x-ray photoelectron spectroscopy/diffraction, photoelectron holography, and high energy ion beam techniques. Dr. Thevuthasan further contributed to the understanding of synthesis and characterization of nanomaterials, ionic transport processes in single- and multi-layer oxide thin film electrolytes, growth and characterization of oxide thin films, and understanding radiation effects in ceramics and oxides. He is an AVS Fellow and thrust area lead for the Chemical Imaging Initiative at PNNL. He is mentoring a number of projects, with a particular focus on the coupling of atom probe tomography, electron microscopy and scanning x-ray transmission microscopy for atomistic imaging at unprecedented levels. He has organized several symposia and workshops as a part of international conferences.

Dr. Vijay Murugesan is a Senior Materials Scientist at Fundamental and Computational Science Directorate (FCSD) in Pacific Northwest National Laboratory (PNNL). He received M.S and Ph.D in Physics from the Bharathiar University, India. He started his postdoctoral research at the Universite du Maine, LeMans of France, working on lithium battery electrolyte materials. Before joining PNNL in 2008, he was doing postdoctoral research at College of William & Mary, Williamsburg and McMaster University, Canada focusing on lithium battery and fuel cell materials.

At PNNL, his work is mainly focused on rational designing of advanced materials for next generation energy storage devices. He is principal investigator of supercapacitors development program, and co-investigator in multiple projects focusing on lithium-ion, lithium-sulfur and redox flow batteries with total funding over $3 million. Dr. Vijay Murugesan was instrumental in developing knowledge based designing of redox flow battery electrolytes, which lead to high performing electrolytes and being commercialized in recent years. His work on flow battery technology is recognized by 'Battelle- Key contributor Award’. Dr. Vijay Murugesan is also part of the team to receive the prestigious R&D-100 award for the development of Graphene Nano-structures for Lithium Battery Technology.
## PARALLEL TECHNICAL SESSIONS I

### Session: 1A: Turbulent Combustion and Propulsion

**Session Chair:** Shaolin Mao  
**Room:** Salon 1  
**Double Tree El Paso**

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<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>8:30 am</td>
<td>Design of High Intensity Turbulence Combustion System</td>
<td>A. Acosta, M. A. Hassan, M. Quiroz, A. Choudhuri, UTEP</td>
</tr>
<tr>
<td>8:50 am</td>
<td>Lox/Methane Reaction Control Thruster Characterization and Performance Testing Utilizing a Torsional Thrust Balance</td>
<td>M.A. Ingle, J.L. Mena, J. Chaparro, and A. Choudhuri, UTEP</td>
</tr>
<tr>
<td>9:10 am</td>
<td>CFD Analysis of a LOX/Methane Pintle Injector Rocket Engine</td>
<td>G.A. Martinez, I. Lopez, J.L. Mena, and A. Choudhuri, UTEP</td>
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### Session: 1B: Wind Power, Energy & Cyber Security

**Session Chair:** Paras Mandal  
**Room:** Salon 2  
**Double Tree El Paso**

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<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>8:30 am</td>
<td>Wind Power Generation Impact on Electricity Market Prices: An Overview</td>
<td>A. Akundi, P. Mandal, E. D. Smith, and B. Tseng, UTEP</td>
</tr>
<tr>
<td>8:50 am</td>
<td>Optimal Placement of Wind Turbines on Non-flat Terrain Using Cluster Identification and Multi-objective Genetic Algorithm</td>
<td>C. A. Garcia-Rosales, J. A. Saavedra, and B. Tseng</td>
</tr>
<tr>
<td>9:10 am</td>
<td>Smart Electricity Market Planning and Operation in a Demand Responsive Environment</td>
<td>D.I. AlHakeem, P. Mandal, A.U.I. Haque, T.I. Tseng, UTEP</td>
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### Session: 1C: Solid Mechanics: Creep, Stress & Noise Control

**Session Chair:** Calvin Stewart  
**Room:** Salon 3  
**Double Tree El Paso**

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<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>8:30 am</td>
<td>Stress Intensity Factor of V-notch for Bonded Aluminum and PMMA</td>
<td>K. Zhao, M. Flores, J. F. Chessa, UTEP</td>
</tr>
<tr>
<td>8:50 am</td>
<td>Creep Rupture Life Prediction of 304 STS Using Larson-Miller Approaches</td>
<td>M.S. Haque, and C.M. Stewart, UTEP</td>
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<tr>
<td>9:10 am</td>
<td>An Inelastic Constitutive Model for Monotonic, Cyclic and Creep Deformation: Summary</td>
<td>L. Varela, C.M. Stewart, UTEP</td>
</tr>
<tr>
<td>9:30 am</td>
<td>Advance Noise Control Fan Test Rig: Analytical Trade Study of the Upstream Rake Assembly</td>
<td>R. Velazquez, C. Stewart, and D. Sutliff, UTEP</td>
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### Session: 1D: Nano-materials and Solar Cells

**Session Chair:** C.V. Ramana  
**Room:** Discovery  
**Double Tree El Paso**

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<th>Time</th>
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<tbody>
<tr>
<td>8:50 am</td>
<td>Evaluation of a Nanomanipulator Station for Characterization of Nanoscale CdTe Solar Cells</td>
<td>R. Aguirre, B. Aguirre, D. Marrufo, A. Vidana, J.C. McClure, and D. Zubia, UTEP</td>
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## PARALLEL TECHNICAL SESSIONS II

### Session: 2A: **Heterogeneous Combustion**  
**Room:** Salon 1  
**Session Chair:** Eric Petersen  
**Double Tree El Paso**

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<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>10:10 am</td>
<td><strong>Combustion Synthesis of Molybdenum Borosilicides for Ultrahigh Temperature Structural Applications</strong></td>
<td>M.S. Alam and E. Shafirovich, UTEP</td>
</tr>
<tr>
<td>10:30 am</td>
<td><strong>Combustion of Lunar and Martian Regolith with Magnesium</strong></td>
<td>A. Delgado, I. Lopez, and E. Shafirovich, UTEP</td>
</tr>
<tr>
<td>10:50 am</td>
<td><strong>Hydrogen Generation From Water Through the Combustion Reactions with Mechanically Alloyed Al/Mg Powder</strong></td>
<td>D. A. Rodriguez, E. Shafirovich, UTEP</td>
</tr>
<tr>
<td>11:10 am</td>
<td><strong>Combustion Synthesis of Magnesium Silicide, a Promising Thermoelectric Material</strong></td>
<td>Delgado, I. Lopez, and E. Shafirovich, UTEP</td>
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### Session: 2B: **Materials, Modeling & Metamaterial Sensor**  
**Room:** Salon 2  
**Session Chair:** Yirong Lin  
**Double Tree El Paso**

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<th>Time</th>
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<tr>
<td>10:10 am</td>
<td><strong>Fabrication and Preliminary Testing of Metamaterial Based Passive Wireless Temperature Sensors</strong></td>
<td>D. Delfin, H. Karim, M. A. I. Shuvo, M. Cadena, S. Gaytan, and Y. Lin, UTEP</td>
</tr>
<tr>
<td>10:30 am</td>
<td><strong>A Double Inclusion Model for Multiphase Piezoelectric Composite</strong></td>
<td>L. Vera, and Y. Lin, UTEP</td>
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<tr>
<td>10:50 am</td>
<td><strong>Concept and Model of a Metamaterial Based Passive Wireless Temperature Sensor</strong></td>
<td>H. Karim, D. Delfin, M.A.I. Shuvo, A. Choudhuri, R.B. Wicker, Y. Lin, UTEP</td>
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### Session: 2C: **Modeling, Fuel Injector, Heat Exchanger & Sensors**  
**Room:** Salon 3  
**Session Chair:** Jack Chessa  
**Double Tree El Paso**

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<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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<tbody>
<tr>
<td>10:10 am</td>
<td><strong>Development of a New Drag Model for Spherical and Nonspherical Particles</strong></td>
<td>R. Chowdhury, C. Rodarte, N. Love and A. Choudhuri, UTEP</td>
</tr>
<tr>
<td>10:30 am</td>
<td><strong>Experimental Evaluation of a Stability Map for a Multitube Fuel Injector</strong></td>
<td>M. de la Torre, S. Maldonado, S. Hossain, N. Love, and A. Choudhuri, UTEP</td>
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<tr>
<td>10:50 am</td>
<td><strong>Effect of Metal Foam on Heat Transfer Rates When Applied to Air Cooled Condenser Tubes</strong></td>
<td>A. Esparza and N. Love, UTEP</td>
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<tr>
<td>11:10 am</td>
<td><strong>Development of a Wireless Temperature Sensor Using Lithium Niobate Pyroelectric Ceramic</strong></td>
<td>M.R. Sarker, S. Sandoval and N. Love, UTEP</td>
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### Session: 2D: **Coatings and Modeling**  
**Room:** Discovery  
**Session Chair:** C.V. Ramana  
**Double Tree El Paso**

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<th>Time</th>
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<tr>
<td>10:10 am</td>
<td><strong>Study of Tungsten-Yttrium Based Coatings for Nuclear Applications</strong></td>
<td>G. Martínez, J. Chessa, S. Shutthanandan, T. Tevuthasan, M. Lerche and C.V. Ramana, UTEP</td>
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<tr>
<td>10:30 am</td>
<td><strong>Selective-Area Growth of CdTe/ZnTe on Micro Patterned SiO2/Cds/ITO/Glass Wafers</strong></td>
<td>A. Vidana, D. Marrufo, B. Aguirre, D. Zubia, and J. McClure, UTEP</td>
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<tr>
<td>10:50 am</td>
<td><strong>Modeling the Interfacial Stresses in Thermal Barrier Coatings</strong></td>
<td>S.K. Gullapalli, J.F. Chessa, and C.V. Ramana, UTEP</td>
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<tr>
<td>Session: 3A: Solid Propellants and Laminar Flames</td>
<td>Room: Salon 1</td>
<td>Double Tree El Paso</td>
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<tr>
<td>Session Chair: Evgeny Shafirovich</td>
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<tr>
<td>1:00 pm</td>
<td>Development of a CO2 Laser Ignition System to Test Solid Propellant Strands</td>
<td>A. R. Demko, T. D. Tran, and E. L. Petersen, TAMU</td>
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<tr>
<td>1:20 pm</td>
<td>Laminar Flame Speed of Methane with Ethane and Ethylene Addition</td>
<td>S. Ravi, T. G. Sikes, A. Morones, C. L. Keese, and E. L. Petersen, TAMU</td>
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<tr>
<td>1:40 pm</td>
<td>Influence of Nano-Aluminum on Stoichiometric Methane O2N2 Laminar Flame Speed</td>
<td>T. Sikes, M. S. Mannan, and E. L. Petersen, TAMU</td>
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<tr>
<td>2:00 pm</td>
<td>Ignition Delay Time &amp; Laminar Flame Speed Measurements of Propene</td>
<td>O. Mathieu, C. L. Keese, A. Morones, S. M. Burke, H. J. Curran, and E. L. Petersen, TAMU</td>
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<tr>
<th>Session: 3B: Numerical Analysis &amp; Modeling</th>
<th>Room: Salon 2</th>
<th>Double Tree El Paso</th>
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<td>Session Chair: Pavana Prabhakar</td>
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<tr>
<td>1:00 pm</td>
<td>Modeling Progressive Damage and Failure for Polymer-Matrix Composites</td>
<td>A. Leanos and P. Prabhakar, UTEP</td>
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<tr>
<td>1:20 pm</td>
<td>Prediction of Damage Due to Compaction During Manufacturing of Textile Composites</td>
<td>M. S. Islam and P. Prabhakar, UTEP</td>
</tr>
<tr>
<td>1:40 pm</td>
<td>Numerical Prediction of Collection Efficiency of a Personal Sampler Based on Cyclone Principle</td>
<td>A. Badhan, L. Bugarin, and S. Mao, UTEP</td>
</tr>
<tr>
<td>2:00 pm</td>
<td>Numerical Investigation of Wet Compression</td>
<td>L. Bugarin, A. Badhan, S. Mao, UTEP</td>
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<tr>
<th>Session: 3C: Propulsion &amp; Cyber Security</th>
<th>Room: Salon 3</th>
<th>Double Tree El Paso</th>
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<tr>
<td>Session Chair: Norman Love</td>
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<tr>
<td>1:00 pm</td>
<td>Experimental Studies of Uni-Element Shear Coaxial Injectors for LOX/CH4 Propulsion Research</td>
<td>L.E. Sanchez, V. Dorado, R. Ellis, G. Trujillo, A. Choudhuri, UTEP</td>
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<tr>
<th>Session: 3D: Design &amp; Numerical Analysis</th>
<th>Room: Discovery</th>
<th>Double Tree El Paso</th>
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<tr>
<td>Session Chair: Vinod Kumar</td>
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<tr>
<td>1:00 pm</td>
<td>Design of Supercritical Carbon Dioxide External Tubular Superheater for Solar Power Towers</td>
<td>A. Castellanos, J. Ortega, V. Kumar, UTEP</td>
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<tr>
<td>1:20 pm</td>
<td>A Heterogeneous Multiscale Method for an Elliptic Reaction Diffusion Equation</td>
<td>P. Delgado, V. Kumar, and S.Y. Yi, UTEP</td>
</tr>
<tr>
<td>1:40 pm</td>
<td>Numerical Analysis of Energy Storage for Nanofluidized Heat Transfer Fluid in Thermocline Thermal Energy Storage System</td>
<td>N. Hossain, S. Afrin, and V. Kumar, UTEP</td>
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<tr>
<td>2:00 pm</td>
<td>Meta-modeling on Building Energy Consumption</td>
<td>C. Cui, C. Su, K. Duggan, T. Wu, ASU</td>
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<tr>
<td>Session: 4A: Energy Storage &amp; Composites</td>
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<tr>
<td>Session Chair: Norman Love</td>
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<tr>
<td>2:40 pm</td>
<td>Enhanced Energy Storage of Dielectric Nanocomposited at Elevated Temperatures</td>
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<td>M.D. Rajib, R. Martinez, M.A.I. Shuvo, H. Karim, D. Delfin, S. Afrin, G. Rodriguez, Y. Lin, UTEP</td>
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<tr>
<td>3:00 pm</td>
<td>An Introduction to Graphene and its Application in Graphene Composites</td>
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<td>G. Rodriguez, M.A.I. Shuvo, and Y. Lin, UTEP</td>
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<td>3:20 pm</td>
<td>Flexible Super-capacitor for Energy Storage Application</td>
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<td>M.A.I. Shuvo, H. Karim, D. Delfin, Y. Lin, UTEP</td>
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<tr>
<th>Session: 4B: Materials Synthesis &amp; Experimentation</th>
<th>Room: Salon 2 Double Tree El Paso</th>
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<tr>
<td>Session Chair: Yirong Lin</td>
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<tr>
<td>2:40 pm</td>
<td>Experimental Study of Structure and Dielectric Properties of Gadolinium (Gd+3) Incorporated Cobalt Ferrite</td>
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<td>M.T. Rahman, and C.V. Ramana, UTEP</td>
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<tr>
<td>3:00 pm</td>
<td>Effect of Tungsten Incorporation on Thermal Stability of Gallium Oxide Thin Films</td>
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<td>E.J. Rubio, A. Miranda Gallardo, and C.V. Ramana, UTEP</td>
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<tr>
<td>3:20 pm</td>
<td>Fabrication and Characterization of Nanocrystalline Hafnium Oxide Thin Films</td>
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<td>M. Vargas, and C.V. Ramana</td>
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<th>Session: 4C: Additive Manufacturing, Design &amp; Analysis</th>
<th>Room: Salon 3 Double Tree El Paso</th>
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<tr>
<td>Session Chair: Sara Gaytan</td>
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<tr>
<td>2:40 pm</td>
<td>Conceptual Design to Fabricate Smart Parts for High Efficiency Energy System Using Electron Beam Melting</td>
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<td>M.S. Hossain, S.M. Gaytan, Y. Lin, and R. Wicker, UTEP</td>
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<tr>
<td>3:00 pm</td>
<td>Analysis of Ferroelectric Ceramic Fabricated by Binder Jetting Technology</td>
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<td>M. Cadenas, S.M. Gaytan, Y. Lin, and R. Wicker, UTEP</td>
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<td>3:20 pm</td>
<td>Literature Review of Mechanical Testing of Ti-6Al-4V Fabricated by Electron Beam Melting</td>
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<td>J.A. Gonzalez, S.M. Gaytan, Y. Lin, R.B. Wicker, UTEP</td>
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<th>Session: 4D: NSF REU</th>
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<tr>
<td>Session Chair: Pavana Prabhakar</td>
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<tr>
<td>2:40 pm</td>
<td>NSF REU Opportunity at TAMU</td>
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<td>E. Petersen, TAMU</td>
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</table>
Abstract
This paper focuses on the design of a high intensity turbulence combustion system. Its focus is on three main components: the combustor design, the experimental set up, and the exhaust section. The design of the combustor was driven by two parameters: the backward-facing step flame stabilization, and the need for optical accessibility features for flow diagnostics. The combustor was designed for compressible flow (M > 0.3), and a maximum operating pressure of 6 bar. The optical access is provided via the use of quartz windows on three sides of the square combustion chamber. A grid, or perforated plate, will be used as the turbulence generator for the experiment. A heating section will be implemented to pre-heat the air which will then be pre-mixed with methane prior to combustion. The exhaust section was designed to control the exit temperature of the exhaust gases to meet laboratory safety specifications. Theoretical and computational analyses were done to validate the design of the aforementioned components in the system.

Introduction
The focus of the project is to study the structure of premixed flames under high intensity turbulent flow. The overall aim is to study structures of backward-facing step stabilized premixed flames in high turbulence flow using optical and laser diagnostics, thus generating experimental flame data at compressible and high Reynolds number conditions to provide a better understanding of turbulent flame structures. The use of a backward-facing step for flame stabilization was used effectively by Takahashi and Schmoll [1]. This paper seeks to provide experimental information on turbulent flame structures, specifically the thickened flame regime. Information on the different flame structures and flame regimes are illustrated in literature [2]. Different length scales and flow characteristics must be dealt with and induced in order to achieve such conditions, therefore the following requirements were established when designing the combustor:

<table>
<thead>
<tr>
<th>System</th>
<th>Requirement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion chamber</td>
<td>Optically accessible</td>
</tr>
<tr>
<td></td>
<td>Grid turbulence generator</td>
</tr>
<tr>
<td></td>
<td>Changeable step size (variable dim.)</td>
</tr>
<tr>
<td></td>
<td>Max Pressure: 6 bar (87 psi)</td>
</tr>
<tr>
<td>Reactants</td>
<td>Air / CH4</td>
</tr>
<tr>
<td>Air</td>
<td>Pre-heated at 400-600 K (260 – 620 F)</td>
</tr>
<tr>
<td>CH4</td>
<td>Flow rate: Variable (based on equivalent ratio)</td>
</tr>
<tr>
<td>Inlet pressures</td>
<td>100 - 600 kPa (14 - 87 psi)</td>
</tr>
</tbody>
</table>

Combustor Design
The combustor section consists of several components; the combustion chamber, an entrance and exhaust regions, a mixing section, a backward facing step, and a grid. The combustion chamber geometry was defined based on existing laboratory flow rate capabilities. The dimensions of the chamber satisfy compressibility conditions of M > 0.3. Fluid flow simulations and literature background defined the geometry of the backward facing step. A backward facing step is a sudden increase in flow area which introduces a recirculation zone in the flow field. This feature has been used for flame stabilization in the past[1]. Prior to designing the combustor,
preliminary fluid flow simulations over a backward facing step with a grid induced turbulence generator were conducted to better understand fluid flow under the desired conditions. A transient Large Eddy Simulation (LES) served to resolve the fluid flow over the step. Figure 1 shows the instantaneous streamline; from this streamline, small vortices downstream of the grid as well as a large vortex in the step were seen (Figure 2). This flow simulation confirms the desired recirculation zone induced by the step in the chamber and velocity fluctuation induced by the grid in the flow field.

![Streamlines over backward facing step](image)

![Vorticity over backward facing step](image)

Fig. 1. Streamlines over backward facing step

Fig. 2. Vorticity over backward facing step

ANSYS computational simulations were used to analyze the structural integrity; thermal deformation, principal stress and strain components considerations further defined the geometry of the chamber design. The maximum deformation (0.000375m) occurs at the combustion chamber. To calculate the structural integrity, a 25 bar static pressure was applied on the surface of the chamber. Results indicate that the maximum principle stress experienced by the combustor yields a factor of safety of 5. In order to avoid velocity fluctuations in the velocity flow, the entrance section was designed based on a fifth degree polynomial curve found experimentally [3]. This design allows the flow to achieve a top head (non parabolic) velocity profile for the combustion chamber. Thus, this velocity profiles provides a uniform velocity distribution at the point where the mixture flows through the grid to ensure all the fluctuation occurs downstream of the grid. This was the same kind of velocity distribution used in the simulations. The same process and assumptions were considered for the exhaust section. The overall design of the combustor can be seen in Figure 3.

![Combustor, entrance and exhaust section cross sectional view](image)

Fig. 3. Combustor, entrance and exhaust section cross sectional view.

**Experimental Setup**

Air pre-heating will be achieved by using a commercially available in-line resistance heater. The air and methane will be pre-mixed using a mixing chamber, which injects methane radially into the axially flowing air. Hydrogen pilot flames will be used as the ignition source for the combustor. In order to have automated control of the system, LabVIEW software will be used in accordance with a PCI card based system in order to formulate a control program. In addition to having an automated system, a manual shut off alternative was also implemented in the design. A flow schematic can be seen in Figure 4. The only part of the system which is independent of the other components is the heater which has its own control panel from the manufacturer. The proper valves and fittings were considered to avoid any safety hazards.
Exhaust Section

The exhaust section was designed around existing laboratory safety considerations. Cold air and water are introduced at different points of the exhaust to regulate the exit temperature. The cold air injection and water section were designed using momentum principles as well as spray atomization. Some preliminary studies on the water spraying show how the multiphase flow affects the temperature. Using standard k-ε model for multiphase flow, a plot of the temperature in the exhaust pipe is generated as seen in Figure 4. It is shown that the temperature stabilizes at a short downstream distance.

Conclusions and Future Work

The design phase of the project has been completed, and the development of the system is currently undergoing. The system design and set up satisfies the requirements needed to achieve the appropriate flame structure. Both theoretical software validations support the functionality of the system. For the future, the focus will shift more to working on the laser diagnostics aspect using a combined PIV and CH-OH PLIF imaging technique. An example of such a technique is illustrated by the works of Böhm et al. [4]. These imaging techniques will be used to investigate the structure of the flame under the previously mentioned conditions.

References
LOx/Methane Reaction Control Thruster Characterization and Performance Testing Utilizing a Torsional Thrust Balance

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Introduction
“Green” propellants such as liquid oxygen (LOx) and liquid methane (LCH₄) are being actively pursued for use in next generation spacecraft propulsion systems [1]. These propellants are relatively new in application, so LOx/LCH₄ thrusters are not as well understood as their more traditional counterparts. Overall spacecraft weight, power consumption, and complexity could also be minimized by feeding both the main engines and reaction control (RCS) thrusters from the same propellant tanks. To achieve all of these objectives, a LOx/LCH₄ benchmark thruster was developed along with a Torsional Thrust Balance (TTB) that employs laser interferometry and a calibration procedure to ascertain thrust production [2]. This study is an extension of the previous work done to develop a test apparatus for the performance evaluation of LOx/ LCH₄ reaction control thrusters. The thrust range targeted spanned from 8 to 36 N (~2 to 8 lb_f). The main objective is to produce a reaction control system that can operate at a variety of propellant inlet conditions without having to precondition the propellant feed system. It is also desired to evaluate the performance of the baseline thruster at liquid propellant conditions since this is where the data is most lacking. It is essential to determine if the thruster will perform with repeatability (thrust, ISP, C*, and C_F) at a variety of inlet conditions. The initial testing of this RCS thruster indicated that it can function with repeatable results for short duration, gaseous, steady-state burns. The test duration was extended to observe both the film cooling and overall thruster performance. A portable LCH₄ condensation unit previously developed by the Center for Space Exploration Technology Research, cSETR, was used in conjunction with a specially designed cavitating venturi to control the supply of the propellants at the correct mixture ratios. Mixed phase propellant inlet conditions will be further explored in future tests.

1 Requirement Overview
The benchmark thruster detailed in this study must meet specific criteria to become actual flight hardware. First, due to the cryogen boil-off in supply tanks, ignition will be expected for a wide-breadth of propellant phases spanning from entirely gas to completely liquid with the inclusion of the mixed phases in between. Furthermore, consistent supply of the propellants at a steady mixture ratio (~2-2.4), thrust production (~2 to 8 lb_f) along with ISP (minimum of 150 sec), C*, and C_F are necessary. These are the ways that thrusters are typically characterized and in order to assess the benchmark thruster correctly, it was necessary to ensure that the measurement devices had the resolution, signal clarity, and data acquisition speed necessary to fully capture the system behavior. There will always be sources of noise, signal interference, and hardware vibrations (as in the case of the torsional thrust balance and feed lines) that make distinguishing physical realities from data uncertainties difficult. To account for this, filtering programs were written in MATLAB to isolate the thrust (displacement) profiles from those produced by noise in the data.
signal and the natural vibrational frequency (~4.7 Hz) of the thrust measurement stand. More specific information regarding the TTB and condensation unit specifications can be found in previous work by Acosta-Zamora, Flores, et al. (2013).

2 Experimental Set Up

2.1 Liquid Methane Production and Propellant Delivery System

The propellant delivery system can be detailed in terms of their source as well as their control/monitoring subsystems. First, the LCH\textsubscript{4} is condensed in a 12 L capacity stainless steel tank fitted with a cavitating nozzle flow control feature on the delivery side. Tank pressurization with Helium provides a constant back pressure to supply the LCH\textsubscript{4} at a consistent mass flow rate. Tank, line, and inlet LCH\textsubscript{4} pressures and temperatures are monitored and later correlated to the thrust data. The LOx is supplied directly from a commercial dewar and is likewise monitored comparably to the LCH\textsubscript{4}. The LOx mass flow is controlled by a cavitating venturi. Both line cooling and safety purges are provided via liquid nitrogen inlets into each of the supply lines and are monitored by their respective LOx and LCH\textsubscript{4} line instrumentation and control features.

2.2 Torsional Thrust Measurement Balance

The TTB that was previously developed using the torsional balance principles demonstrated in the cited works [2-7], accurately measures thrust in ranges from 8.9 to 35.6 N (2 to 15 lb\textsubscript{f}) with a 0.09 N resolution [2]. The advantages of the TTB system include its ability to reduce the effects of gravity-induced tare, movable counterbalance to account for thruster weight, and its proven repeatability through calibration studies [8]. It is important to note that this TTB measures thrust indirectly. Through a calibration process, a correlation is made between a displacement of the moment arm measured through laser interferometry and a known applied loading.

2.3 Propellant System and Thrust Measurement Interface

All of the required data acquisition, valve controls, and automated test operation/monitoring functions were included in a LabVIEW based graphical user interface (GUI). Specific valve and igniter operations as well as automatic emergency shutoff commands are all initiated from the GUI and are based on a series of inputs unique to the conditions specified in the test matrix. To be clear, the GUI facilitates the automation of the tests and the acquisition of mass flow, pressure, temperature, and displacement data in real-time.

3 Results and Discussion

This investigation consisted of 3, 5, and 10 second steady state burns of liquid state propellants. The inlet pressures were approximately 180 psia for the LOx and 130 psia for the LCH\textsubscript{4}. Tests were run after precooling the lines and when the propellant feed lines were unconditioned. During a previous 10 second test, the thruster exhibited signs of extreme and uneven heating in the combustion chamber and nozzle as seen in Figure 1. For this reason all subsequent tests were limited to 3 and 5 second burns to prevent damage to the thruster. The graphs show the filtered

Fig.1. 10 second steady-state thruster operation test.
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March 22, 2014, El Paso, TX

thrust data from two of the liquid propellant tests (3, 5 sec.). As can be seen in the figures, the average maximum thrust was approximately 10 N and 6 N for the 3 and 5 second burns respectively. The initial peaks were not considered as they represent the initial overshoot in displacement caused by the injection of the propellants.

4 Conclusions
The initial phases of the performance evaluation testing were completed. A LOx/LCH4 thruster was successfully fired at liquid-liquid propellant conditions producing a thrust value within the desired range. However the test results have not yet achieved the level of repeatability needed to calculate and average maximum thrust value for the given burn durations. So for this reason characteristic thruster calculations such as ISP, C* and C_F have not yet been computed. Furthermore, longer duration tests will be required to better assess the performance of the film cooling features of the benchmark RCS thruster.

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References
CFD Analysis of a LOX/Methane Pintle Injector Rocket Engine

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1 Introduction

The design of rocket engine injectors has been of the utmost importance for rocket engineers, due to the fact that most of the combustion instabilities generated throughout the ignition and steady state firing originate from the injector’s pressure drop. Several types of injectors have been developed throughout the years; these include showerhead injector, impinging injectors, coax injectors, etc. The pintle injector, however, was developed during the mid-1950’s. The pintle injector was developed in order to test and study propellant mixing and combustion reaction times of hypergolic liquid propellants. Engineers discovered that the pintle injector showed a very high combustion efficiency comparable to coaxial or showerhead injector [3]. Using such knowledge, the pintle injector has been used since then in several engines, including the Lunar Module Descent Engine (LMDE) used during the Apollo missions. One of the advantages of using pintle injectors is that it is very easily throttleable. Compared to other injectors where the throttling mechanism might create combustion instabilities, the pintle injector has excelled in this subject, maintaining high combustion efficiency and no combustion instabilities recorded throughout the 60 years of its development [3]. The pintle injector has been developed for a wide range of thrust levels (5 lbf – 650 klbf) and for 25 different propellant combinations, including hypergolic propellant combinations such as monomethyl hydrazine (MMH) and nitrogen tetroxide (N₂O₄), and cryogenic propellants such as liquid oxygen (LOX) and liquid hydrogen (LH₂). Throughout the history of pintle injector engines, it has never been used to mix “green” propellants such as LOX and liquid methane (LCH₄). Due to the fact that the green propellant technology is relatively new compared to other cryogenic fuels, the mixing, ignition, and combustion properties of LOX/LCH₄ thrusters or engines are not very well understood; therefore, it is the main objective of this study to understand how the variations of propellants mass flow affects the cone angle formed by a LOX/LCH₄ pintle injector via CFD analysis.

2 Pintle Geometrical Characteristics

Pintle injector geometry, unlike other injectors such as coaxial injectors or showerhead injectors, has been shown very stable throughout it usage history; therefore, the geometrical characteristics of the pintle injector has not been drastically modified. In order to design a pintle injector’s geometry, a decision of whether throttling capabilities are required must be made. As mentioned before, pintle injectors have been proven to have excellent combustion efficiency and stability when throttled; therefore, there have been several mechanism developed in order to throttle the engine (see Fig. 1).
Although a pintle injector might change whether it is throttleable or not, the actual pintle of the injector does not vary too much. Pintle geometry has always consisted of a concept called crossflow injector (a radial jet is “splashed” perpendicularly across an axial jet, as seen in Fig. 2. This concept has led engineers to develop several different types of pintles in order to optimize the injection of both flows.

Pintle geometry is mainly characterized by three aspects: what propellant flow inside the pintle (normally referred to as ox-centered of fuel-centered), radial injection type (holes, slots, or annulus), and skip distance. Usually, the first two depend on the most important factor in the design of pintle injectors, the total momentum ratio (TMR), which is the ratio of the mass flow rate of the radial jet times its velocity and the mass flow rate of the axial jet times its velocity:

$$TMR = \frac{\dot{m}_r U_r}{\dot{m}_z U_z}$$

The cone spray half angle, $\varphi$, depends extremely on the TMR. When TMR increases, $\varphi$ increases, letting the cone spray created by the pintle open up and spray directly on the engine’s combustion chamber walls. This creates several problems during ignition and steady state firing. First, if the pintle is ox-centered, it can create a high oxidizer concentration on the walls of the engine while creating combustion temperature concentrations on the wall. Second, combustion instability issues can occur; therefore, it has been shown that a TMR of unity can tend to optimum engine performance [2].

### 3 Requirements Overview

As mentioned before, preliminary two dimensional CFD analysis of a pintle injector has been done in the center for Space Exploration Technology Research. The effects of TMR on $\varphi$ were studied using ANSYS Workbench and Fluent’s turbulence and species transport modeling. The requirements of the pintle injector are very few but can completely define the engine where the injector will be used. Using the requirements shown in Table 1, a weight flow rate of both propellants was calculated in order to calculate the injection diameters of the pintle injector. The weight flow rates calculated were: 6.76 lbf/s for LOX and 2.50 lbf/s for LCH4.

Using the aforementioned parameters, the area of injection of both propellants was calculated for a given pressure drop using Eq. 2 [1]:

$$A_{inj} = \dot{W} \sqrt{\frac{3.805}{\rho \Delta P}}$$

<table>
<thead>
<tr>
<th>Max Thrust (lbf)</th>
<th>2000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burn Time (s)</td>
<td>180</td>
</tr>
<tr>
<td>Minimum Operating Altitude (mi)</td>
<td>15.5</td>
</tr>
<tr>
<td>Specific Impulse (s)</td>
<td>216</td>
</tr>
</tbody>
</table>

Table 1. Engine requirements list
The calculated injection areas for a 40 psi pressure drop were: 0.247 in$^2$ for LOX and 0.150 in$^2$ for LCH4. Using the area of injection, plus the propellant mass flows, the injection velocities were calculated for both propellants: 55.34 ft/s for LOX and 90.99 ft/s for LCH4.

4 Fluent Setup

4.1 Mesh and Boundary Conditions

As mentioned before, the CFD simulations that will be discussed in the Results section were preliminary; therefore, the mesh density was chose to be of at least 300,000 elements in order to ensure sufficient solution accuracy. For the boundary conditions, the velocities of the solutions were kept constant for all simulations but the injection fluids were changed in order to save computational time; therefore, 3 simulations were run using water as the injection fluid on both inlets, and 2 simulations were run using LOX and LCH4 on the respective entry holes. For a sample of the geometry used in all simulations, see Fig. 3.

4.2 Model Setup

Due to the turbulent nature of injection physics, a turbulent model had to be used for the CFD analysis of the pintle injector. The Standard $\kappa - \varepsilon$ model was used in order to deal with the turbulence part of the simulations. To run the simulations that required two different fluids, a species transport model was used.

5 Results

In order to compare the TMR- $\phi$, a relation between the radial and axial jets was developed. A linear relation between angle and momentum was assumed:

$$\phi = \tan^{-1}(TMR)$$

The following table illustrates the results yielded by 5 different simulations:

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Fluids Used</th>
<th>TMR</th>
<th>Linear $\phi$ Approximation</th>
<th>CFD $\phi$ Approximation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Water-Water</td>
<td>7.11</td>
<td>82.00</td>
<td>89.30</td>
</tr>
<tr>
<td>2</td>
<td>Water-Water</td>
<td>0.017</td>
<td>0.97</td>
<td>0.27</td>
</tr>
<tr>
<td>3</td>
<td>Water-Water</td>
<td>0.607</td>
<td>31.27</td>
<td>35.45</td>
</tr>
<tr>
<td>4</td>
<td>LOX-LCH4</td>
<td>1.63</td>
<td>58.47</td>
<td>57.09</td>
</tr>
<tr>
<td>5</td>
<td>LOX-LCH4</td>
<td>1.65</td>
<td>58.78</td>
<td>54.75</td>
</tr>
</tbody>
</table>

Table 2. CFD and Analytical Results of the spray half angle.

6 Conclusions

Comparing the linear approximation and the CFD results for the half angle, it can be seen that there is very little error between both of them, proving that the linear relation of the momentums can be used as a rough approximation of the angle. Furthermore, three dimensional simulations are being done to fully understand a pintle injector.
7 References

Experimental Studies of Uni-element Shear Coaxial Injectors for LOX/CH₄ Propulsion Research

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1 Introduction

This experimental investigation is a small part in a larger effort to characterize LOX/CH₄ as an alternative propellant combination and to expand the experimental knowledge that can be used directly in the development of hardware optimized for this propellant combination. Among the published efforts to model the spray atomization process for rocket fuel injection are the studies conducted by Woodward et al., in which several tests at high momentum flux ratios (ranging from 20 to 150) were conducted to compare the core breakup length (L/D) in shear coaxial LOX/GH₂ injection to the established mathematical models of L/D in conditions relevant to real space applications [3]. Like the experiments described in this article, the Woodward et al. testing was conducted in non-combustion conditions and analyzed using shadowgraph as a flow visualization technique. Two applicable models developed for the prediction of core breakup length have been chosen as baselines to compare the measurements obtained at cSETR for experimental shear coaxial studies.

Woodward model:

\[ \text{Woodward model: } 0.0025 \left( \frac{\rho_G}{\rho_L} \right)^{-0.44} R \epsilon_D^{0.76} W \epsilon_G^{-0.22} \]  

Davis model:

\[ \text{Davis model: } \frac{25}{J^{-0.2}} \]  

2 Methodology

All testing was conducted with non-ignitable mixtures (LN₂/GCH₄) at near ambient conditions (P\text{avg}= 17psia) in an atmospheric aluminum rig at the Goddard Laboratory in the University of Texas at El Paso. The testing conditions were selected to obtain relatively fuel-rich MR ranges observed in standard methane propulsion applications. Interfacing with the geometry of an optically accessible combustor (MOAC) led to the unique design of the injectors.

2.1 Shear coaxial injector geometry

Each of the three injectors developed for this testing program has a 316 Stainless Steel body and an assembly containing four separate parts joined by braze welding. The injectors are labeled as A, B and C, and each is identical to the others in all but one respect. For all three injectors, the central orifice has a diameter of 2 mm (0.0787 in) and an area of 3.14 mm², while the co-annular injection port has a co-annular area of 2.84 mm². The central orifice pertains to the liquid jet and the surrounding annulus to the gaseous fuel. The baseline plate geometry A has a fuel outer annulus diameter of 5.2 mm [1]. The parameter variations featured in each injector are shown in Table 1.

| Table 1 Variable Parameters in Plate Geometry |
|---|---|---|---|
| Injector | Variable | Central post Thickness, τ₀ | Recession Length, τ_L |
| A | Baseline | 1.42 mm | 0 mm |
| B | τ₀ | 2.26 mm | 0 mm |
| C | τ_L | 1.42 mm | 5 mm |
2.2 Test flow conditions

Liquid nitrogen was used as a substitution for liquid oxygen for cold flow tests in combination with gaseous methane under the considerations that its behavior in a cryogenic state would be satisfactorily similar to that of LOX and that further tests, i.e. high pressure and hot firings, would be conducted with LOX and its results compared to these experiments to verify this assertion. Flow conditions were replicated for each injector to isolate the effects of the geometrical variation in place. The three flow conditions tested on each injector are shown in Table 2 along with the targeted J numbers. The test matrix constructed for this purpose showcased a total mass flow rate range of 0.0125-0.0145 kg/s and a MR range of 2-4. The tests were also developed to study a momentum flux ratio considered much greater than existing rocket engines (>20).

<table>
<thead>
<tr>
<th>Case #</th>
<th>GCH4 Mass Flow rate, kg/s</th>
<th>LN2 Mass Flowrate, kg/s</th>
<th>MR</th>
<th>Vr</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0025±0.005</td>
<td>0.01±0.002</td>
<td>~4.0</td>
<td>105</td>
<td>30</td>
</tr>
<tr>
<td>2</td>
<td>0.0035±0.005</td>
<td>0.01±0.002</td>
<td>~3.0</td>
<td>145</td>
<td>55</td>
</tr>
<tr>
<td>3</td>
<td>0.0045±0.005</td>
<td>0.01±0.002</td>
<td>~2.0</td>
<td>230</td>
<td>150</td>
</tr>
</tbody>
</table>

3 Results

3.1 Shadowgraph Results

The images of the LN\textsubscript{2}/CH\textsubscript{4} flow were obtained for all three flow conditions cases with an area of interest that encompassed from the injector face plate to the opposite end of the MOAC. Core length (liquid breakup length normalized by core diameter) was measured at three different instants during steady state in each shadowgraph recording, and the average of these was the recorded core length for its corresponding injector geometry.

From the captured images (1001 per run), the liquid nitrogen core region can be seen to be confined in a slender region downstream of the injector face plate. This reinforces the traditional model attributing the changes in core break up length to the high shearing velocities from the momentum flux of GCH\textsubscript{4}. A sample of the liquid/gas interaction in the wake of the injection plate is shown in Figure 1.

![Figure 1 Case #1, Injector A, Image 500](image1.png)

3.2 Core Length Analysis

A comparison of core fragmentation models from Woodward and Davis to the measured values in this study is imperative to correlate the obtained results with existing literature on jet core length analysis [3]. Figure 2 presents a plot of LN\textsubscript{2} core length against J number. Davis’ two-phase jet flow equation and Woodward’s intact core correlation equation are represented in the plot, as well as experimental data published by Bonafice, Reed, and Woodward et al. Core
length measurements for Injector A are the ones that most closely resemble the Davis subcritical two-phase core length model [3].

Figure 2 Plot of LOX core length measurements from Boniface et al.⁴, Reeb⁵, Woodward et al.⁶, and this study against gas-to-liquid momentum flux ratio

4 Conclusions

Preliminary results of core flow field in a uni-element shear coaxial injector for LOX/CH₄ under unpressurized cold flow conditions has been characterized by shadowgraph imaging and core length analysis. Correlations of existing literature for predicting core length for shear coaxial injectors with the measured core lengths serve as an ideal comparison for this study. Results support classical liquid core fragmentation models and suggest that changes in central post thickness and co-annular orifice recession length with respect to the injection plate have visible effects in the generated spray flow field despite being unaccounted for in the parameters traditionally used to describe the spray atomization process. The differences in cold flow analysis to the hot fire testing must be analyzed and compared to provide deeper understanding of how hot fire testing affects the injection, droplet atomization and evaporation.

References

An Experimental Investigation of the Heat Transfer Effects on the Internal Forced Convection of Liquid Methane

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1 Introduction

The Center for Space Exploration Technology Research (cSETR) has focused on research pertaining to liquid methane (LCH₄) for propulsion systems and cooling applications. Currently, the heat transfer characteristics of LCH₄ have been researched due to the lack of empirical data. The use of LCH₄ in regeneratively cooled rocket engines (regen engines), has proven to have many advantages concerning deep space exploration. These advantages include comparable storage temperatures to liquid oxygen (LOX) as opposed to the widely used and researched liquid hydrogen (LH₂) and material compatibility [1]. For this reason, the cSETR laboratory has developed a High Heat Flux Test Facility HHFTF for the purpose of testing the internal forced convection of LCH₄ at turbulent conditions when flowing through a 1.8 mm x 4.1 mm channel.

2 Experimental Design

2.1 High Heat Flux Test Facility

The HHFTF is capable of handling temperatures as low as 77 K and temperatures as high as 723 K. High temperatures are achieved by maintaining a copper heating block directly in contact with the test section where a copper cooling channel is held firmly in place with an aluminum cradle. A heating block with up to 25 heating cartridges supplies a constant heat flux to the test section asymmetrically providing an environment similar to that of a rocket engine.

The cooling channel is designed to hold six E-type thermocouples measuring the wall temperature in addition to one inlet and one outlet thermocouple measuring the fluid temperature passing through the test section. A detailed illustration of HHFTF is shown in Fig. 1 showing all parts associated with the HHFTF. A further detailed description of the HHFTF can be found in reference [2].

![Fig. 1. CAD model of the High Heat Test Flux Facility.](image-url)
2.2 Methane Condensing Unit

A Methane Condensing Unit (MCU) designed to condense up to 13 L of LCH₄ is piped directly into the propellant line of the HHFTF to supply the system with sufficient LCH₄ and support steady state wall temperatures of the cooling channel. Fig. 2 shows the MCU coupled with the HHFTF during an actual test run. The MCU condensing tank utilizes a shell and coil heat exchanger by flowing LN₂ through coils inside the condenser liquefying CH₄ pressurized inside the tank. Typical condensing times run approximately one hour to condense all 13 L of CH₄.

Fig. 2. Experimental setup of the MCU paired with the HHFTF.

3 Results and Discussion

Fig. 3 shows a steady state run for a test condition of 1.03 MPa tank pressure and 7500 kW/m² heat flux. The plot also shows the method in which the analysis is performed. For the series of tests, the fragment that is of most importance is the section at which steady state wall temperatures are achieved. At this point, 10 seconds of steady state data is averaged to attain the fluid properties (taken at the bulk temperature) and average wall temperatures when employing the final heat transfer analysis. The test conditions chosen contain a heat flux within the range of 4.8 to 14.5 MW/m² and test pressures ranging from 1.03 MPa to 2.07 MPa.

The test data is analyzed to produce a Nusselt (Nu) number correlation based off a Nu vs Reynolds (Re) number plot. Several Nu number correlations from literature were studied to choose the appropriate Nu correlation for the test conditions and data produced [3]. Fig. 4 shows the final Nu correlation most representative of the data presented from the HHFTF. The NASA
Rocketdyne model showed the best correlation [4]. This correlation has been used previously when investigating CH$_4$ heat transfer and has continued to correlate well for sub-critical data flowing through a channel with a rectangular cross section. Eqn 1 shows the Nusselt number correlation used for this data where $T_b$ is the bulk temperature and $T_w$ is the average wall temperature.

\[
Nu = 0.0187 Re^{0.8} Pr^{0.4} \left(\frac{T_b}{T_w}\right)^{0.45}
\]  

(1)

![Graph showing measured Nusselt number vs. theoretical Nusselt number.]

4 Conclusion

The development of the HHFTF paired with the MCU provided steady state heat transfer results for LCH$_4$. For the test conditions mentioned above, a Nu number correlation was generated for predicting the heat transfer behavior and will be compared with other cooling channel geometries. Future work involves developing cooling channels with various surface roughnesses to observe the heat transfer effects and the resultant pressure drop encountered. Other channels currently in development include longitudinal fins within the channel and high aspect ratio cooling geometries.

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References

Combustion Synthesis of Magnesium Silicide, 
A Promising Thermoelectric Material

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1 Introduction

Magnesium silicide (Mg$_2$Si) is a promising thermoelectric (TE) material for harvesting energy because it could be used at 300–600°C, i.e., in the operation domain of TE generators used in exhaust systems and other high-temperature applications [1]. Magnesium and silicon are non-toxic, abundant, and relatively inexpensive.

Mg$_2$Si-based compounds are typically synthesized on a small scale via melt synthesis or casting. Scaling up these methods is problematic due to the high vapor pressure and reactivity of Mg, which can lead to the loss of Mg and poor control over stoichiometry [2]. Mechanical alloying has been considered, but this method requires long milling times, leading to contamination from the milling media [3-5]. One promising alternative is the so-called self-propagating high-temperature synthesis (SHS), which is recognized as a cost-effective, efficient, and clean method for the production of advanced materials [6]. A major advantage of SHS is low energy consumption – the process is sustained by the heat of the exothermic reaction between constituent powders.

Unfortunately, the reaction between Mg and Si is not very exothermic and it is difficult to ignite their mixture. To overcome this problem, in the present paper, Mg$_2$Si is fabricated using mechanically activated self-propagating high-temperature synthesis (MASHS) [7]. The method adds a short-duration, high-energy ball milling step, which precedes the combustion process. The high-energy milling (mechanical activation), rapidly produces nanostructured powders, so that intermixing of reactive components is obtained on a nanometric scale. The fracture-welding process during milling increases the contact surface area between reactants and destroys the oxide layer on their surface. As a result, mechanical activation improves the reaction kinetics, leading to an easier ignition and stable combustion. Also, the short milling time eliminates the problem of Mg$_2$Si contamination by milling media.

2 Method

Magnesium (–325 mesh, 99.8% pure, Sigma-Aldrich) and silicon (–325 mesh, 99.5% pure, Alpha Aesar) powders were used in this study. A mixture of 2 mol Mg and 1 mol Si was prepared using a three-dimensional inversion kinematics tumbler mixer (Bioengineering Inversina 2L) and compacted into 3.7-g cylindrical pellets (diameter: 13 mm, height: 20-21 mm) in an uniaxial hydraulic press. Combustion of the pellets was studied in a windowed stainless steel chamber (diameter 30 cm, height 40 cm), connected to a compressed argon cylinder and a vacuum pump. The pellet was placed on top of a brass holder, insulated with ceramic fiber paper, and ignited with a tungsten coil, heated from a DC power supply. Before the experiment, the chamber was purged three times and filled with argon at 1 atm pressure.
For MASHS experiments, the mixture was treated in a planetary ball mill (Fritsch Pulverisette 7 premium line) using zirconia-coated grinding bowls and zirconia grinding balls (diameter: 3 mm). The balls-mixture mass ratio was 5:1. The milling was conducted in an argon environment at 750 rpm for 5 min. The obtained powder was compacted into pellets and ignited in argon environment as described above.

Compositions of the milled powders and combustion products were studied using X-ray diffraction analysis (Bruker D8 Discover XRD). Particle size distributions in these powders were studied with a laser diffraction particle size analyzer (Microtrac Bluewave).

3 Results

In the experiments with unmilled Mg/Si mixture, ignition was observed for only 3 out of 7 samples. In contrast, for the mechanically activate mixture, a steady propagation of the combustion front was observed for all samples (Fig. 1). The average velocity of the front was 6 mm/s. The pellet expanded during combustion. Although the product pellet maintained the cylindrical shape, it was very fragile.

![Fig. 1. Self-sustained propagation of the reaction wave over mechanically activated Mg/Si mixture. The pellet diameter: 13 mm.](image)

XRD of the milled powders (before the combustion) shows that no significant reaction occurred during the milling process (Fig. 2). XRD of the products after combustion of the milled sample has shown Mg$_2$Si with no initial reactants (Fig. 3).

![Fig. 2. XRD pattern of Mg/Si mixture after 5-min milling at 750 rpm.](image)

![Fig. 3. XRD pattern of the combustion products.](image)
Figures 4 and 5 show the particle size distributions for the milled powder and the product, respectively. The bimodal distribution observed for the milled powder, with maxima at 20 µm and 356 µm, is apparently explained by agglomeration of magnesium particles during milling. In contrast, the particle size distribution for the product is rather narrow, with a single peak at 17 µm (the median diameter: 17 µm, the mean volume diameter: 18 µm).

**4 Conclusions and Future Work**

Magnesium silicide was been fabricated from magnesium and silicon powders by MASHS technique. Without mechanical activation, samples were hard to ignite due to their low exothermicity.

Future work is needed to understand the effect of mechanical activation, i.e. milling time and media. To produce dense and stronger Mg$_2$Si products, it is planned to use SHS compaction.

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**References**

Stress Intensity Factor of V-notch for bonded Aluminum and PMMA

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1 Introduction

Composite Materials has extensive applications in many engineering fields, including aerospace, aircraft, automotive, marine, energy, infrastructure, armor, biomedical, and sports applications [1]. There exists an interface between the matrix and fibers since composites are made of two or more materials. This interface is usually the weakest link and hence it becomes very important to characterize its mechanical properties [2]. Failure of composite materials usually characterized by delamination of layers between fibers and matrix. There is an angle that is similar to V-notch between fibers and matrix after the delamination. It is very critical to study the V-notch under shear loading due to the fact that the stress intensity factor is the key to help us understand stress field around the V-notch, however it is still unknown for this special configuration. In order to study the stress intensity factor of V-notch between two materials, we simulate the actual composites to two bonded short beams which are made from Aluminum and PMMA.

It is not straightforward to create a pure shear loading state. This is a result of the difficulty of subjecting a composite material to a pure and uniform shear stress state while avoiding complications caused by machining, high costs, and the effect of other stresses [3]. A new approach – short beam shear test (Fig. 1, Fig. 2) – was developed to provide pure shear loading which has advantages of low machining, fixture cost and shorter time for preparation. The advantage of having zero interfacial normal stress (zero bending moment) at the specimen center is used to develop an efficient experimental method to determine the mode II stress intensity factor of bonded Aluminum and PMMA.

Fig. 1. Schematic diagram of the short beam shear test with loading blocks in the Iosipescu shear fixture.
2 Theoretical Background

Williams [4] showed that a universal singular stress field of the form

$$\sigma_{\alpha\beta} = Kr^{\lambda-1} f_{\alpha\beta}(\theta)$$

exists in the region surrounding a sharp notch. $$\lambda - 1$$ is the order of the stress singularity, depend on notch geometries. $$K$$ is the stress intensity, a function of the geometry of the solid and the far-field loading (Fig. 3).

3 Experimental Procedure

Each short beam has a center length of 38.1mm and the height is 19.1mm. The included angle between Aluminum and PMMA varies from 5 degrees to 60 degrees. Loctite Ultra Gel Control Super Glue is chosen as the adhesive to bond two parts. Every specimen was bonded together from separate halves to enable an interfacial failure and all of the individual bonding surfaces were sandblasted. Prior to bonding, PMMA and aluminum were cleaned and degreased by alcohol and acetone respectively in order to improve the bonding quality. The specimens were cured for a period of 24 hours before removed from the fixture in order to achieve the bonding strength under
room temperature.

Digital image correlation method (Fig. 4) will be adopted to record strains during loading. From the recorded strain, we can calculate the stress field around notch tip. The order of the stress singularity and stress intensity factor will be determined through curve fitting based on the calculated stress field.

Fig. 4. Strain contour around notch tip by DIC

References

Creep Rupture Life Prediction of 304 STS Using Larson-Miller Approaches

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Abstract:
The Larson-Miller relation (LMP) was used to develop a general (any stress and temperature) approach for predicting creep rupture life of 304 STS. Fourteen sets of experimental data taken from 1971 to 2008 were collected from literature and used in this study. The experimental data includes low stress (4.7767 MPa) and high stress (320.26 MPa) at low homologous temperature ranging from (0.4 T_m to 0.65 T_m). MATLAB curve fitting tool was used to find the optimum value of constant C and set up an LMP equation where LMP is depending on stress only. A comparison of rupture life prediction model and experimental data is shown. Finally, critical issues and limitations of LMP were discussed and a new approach is proposed.

1 Introduction:
Materials that are used in high temperature (>0.4 T_m) environments often exhibit time dependent deformation[1]. For example cracks form in the airfoils of aero-turbines due to thermo-mechanical fatigue. Over time if inspections are not performed the crack can reach the critical crack limit leading to fracture. This fracture can cause a chain reaction of collateral damage which can cost power plant operators millions of dollars. This problem can be avoided if the rupture life of the operating component under specific temperature and stress can be accurately predicted. Larson-Miller is one of the earliest (1952) and widely used creep rupture (time-to-failure) prediction approaches[2]. This simple but useful approach can be used to predict rupture life of 304 STS.
Researchers have fit the Larson-Miller approach to experimental data [1,4] and some have tried to modify it [7] but there is little or no work on generalizing this approach. Here fourteen data sets of wide temperature and stress range were used to develop a general approach by which anyone can predict the rupture time given the operating temperature and stress. Fig.1 & 2 shows that the general model matches with the experimental data. In the process the critical issues of each stage is discussed in detail.

2 Larson-Miller Approach:
The Larson-Miller approach is based on a time-temperature relationship as follows:

\[ LMP = T(\log t_r + c) \]  \hspace{1cm} (1)

where \( T \) is temperature in Kelvin (K), \( t_r \) is rupture time, \( C \) is a constant, and LMP is the Larson-Miller parameter [6]. For metals, \( C \) can be set 20 universally. Fixing \( C=20 \) is no longer acceptable to the researchers. Furillo [3] et al. reported \( C \) values ranging from 10 to 50 in many cases of metal alloys. Vasudevan [4] et al. reported they have found \( C \) value 13.5 for austenitic stainless steel. When LMP is set up as a function of applied stress [Equation (2)] \( C \) valued is determined by experimental data fitting analysis

\[ LMP = f(\sigma) \]  \hspace{1cm} (2)

rupture time can be predicted by [equation (3)] (given that operating temperature is known).

\[ t_r = 10^{\frac{LMP - T c}{T}} \]  \hspace{1cm} (3)
LMP Vs Stress (square root formula)

Fig.1. LMP vs Applied Stress. The points represents the LMP values at different temperature and the line represents the developed model.

Applied Stress Vs Rupture Time (Log Scale)

Fig.2. Stress Vs Rupture time. By using [Equation (3) and (4)]. The solid lines are modeled curve and the dot points are experimental data.

3 Experimental Result:
All fourteen data set were used to calculate the LMP assuming $C$=[18.5,19,19.5 and 20]. MATLAB curve fitting directed that minimum residual is observed at $C=19$. During fitting it was observed that the difference between maximum and minimum LMP values remains the same for all $C$ values. After selecting the $C$ value the LMP values evaluated from experimental value were plotted against applied stress and the EUREQA [8] symbolic regression software was used to find an equation of LMP versus applied stress. EUREQA fits [Equation (4)] as best fit.

$$LMP(\sigma )=31250 + 41.8623767711648*\sigma - 1491.91139306372*\sqrt{\sigma}$$  \hspace{1cm} (4)

DiMelfi [5] states that [Equation (2)] can take any form but the most popular form is a polynomial. While generating an universal form of LMP equation it was found that the new form [Equation (4)] gives much better prediction of LMP. The polynomial equation gives less accurate predictions compares to the square root equation because in the Larson-Miller equation the LMP value acts as a power of ten. Small deviation in LMP leads to very large deviation in life prediction.
4 Result Analysis:
The developed model matches with the experimental data (Fig. 2). However at very low
temperature and very high stress (near to UTS) the curve cannot predict the rupture life. For the new
square root equation the first derivative is
\[ \frac{d(LMP)}{d\sigma} = a_1 + a_2 \cdot 0.5 \cdot \sigma^{-0.5} \] (5)
Setting the derivative equal to zero (where the curve will reach at maximum point) and solving for \( \sigma \) results is \( \sigma = 317.56 \text{MPa} \), The model has a inflection point at 317.56 MPa which results in
fictitious prediction of life above this stress value.

5 Future work:
To avoid this limitation a new approach is planned [Equation (6)]. where \( n \) is function of
temperature
\[ \text{stress} = \frac{a}{t^{n} + b} \] (6)
and the ratio \((a/b)\) determines the maximum stress applicable (which is the Ultimate tensile strength
(UTS)) and will be treated as a function of temperature, \( a / b = f(T) \) (fig. 3). The main advantage is
it will generalize the model from UTS to low stress (where life will be theoretically infinite), unlike
Larson-Miller approach, this model will use UTS as a function of temperature (\( UTS = f(T) \) ),
means the UTS will be different for same material at different temperature which will give the safe
operating stress limit for that specific temperature.

Fig.3. Planned stress vs rupture life model curve

6 Reference:
An Inelastic Constitutive Model for Monotonic, Cyclic and Creep Deformation: Summary

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1. Introduction

Materials subjected to extremely high temperatures and cyclic loads for example, the hot-end components of industrial gas turbines exhibit nonlinear deformation behavior, making it difficult to predict damage and failure of the material. The prediction of these material’s states becomes difficult because multiple phenomena contributes to the deformation of the material; therefore, a unified model that incorporates multiple phenomena into one set of equations is required to accurately predict deformation and damage.

2. Miller’s Model

Miller’s model [1] is a mathematical model proposed in 1976 that describes the viscoplastic behavior of a material exposed to high temperature and cyclic loading. This mathematical model does not just consider creep and fatigue caused by the exposure to high temperature, but takes into consideration numerous mechanisms of deformation such as transient (primary) creep, steady-state (secondary) creep, monotonic short-time plastic deformation, cyclic hardening and softening, Bauschinger effect, rate effects, temperature effects, annealing and the accumulation of these effects though time. Individual mathematical consideration of each mechanism will be a more accurate in an individual scale, but this model attempts to bring them together towards a more realistic structural analysis by the interaction among the mechanisms [2].

Miller’s unified model consists of a set of three equations, characterized by a total of ten constants that can be characterized using creep-fatigue test data Eq. (1-3). These equations were formulated based on the individual mechanisms that cause the deformation of the material.

\[
\dot{\varepsilon} = B_0 \sinh \left( \frac{\sigma - R}{D} \right) \text{sgn}(\sigma - R) 
\]

\[
\dot{R} = H_1 \dot{\varepsilon} - H_2 B_0' \sinh \left( \left| R \right| \right) \text{sgn}(R) 
\]

\[
\dot{D} = H_3 \dot{\varepsilon} \left[ C_2 + \left| R \right| - \left( \frac{A_1}{A_2} \right) D \right] - H_3 C_2 B_0' \sinh \left( \left| A_1 A_2 \right| \right) 
\]

Eq. (1) describes the strain rate $\dot{\varepsilon}$ of the material as a function of applied stress $\sigma$, a temperature dependent factor $\theta'$, rest stress $R$, characteristic drag stress $D$ and material constants $B$, $n$. The signum function and absolute values were added so that this equation can take into consideration both positive and negative stresses and strains. Eq. (2) and Eq. (3) describes transient behavior of rest stress rate and drag stress rate, respectively; as a function of strain rate $\dot{\varepsilon}$, steady state Rest Stress $R$, temperature dependent factor $\theta'$, steady state drag stress $D$ and material constants $H_1$, $B$, $A_1$, $n$, $A_2$, $C_2$, $H_2$. 
2.1 Calculation of Material’s Constants

In order to solve for all the material variables required by this unified model, it is required to solve for them in a specific order so that all the variables can be found and all the equations can be solved.

The first step is to find the constants responsible for the steady state creep which are: \( \theta' \), B, Q, A, n, \( A_1 \), and \( A_2 \). Q and \( \theta' \) stands for activation energy for plastic flow at high temperature and temperature-dependent factor, respectively; these constants are calculated using creep test data and plotting the minimum creep strain rate \( \dot{\varepsilon}_{ss} \) versus applied stress \( \sigma_{ss} \) with temperature as a parameter. Then by using Eq. (4), dividing the minimum creep rates by \( \theta' \) and trying different values of \( \theta' \) until all the minimum creep data for the different temperatures coalesce in a narrow rectangular area, a best fit value of \( Q \) can be found.

\[
\theta' = \exp\left(-\frac{Q}{kT}\right) \tag{4}
\]

Then the next step is to find a value for the A constant, which is not clearly present in the model’s formulas but it is required to calculate constants \( A_1 \) and \( A_2 \). Constant A is calculated by using Eq. (5) and using trial and error method, until Eq. (5) results in a straight line when plotted \( \log(\dot{\varepsilon}_{ss} / \theta') \) versus \( \log[\sinh(A\sigma_{ss})] \). The slope of this straight line is what defines the value of \( n \) and the value of \( \dot{\varepsilon}_{ss} / \theta' \) at \( \log[\sinh(A\sigma_{ss})]=1 \) is the value of B.

\[
\log(\dot{\varepsilon}_{ss} / \theta') = \log(B) + n\log[\sinh(A\sigma_{ss})] \tag{5}
\]

The second step is to calculate the constants responsible for the cyclic stress-strain behavior which are \( C_1 \), \( H_1 \) and \( C_2 \). These constants are calculated from cyclic stress versus cyclic strain and by best-fit procedure as shown in Fig. 1 [1]; the arrows indicate the effect of an increase in each constant.

With a proper value for \( C_1 \), the values of \( A_1 \) and \( A_2 \) can be calculated using Eq. (6) and Eq. (7), which maintain a balance relation to \( C_1 \) and A.

\[
A_2 = \left[A/(1-C_1)\right]^3 \tag{6}
\]

\[
A_1 = A/C_1 \tag{7}
\]
By using Eq. (8) where Y is the 0.2 percent yield strength, the $D_o$ constant can be found. This constant determines the initial value for the history of the drag stress.

$$D_o = (Y - 0.02H) / \left( \frac{\sinh^{-1} \left( \frac{\varepsilon \cdot B^2}{BP} \right)}{5.0677} \right)$$

(8)

In Summary with experimental data, constants can be calculated by best-fit in a plot method and by using the exact equations explained above. By plugging in all the constants into the main model’s equations, the strain rate due to a multiple deformation mechanisms acting at the same time on a material can be calculated.

3. Conclusion

This unified mathematical model results are dependable, since its development is based on the individual deformation mechanisms or phenomena that create plastic deformation of the material and consider the interaction among them to calculate the final strain rate. This unified model is reliable because the only experimental information required for the calculation of variables consists of creep, cyclic stress-strain, and tensile-test.

4. Future Work

ANSYS Mechanical APDL is a general purpose finite element software able to simulate deformation of CAD objects, ANSYS has a library of constitutive laws which allow it to model mechanical stresses, thermal stresses, fatigue, creep, etc. An example of the simulation results for a simple truss is given in Fig. 2. While ANSYS has many built in constitutive laws; it does not have Miller’s law. ANSYS allows the user to create custom constitutive laws through user programmable features (UPF). In the future, Miller’s model will be programmed into ANSYS; simulations performed and compared to experimental data towards qualify the performance of Miller’s equations.

Fig. 2. ANSYS simulation, displacement contour.

References
ADVANCE NOISE CONTROL FAN TEST RIG:
ANALYTICAL TRADE STUDY of the UPSTREAM RAKE ASSEMBLY

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Aircraft designed in the 21st Century are measured quieter than the aircraft designed from the past. This could be attributed to Advanced Noise Control Test Rig (ANCTR), which is used to develop technology to reduce acoustic noise level within aircraft engines and airframes. As deposited in Fig. 1. ANCTR is a platform for recording the acoustic behaviors of aircraft. The baseline design for the ANCTR is a 48’ diameter fan (16 blades), 10 ft. fan centerline to ground, inflow control device, rotating rake at inlet and exhaust, and electric motor at 75 hp and 2200 rpm, removable fan exit guide vane design and a Shafts, bearings, belts and coupling provide fan drive from “hidden” electric motor. Within ANCTR there is a component called the Upstream Rake Assembly (USRA). This is shown in Fig.2, the conception design uses a material of Aluminum 6061. The material mechanical properties of Aluminum 6061 (AL 6061) are a density 0.0979 lbm/in^3, Young’s Modulus 3.86E9 lbm/in s^2, Poisson Ratio 0.30, Thermal Expansion 1.3E-5 F, and a Shear Stiffness 1.484E9 lbm/in s^2. The dimension called for a length of 15.92 in., the base plate 5.00 in. x 3.500 in. with a curve radius of 24.00 in. Inside the USRA is located a channel where there will be placed (6) microphones shown in Fig.3, with a dimensions 5.56 mm x 3.98 mm x 2.21mm. The purpose of the KA & KE mic is a time-tested electret condenser microphone, used for sensitive applications measuring low-level noise. In which has a wide range of frequency response. The distance between each mic is 3.00 in. and a diameter of 0.129 in. The baseplate will be fix inside the ANCTR call for 4x diameter 0.2150 in. thru 82° x diameter 0.5000 in. bolt location. The baseline design of the USRA is used to measure the airflow while rotating from 1 RPM to 2200 RPM inside the ANCTR. The manufacturing process called for 175-210 machining hours, creating (5) individual part (Rake Body, Baseplate, Mic tube, Bracket, and Rake Cover) on a STEP/STL file along with conception drawing and an isometric view. Due to the complicity of each part they had to be machined correctly and precisely. They also had to pass the quality assurance (QA) process to be cleared therefore the cost of the USRA is high.

The project was calling for a different approach to achieve the goals of understanding the acoustics noise level at a low price, faster manufacturing process, and to consolidate 5 individual parts to 2 parts (Rake Body and Cover). A new design of the USRA was created using Pro Engineer/CREO shown in Fig.4. modification was implement base on the new design requirements. The length of the rake was reduced to 5.714 in., the baseplate thickness to 0.215 in. and a round over of 0.060 in. that will be connecting the
baseplate of the rake body. The dimensions of the baseplate are 5.000 in. x 3.500 in. and 4x diameter 0.2150 in. thru 82° x diameter 0.5000 in. From the center of the rake body to the center diameter is 1.750 in. with the bolt location distance of 3.500 in. Each mic will have a distance of 0.946 in. starting from the bottom of the baseplate to the center of the (6) mic tube. The tubes outside diameter of 0.125 in. and a inside diameter 0.075. A factor of the consolidating development was to include a round over of 0.060 in. connecting the mic tubes to the rake body to allowing a simpler airflow pattern. A diameter of 0.106 in. is located on the back view. The diameter is used to fasten the mic into place at a fixed position during testing. The width of the rake body to 0.500 in, making the channel wider for easy installation of the mics and cables. The cables will be exiting from the rear of the device at a measurement of 0.750 in. x 0.250 in. rectangular shape. Inserting a dado cut of 5.204 in x 0.2500 in x 0.0625 in. underneath the rake cover in which would allow the cables that are protruding to be protected during test. Investigating different approaches of the manufacturing process and meet the goals of the project.

One of the many goals of this research is to perform an analytical trade study implementing a 3-D printing process shown in Fig.5, of the USRA. The material that was selected for this analytical trade study is ABSPLUS 2. It is a production-grade thermoplastic that is durable enough to perform virtually the same as production parts. ABSPLUS is an ideal material for functional prototyping and manufacturing parts. The material mechanical properties of ABSPLUS are a density 1.04 lbm/in^3, Young’s Modulus 2.007E6 lbm/in s^2, Poisson Ratio 0.30, Thermal Expansion 4.9E-05 F, and a Shear Stiffness 72,177 lbm/in s^2. Understanding materials behavior while rotating 1 RPM to 2200 RPM and the tendency of drag and pressure to rotate about a point that is not on the line of action of the force. For the initial research of the USRA will be to measure the airflow while rotating 1 RPM to 50 RPM (roughly statically fix) in sync with the fan, the velocity/speed of the sound at sea level will be mock 0.1 = 76.1 mph to convert to velocity = 34.029 m/s. The method of calculating drag was used from the given equation.

\[ D = C_D(0.5)pV^2A \]  

Where \( D \) is the drag force, which is by definition the force component in the direction of the air velocity, \( p \) is the density of the air, \( V \) is the velocity of the object relative to the air, \( A \) is the area, and \( C_D \) is the drag coefficient. Based on the geometry of the USRA, the data was used in the drag equation. When analyzing the USRA it was taken into account there would be (2) different areas of drags. The first is \( D_1 \), length 5.499 in. of the rake body called “Bullet” and a \( C_D = 0.295 \). The second is \( D_2 \), cylinder flat plate of the mic tubes called “Flat Plate”. The area of the cross-section inside diameter 0.075 in., outside diameter 0.125 in., and \( C_D = 1.28 \). Being able to solve for \( D_1 \) and \( D_2 \), was able to calculate Pressure. The following is the equation used to find pressure.

\[ P = D/A \]  

Where \( P \) is the pressure, \( D \) is the normal force, and \( A \) is the area of the surface contact. Given \( D_1 \) and \( D_2 \) resulted in solving for \( P_1 = 3.02E-2 \) psi and \( P_2 = 0.129 \) psi. In Fig.6.
illustrates the location where the pressure was applied. $P_1$ is a distributed load, pressure which acts on the length, in this case length of the bullet of the USRA. $P_2$ is a concentrated force, but for this research is the concentrated pressure, acts along the surface cylinder flat plate of the mic tubes. A constraint was applied in the location of the 4x diameter 0.2150 in. thru 82° x diameter 0.5000 in.

The analytical trade study approach that was used to answer the unknown factors from this research was a Cantilever beam method. Because of the rake body, is anchored (fixed) at only one end it carries the load to support the pressure by a moment and shear stress. Future research of the USRA will be introducing an equation of moment. Taking into account that the USRA is homogeneous with a length of 5.499 in. and a uniform cross section of the area subject to a centric axial load pressure. This will allow finding the deformation of the USRA under an axial load introducing Hooke’s Law. The USRA is loaded at different points and consist of several portions of various cross sections introducing the following equation.

$$\delta = \frac{PL}{AE}$$  \hspace{1cm} (3)

Where $P$ is the pressure, $L$ is the length, $A$ is the uniform cross-section of the area, and $E$ is the modulus of elasticity.

Performing the analytical trade study was to comprehend Displacement, Stress, Vibration and Fatigue behavior. Using the newly designed USRA and comparing Aluminum 6061 vs. ABSPLUS 2 to optimize the final design base on weight and stiffness per engineering best practices. The assumption that were made based on the data and boundary condition (BC), using 3-D printing of material ABSPLUS 2 can only with stand a certain amount of pressure before showing signs of fatigue and deformation. Analyzing the data from displacement, the USRA at an erect position examining from the initial to the final position. Material AL6061 demonstrated an insignificant $\Delta$ in length of 5.025E-06 in. while ABSPLUS 2 material confirmed a substantial $\Delta$ in length of 9.55E-03 in. shown in Fig.7. The stress expressing the internal forces results conclude for both materials fatigue and deformation will appear in the same location, at the aft end of the rake body attached to the baseplate. Studying the behavior of the vibration, investigating the oscillation about an equilibrium point. The location is determined at the top of the USRA will establish major changes. The BC: 0.0166Hz to 0.8333Hz for AL6061 the first mode (1) at 3.44E02Hz and ABSPLUS 2 was at mode (1) at 2.41Hz.

Future work of the USRA will include investigating different material with a great stiffness for 3-D printing. By increasing the velocity and monitoring the displacement of the maximum breaking point about a location. Reinforce and redesign areas of maximum stress location. Apply the moment and deformation equation to understand the behavior of mechanical properties of the USRA while in testing.
FIGURES

Fig. 1. Baseline Configuration of the Advance Noise Control Test Rig

Fig. 2. Upstream Rake Assembly AL 6061

Fig. 3. KA & KE microphone

Fig. 4. Mechanical Model of the USRA

Fig. 5. 3-D Model of the USRA

Fig. 6. Applied $P_1$, $P_2$, and constraints of the USRA

Fig. 6. ABSPLUS 2 3-D printing Displacement results
Indexing and TEM Sample Preparation of Isolated CdTe/CdS Nano-Islands

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Abstract

Nano-arrays of CdTe can be used for deep understanding of defects in CdTe/CdS solar cells. In this work, CdTe/CdS nano-islands were indexed and prepared for transmission electron microscopy analysis. A focused ion beam (FIB) system was used to make micro and nano-marks on samples and identify single islands within groups of thousands of islands. CdTe islands were then thinned for electron transparency, detached from the glass/ITO/CdS substrate and placed in a TEM grid using an omniprobe. CdTe nano-islands were successfully indexed and prepared for TEM analysis.

Fig. 1. Schematic representation of CdTe selective growth on glass/ITO/CdS patterned substrates

Fig. 2. a) Micro marks and b) nano-marks made on the surface of a sample shown using a FIB system
1 Introduction

In the last years, CdTe solar cell efficiencies have approached 20% [1]. Most of the research efforts have been made on increasing the short circuit current [2] while the open circuit voltage has remained almost constant for decades [3]. Simulations and recent experimental work have predicted that open circuit voltage depends on defect density and quality of CdTe [2, 3]. Research groups have tried to study the impact of defects on the electrical performance of CdTe solar cells but a technique with high resolution is still needed to decouple the electrical impact of different kinds of defects. We use selective area growth to isolate single CdTe grains and study their microstructure and electrical performance. In this work, a method is presented to index isolated CdTe/CdS junctions and then prepare them for transmission electron microscopy. A schematic presented in figure 1 shows the layers of the samples as well as the selective area growth of CdTe on patterned substrates.

2 Experimental Procedure

CdTe was selectively grown on glass/ITO/CdS nanopatterned substrates using close space sublimation. The nanopatterned structures consisted on 300 nm-sized windows and CdTe nucleated as single grain inside each nano-window. More information on the fabrication procedure can be found somewhere else [4]. A dual beam SEM/FIB system from
FEI with a resolution close to 1 nm was used to see the nano-CdTe islands and prepare samples for TEM. The FIB system consists of an electron gun used for imaging and a Gallium ion gun used for milling placed 52° from each other. The sample is positioned 5 mm away from the electron gun and then tilted 52°. This makes the surface of the sample perpendicular to the ion beam and ready for milling. A fine adjustment is then made to the height of the sample such that both beams aim at the same point. This gives the capability of real time imaging while the sample is being milled. Two rectangular micro-marks were made on the substrate (150 um x 15um) by removing material from the sample. Then, two rectangular nano-marks were made next to one of the micro marks (50 um x 2000 nm) as shown in figure 2 a) and b). The purpose of these marks is to identify specific islands within thousands of islands in a single sample. Since different characterization techniques will be used to characterize a single CdTe nano-island, this technique was developed for CdTe nano-island indexing. An example of island indexing is shown in 3 a). Sample preparation for TEM consisted on 4 steps. First, a platinum protective layer was placed on top of the nano-islands of interest (Figure 3b). Second, two areas are milled on the sides of the islands of interest using the FIB system (figure 4a). Third, a “u” cut is made underneath the islands of interest (figure 4b) and finally the sample is detached from the substrate using an omniprobe (figure 5a) and placed on a TEM grid (figure 5b)

3 Results and Discussion

CdTe nano-islands were successfully indexed and prepared for TEM analysis. Indexing of nano-islands using a dual beam system helped us to orient our sample and identify the same CdTe nano-islands with two different characterization tools (SEM and TEM). A group of CdTe nano-islands were entirely removed from the substrate and thin enough for TEM characterization. The indexing and sample preparation method presented in this work proofs to be a key process for analyzing and correlating the microstructure, electrical performance and atomic defects of single CdTe grains with different characterization techniques.

Acknowledgements

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References

Characterization Methods used on a Multi-layered CdTe/ZnTe Film for use in Solar Cells

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\textbf{ABSTRACT}

Thin films of ZnTe and CdTe have been grown in a close space sublimation reactor for use in a CdTe solar cell device. Due to the complex structure of the films it has been found that simple analysis methods do not always work to provide information to the composition, physical structure or quality of the films and that a combination of SEM images, XRD data, XPS and SIMS must be used. We will show each method and the types of unique results that they can obtain to better characterize a film.

1 Introduction

A close space sublimation (CSS) reactor has been used to create thin films of ZnTe and CdTe for use in solar cells. This type of solar cell is made from depositing a film of CdTe onto a film of CdS creating the PN junction of the device. However, a large lattice mismatch between the two materials leads to a high defect density reducing the efficiency of the device. A ZnTe buffer layer which has been proposed between the CdTe and the CdS to alleviate stress in the interface and reduce the defect density \cite{1} has been grown using a specialized CSS \cite{2} in many arrangements. However, due to the complexity of the layers in the device, analysis of a single sample has become a major challenge on its own since no single characterization method can provide all the relevant data to make an accurate description of the multi-layered film. In this paper we discuss the observations made in these multi-layered structures with SEM, XPS, SIMS and XRD and their place in the characterization.

2 Sample Preparation

All samples were grown inside a specialized CSS reactor containing two independently heated powdered sources of ZnTe and CdTe and the deposition target substrate. An intended layer of ZnTe \textasciitilde{}160nm thick was first deposited followed by \textasciitilde{}100nm of CdTe resulting in a final CdTe/ZnTe/CdS/ITO/Glass multi-layer structure.

3 Characterization

3.1 Scanning Electron Microscope

By using SEM, grain size and quality of the film can be determined very easily from the surface, but no information can be obtained from layers below the surface which in the case of a multi-layered structure lowers the effectiveness of the SEM. In order to obtain relevant information to the complex structure, the sample must be cleaved, or cut with special tools like a focused ion beam (FIB) so that the sample is not damaged and a profile of the thin layers can be viewed. In the sample shown in Figure 1, a FIB was used inside an SEM where a layer of platinum was deposited to protect the surface before milling into the sample;
afterwards, SEM pictures of the profile were obtained where all the layers can be identified except between the CdTe and ZnTe which could indicate a ternary alloy of Cd$_x$Zn$_{(1-x)}$Te and possible grading that cannot be determined with the SEM.

![SEM picture of milling process with FIB and profile view of the sample](image)

**3.2 X-Ray Photoelectron Spectroscopy**

In a multi-layered structure, XPS has a limited function since it only provides data on the first ~10nm of material from the surface. In our sample, XPS was able to accurately give the composition of the top layer of the structure without penetrating into other layers which was Cd 44.91%, Zn 5.92%, and Te 49.17% or approximately Cd$_{0.90}$Zn$_{0.12}$Te$_{0.98}$

**3.3 Secondary Ion Mass Spectrometry**

Since it is a multi-layered film and grading is already suspected SIMS is a method to analyze composition as a function of depth. In this case the sample was analyzed and the raw data is shown on the left image of Figure 2. Unfortunately, the raw data of SIMS is difficult to interpret since the counts don’t exactly represent the composition but also take into account the composition of the matrix bulk matrix. In our case the composition of the bulk matrix is constantly changing so finding correction factors was difficult and so a simple workaround was found by using the values obtained using XPS and using them to normalize the relative atomic percentage of Cd to Zn in the first 10 nm of the material. By doing this and normalizing the composition of the other layers an atomic percentage vs. depth graph was obtained shown in the right side of Figure 2.

![Raw SIMS data and calibrated SIMS data using XPS information](image)

**3.4 X-Ray Diffraction**

The last method used was X-ray diffraction which due to the penetration of the ray analyzes the crystal structure of the entire film down the glass substrate. This introduces many
variables but also provides the opportunity to analyze the sample quickly and non-destructively. When analyzing the XRD data for the sample shown in Figure 3 it is possible to observe that unlike a regular XRD scan which shows distinct single and mostly independent peaks we obtained a range of counts between the <111> peak location of CdTe and ZnTe. Furthermore, when comparing the two strongest peaks of the XRD to the independently calibrated SIMS data of Figure 2 we arrive at similar atomic percentage values at depth ~30nm and ~130nm giving us some confidence in the analysis of the data.

Fig.3. XRD data showing an array of compositions between the <111> peak location of CdTe (blue line) and ZnTe (orange line). Two strongest peaks marked with their composition.

4 Conclusion

We have reached a point where we are capable of growing the complex structures and are about to use these structures to build complete solar cell devices, but we don't know all of the characteristics of the films. All the characterization methods used in this article have they're place but to know the composition of the entire device and the exact grading of the films tools like SIMS, or TEM need to be used which destroy the sample or alternatively use a non-optimal tool like XRD to approximate a value and continue with the process of using a sample in a finished device.

Acknowledgements

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References


Evaluation of a Nanomanipulator Station for Characterization of Nanoscale CdTe Solar Cells

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Abstract

Selective area growth (SAG) has the potential to reduce the number of defects in CdTe and increase the efficiency of CdTe-based solar cells. Electrical characterization of planar CdTe solar cells was performed in this work as to evaluation for future usage on nanopatterned samples. Current vs. Voltage (I-V) measurements were made inside a scanning electron microscope (SEM) using a nanomanipulator station. Samples were placed in a nanomanipulator stage which has nanopores capable of contacting CdTe grains with few nanometers in diameter. Preliminary results show that this setup is an ideal approach to test solar cells at the nano-scale level.

1. Introduction

CdTe solar cells are among the cheapest solar cells in the world because of its cheap fabrication cost. CdTe has a direct band gap of 1.44 eV, close to the optimum for photo conversion, and a very high optical absorption [1]. The theoretical efficiency of CdTe solar cells is 29% and the maximum world record efficiency is of 19.6 % [2]. Fabrication of CdTe solar cells is usually planar. Laboratory planar CdTe solar cells are typically 0.25 cm² big and the contact area is defined by photolithography. Film thicknesses are approximately 100 nm and 4 um for CdS and CdTe respectively [3]. On the other hand, SAG can be used to control the growth of CdTe at the nanoscale and grow single CdTe nano-crystals for CdS/CdTe solar cell applications [4]. By doing this the dislocation density is decreased, thus increasing the efficiency of the overall solar cell. By using SAG of CdTe in nanopatterned glass/ITO/CdS substrate, correlation between electrical performance and microstructure could be made if characterization techniques with high resolution are used. Fig. 1 shows diagram of the idealized nanopatterned ZnCdTe solar cell with CdS substrate. However, characterizing nanoscale solar cells is difficult due to their small size. Also, it is necessary to perform test of light and efficiency in order to simulate their application. Previous measurements showed noise and error giving a V_OC close to 4 volts.

In this work, factors producing noise and errors such as resistance on measurement wires and type of measurement were addressed, thus evaluating its use for IV characterization of CdTe solar cells at the nanoscale level.
2. Methodology

The planar CdTe sample is mounted on the nanomanipulator stage (seen on Fig. 2) and then placed inside the SEM. Planar CdTe sample is used for reference for future measurements on nanoscale solar cell samples. Nanomanipulator stage uses the Zyvex S100 system with driving electronics for positions, connector patch panel interfacing Zyvex probes with other instruments, a joystick for remote control of the probes and a power supply rack to power positioners. Nanoprobes are polycrystalline tungsten wire, 14mm length, shank diameter 0.25mm, and average tip radius of 40nm. Zyvex S100 system is then interfaced with Keithley 2400 general purpose source meter for measurement. Two and four wire measurements with no light are performed on samples for comparison. Also, additional measurements of resistors were performed to ensure measurement reliability.

3. Result and Discussion

Planar CdTe solar cells were measured and recorded in this research. Similar I-V graphs were obtained contacting different parts of the sample. Two and four wire measurement show different results. As seen in Fig. 4, two wire solar cell measurement shows p-n junction behavior with a right shift from the origin. Also, in the same figure, four wire measurement shows that the measurement starts in the origin. It is then seen that noise is introduce when performing an
ordinary two wire measurement. This is confirmed by testing a conventional 5.5kΩ resistor. Fig. 3 shows how a resistor measurement also experiences a shift to the right from the origin. In contrast, four wire measurement passes through the origin. The reciprocal of the slope of the voltage vs. current graphs of resistor show that the value of the resistance closer to the true value is the one made by a 4-wire measurement. It is seen that this shift is of about .75 volts. This shift could be because of the resistances introduced in the overall circuit and contact capacitance. A deep understanding and analysis of the reasons why this shift is introduced will be perform in future trials. However, four wire measurement is shown to be ideal for doing measurements in the nanoscale since noise and additional resistances are removed.

4. Acknowledgements

This work was supported in part by the following grants: NSF/IGERT: DGE-0903670, and DOE/BRIDGE: DE-EE0005958. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

References


Combustion Synthesis of Molybdenum Borosilicides for Ultrahigh-Temperature Structural Applications

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1. Introduction

The ever present aspiration to enhance the efficiency of gas-turbine power plants by operating at higher temperatures leads to the demand for new, ultrahigh-temperature structural materials. In current turbines, components made of nickel-based superalloys can reach temperatures approaching 1150 °C, which is about 200 °C below their melting points [1]. Gas temperatures within the turbines can be higher when the parts are protected by cooling systems and thermal barrier coatings, but cooling drastically reduces the actual engine performance [1, 2]. A preferred solution is the development of new structural materials, based on molybdenum borosilicides, which can operate at temperatures higher than 1300 °C without the need for cooling [1−4]. Molybdenum borosilicides are promising structural materials for gas-turbine power plants. A major challenge, however, is to simultaneously achieve high oxidation resistance and acceptable mechanical properties at high temperatures. For example, molybdenum disilicide (MoSi$_2$) has excellent oxidation resistance and poor mechanical properties [5], while Mo-rich silicides such as Mo$_5$Si$_3$ (called T$_1$) have much better mechanical properties but poor oxidation resistance [4, 5]. One promising approach, explored in the present paper, involves the addition of boron to Mo-rich silicides for improving their oxidation resistance through the formation of a borosilicate surface layer [1]. In particular, Mo$_5$SiB$_2$ (called T$_2$) phase is an attractive material. In the present paper, mechanically activated self-propagating high-temperature synthesis (SHS) [6] of materials based on T$_2$ phase is investigated. This process involves a self-sustained combustion of Mo/Si/B mixture due to exothermic reactions between these powders. High-energy ball milling (mechanical activation) of the mixture is used to facilitate the ignition.

2. Experimental Procedure

Molybdenum (99.95% pure, Climax Molybdenum), silicon (crystalline, 99.5% pure, Alfa Aesar), and boron (amorphous, 94–96% pure, Alfa Aesar) powders were used in this study. The powders were mixed in a three-dimensional inversion kinematics tumbler mixer (Bioengineering Inversina 2L), with the mixing time of 1 h, and then milled in a planetary ball mill (Fritsch Pulverisette 7 premium line). The as-milled powders were compacted into cylindrical pellets in a uniaxial hydraulic press (Carver; force: 10–40 kN). The pellet was installed on a ceramic fiber insulator (Fiberfrax) in a 30-L stainless steel reaction chamber. A booster pellet, prepared from titanium/boron (1 mol Ti + 2 mol B) mixture, was placed at the top of the sample. The chamber was evacuated and filled with ultrahigh purity argon at 1 atm. The booster pellet was heated by a tungsten wire connected to a DC power supply. After fast combustion of the booster mixture, propagation of the combustion front over Mo/Si/B mixture was observed. The as-milled powders and combustion products were analyzed using X-ray diffraction (Bruker D8 Discover XRD). A thermogravimetric analyzer (Netzsch TGA 209 F1 Iris) was used to study the oxidation resistance of the obtained materials.
3. Results and Discussion

The attempts to ignite a mechanically activated mixture of Mo, Si, and B that corresponds to Mo₅SiB₂ phase were unsuccessful. To increase the exothermicity, the composition of the initial mixture was designed according to the stoichiometry of reactions that produce two phases: Mo₅SiB₂ and MoB. The idea of adding more boron is based on the higher exothermicity of Mo–B mixture: the adiabatic flame temperature of Mo–B equimolar mixture is equal to 2310 K, i.e., by 400 K higher than for Mo–Si (1:2 mole ratio) mixture. Table 1 shows the compositions of the prepared mixtures and of the expected products.

Table 1: Compositions and combustion characteristics of the tested Mo–Si–B mixtures.

<table>
<thead>
<tr>
<th>No.</th>
<th>Initial mixture</th>
<th>Expected product</th>
<th>( u )</th>
<th>( z )</th>
<th>( f )</th>
<th>( n )</th>
<th>( v )</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td>( \text{mol}% )</td>
<td>( \text{mol}% )</td>
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<td>-</td>
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</table>

* Accurate measurements were impossible in this case.

The combustion experiments confirmed that the proposed method for increasing the mixture exothermicity works: mixture #2 (see Table 1) ignited and the combustion front stopped before reaching the middle of the pellet, while for mixture #3, the front traveled 90% of the pellet height and for mixtures 4–7, the front reached the bottom of the pellet. All the pellets burned in the spin combustion regime where the combustion wave propagates as the motion of one or several hot spots along a helix on the pellet surface.

The measured characteristics of the spinning front such as the axial velocity \( (u) \), pitch \( (z) \), frequency \( (f) \), number of spin heads \( (n) \), and tangential velocity \( (v) \), are shown in Table 1. A simplified theory of spin combustion developed by Novozhilov [7] predicts that the product \( u \cdot z \) (or \( u^2 f^{-1} \)) is constant and of the same order of magnitude as the thermal diffusivity of the medium. The obtained values of \( u \cdot z \) are, indeed, close to each other (see Table 1). In addition, the measured values of the tangential velocity \( v \) for mixtures 3 and 4 (121 and 47 mm/s, respectively) correlate with the values 106 and 45 mm/s, respectively, obtained using the mass conservation equation: \( v = \pi d u n^{-1} z^{-1} \), where \( d \) is the pellet diameter. Thus, the obtained characteristics of spin combustion are in good agreement with Novozhilov’s theory.
X-ray diffraction analysis of the combustion products has shown that with increasing the content of MoB in the product composition, the content of Mo phase decreases. It is well known that increasing the amount of Mo phase improves mechanical properties of molybdenum silicides and borosilicides, but decreases the oxidation resistance because of the formation and volatilization of MoO₃ [1–5]. To determine the effect of Mo phase on the oxidation resistance of the obtained materials, mixtures 3, 4, and 7 were subjected to thermogravimetric analysis in oxygen–argon flow. For all three samples, the thermogravimetric and calculated differential thermal analysis (c-DTA) curves were virtually identical. Thus, it can be concluded that oxidation resistance of the obtained Mo–Si–B materials is independent on the concentration of Mo phase in the products so that the materials with higher Mo contents are preferable because of better mechanical properties.

4. Acknowledgments

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5. Conclusions

Materials based on Mo₅SiB₂ phase have been obtained by mechanically activated SHS. Combustion of Mo–Si–B mixtures for the formation of Mo₅SiB₂ phase becomes possible if the composition is designed for the addition of reactions leading to the formation of molybdenum boride. These mixtures exhibit spin combustion, the characteristics of which are in good agreement with the spin combustion theory. Oxidation resistance of the obtained Mo–Si–B materials is independent on the concentration of Mo phase in the products so that the materials with a higher Mo content are preferable because of better mechanical properties.

References

Combustion of Lunar and Martian Regolith with Magnesium
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1 Introduction

In-situ resource utilization (ISRU), i.e., the use of lunar and planetary resources for the production of oxygen propellants, and materials is an attractive concept for future space exploration missions. Previous research has shown that lunar regolith forms thermite mixtures with magnesium. Once these mixtures are ignited, they exhibit a self-sustained combustion that leads to the formation of ceramic composites that could be used as construction materials on the Moon [1-4]. In the present paper, this research is expanded to the Martian regolith, with the goal to explore the feasibility of producing construction materials on Mars. Combustion experiments with one lunar and two Martian regolith simulants are also complemented by thermogravimetric analysis, with the goal to reveal the reaction mechanisms.

2 Experimental Procedures

Two Martian regolith simulants (JSC-Mars-1A and Mars Mojave) as well as JSC-1A lunar regolith simulant were studied in the present research. These powders were milled in a planetary ball mill as described elsewhere [2], and then mixed with magnesium powder (−325 mesh, 99.8% pure, Sigma-Aldrich) at different mixture ratios in a three-dimensional inversion kinematics tumbler mixer (Bioengineering Inversina 2L). The mixtures were then compacted into cylindrical pellets (diameter 13 mm) using a uniaxial hydraulic press.

To study the combustion process, the pellet was placed inside a steel chamber (diameter 30 cm, height 40 cm), connected to a compressed argon cylinder and a vacuum pump. The pellet was ignited at the top by a tungsten wire heated using a DC power supply. A C-type thermocouple measured temperature in the middle of the pellet during combustion. Digital video recording was used for observations of the combustion propagation over the pellet and for the determination of the front velocity. All experiments were conducted in an argon environment at atmospheric pressure.

To investigate the reaction mechanisms in the regolith/magnesium mixtures, thermogravimetric analysis (Netzsch TGA 209 F1 Iris) was used. The mixture of 26 wt% Mg and 74 wt% JSC-1A was prepared as described above. The mixture samples placed in alumina crucibles were heated in an argon flow (20 mL/min). The heating process was terminated at different temperatures and the condensed products were cooled in argon. The product compositions were studied with X-ray diffraction analysis (Bruker D8 Discover XRD).
3 Results and Discussion

Figure 1 shows the maximum temperatures during combustion in the mixtures of Mars Mojave regolith with Mg and the adiabatic flame temperatures of this system calculated using THERMO software. A reasonable agreement between experimental and predicted data is observed. Figure 2 shows the front propagation velocity in these mixtures as a function of Mg concentration. For the mixtures based on JSC-Mars-1A, the maximum temperatures and the front velocities are lower.

Figure 3 shows the TG and c-DTA (calculated differential thermal analysis) curves obtained for JSC-1A/Mg mixture at a heating rate of 10°C/min when the process was stopped at 1000°C. The c-DTA curve has a distinct exothermic peak at about 550 °C, i.e., at temperatures below the melting point of magnesium (650 °C).

To investigate this reaction, the heating process, conducted at a heating rate of 5°C/min, was stopped at three different temperatures (500 °C, 550 °C, and 590°C). XRD of the obtained products (Fig. 4) revealed that there is no MgO at 500 °C, while all Mg is converted to MgO at 590°C. At 550 °C, there is a partial conversion of Mg to MgO. These results clearly indicate that the reaction between JSC-1A and Mg occurs at relatively low temperatures when Mg is still solid.
4 Conclusions and Future Work

It has been shown that Mars Mojave and JSC-Mars-1A regolith simulants form combustible mixtures with magnesium. Thermogravimetric analysis conducted for the mixture of JSC-1A lunar regolith simulant with magnesium revealed an exothermic reaction at 550 °C, below the melting point of Mg. Ongoing research focuses on the determination of the reaction mechanisms during combustion of lunar and Martian regolith simulants with magnesium.

Acknowledgments

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References


Hydrogen Generation from Water through the Combustion Reactions with Mechanically Alloyed Al/Mg Powder

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1. Introduction

Hydrogen can be produced from water through the reactions with some metals for space propulsion and fuel cell application. Several research teams have investigated combustible mixtures of water with aluminum powders [1–9]. It was determined, however, that for a self-sustained combustion of such mixtures, nanoscale aluminum powders must be used. These powders have a drawback of the reduced content of free metallic aluminum due to the surface layer oxidation. Also, they are quite expensive.

Recently, mechanically alloyed Al/Mg powder has been fabricated at New Jersey Institute of Technology [10, 11]. This powder is micron-sized, which eliminates the drawbacks of nanoscale Al powders. At the same time, it has a high reactivity. Also, it is expected that it has excellent storage characteristics. The objective of the present paper is to explore the feasibility of using mechanically alloyed Al/Mg powder as an energetic additive in mixtures with water for hydrogen generation.

2. Experimental Procedure

The mechanically alloyed Al/Mg powder was prepared at New Jersey Institute of Technology. This powder was mixed with deionized water. To prevent sedimentation of relatively coarse Al/Mg particles, water was gelified by adding a small amount of poly(acrylamide-co-acrylic acid) (Sigma Aldrich), for simplicity called polyacrylamide in the present paper. First, the gellant was added to distilled water and then the Al/Mg powder was mixed with the obtained gel. The mass fraction of water in the metal-water mixture was varied from 10 to 60%. Two concentrations of polyacrylamide in water were tested: 1 wt% and 3 wt%. A sample of the resulting mixture was then placed in a quartz tube (height 25.4 mm) for the combustion experiments.

Combustion of the obtained mixtures was investigated using an experimental setup with laser ignition (Fig. 1). The setup includes a stainless steel chamber (volume: 11.35 L), equipped with a door port, three windows for observation and video recording, a zinc selenide window for introducing the laser beam, and a pressure transducer (Omegadyne PX-409-030AI). The chamber is connected to a mass-spectrometer (Pfeiffer Omnistar GSD 320) for analysis of gases generated during combustion. The pellet or the quartz tube with the mixture was installed vertically on a brass pedestal.
Before each experiment, the chamber was evacuated and filled with ultra-high purity argon to a pressure of 1 atm. An infrared beam (wavelength: 10.6 µm, diameter: 2.0 ± 0.3 mm) of a CO₂ laser (Synrad Firestar ti-60) was introduced into the chamber vertically through the ZnSe window, located at the chamber lid. The beam was directed to the top of the pellet. For alignment of the optical system, a laser diode (Synrad Diode Pointer) was used. The power of the beam after passing the beam delivery system and ZnSe window was measured with a powermeter (Synrad PW-250) and controlled using a laser controller (Synrad UC-2000), while the duration of the laser pulse was controlled using LabVIEW (National Instruments) software. After ignition, the combustion front propagated downward through the sample. The propagation was monitored using a digital video camera (Sony XCD-SX90CR).

3. Results and Discussion

Initially, experiments were conducted at 3 wt% polyacrylamide. Experiments have shown that mixtures with water concentration up to 60 wt% are combustible. Figure 2 shows the measured combustion front velocities in mixtures with different concentrations of the energetic additive. Hydrogen yield was initially calculated based on the pressure increase after the combustion, measured with the pressure transducer. Figure 3 shows that, with this approach, the experimental values were higher than theoretically possible, which is obviously impossible.

Mass-spectroscopic analysis of the gas environment in the chamber after combustion has detected peaks at 31 and 44 in addition to argon, hydrogen, and air traces. This confirms the presence of gases evolved from polyacrylamide. Calibration of the mass-spectrometer was done for measuring the amount of hydrogen produced. Figure 3 shows that at 46.5 wt% H₂O the H₂ yield is below the maximum theoretical value, which confirms that polyacrylamide produces gases.
Fig. 2. Combustion front velocities in Al/Mg-water mixtures at 3 wt% polyacrylamide with respect to water.

Fig. 3. Hydrogen yield in Al/Mg-water mixtures at 3 wt% polyacrylamide with respect to water.

4. Conclusions and Future Work

Mixtures of gelled water and mechanically alloyed Al/Mg powder are combustible. Upon ignition by a laser beam in an argon environment, a self-sustained propagation of the combustion front occurs, leading to hydrogen generation. The use of polyacrylamide as a gellant increases the burn rate, but its decomposition produces significant amounts of gases. Future work will identify these gases and determine the optimal conditions for hydrogen generation.

5. Acknowledgments

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6. References

Development of a CO₂ Laser Ignition System to Test Solid Propellant Strands

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1 Introduction

This study focused on the development of a new method to ignite solid propellants produced in the authors’ laboratory. Currently, the solid propellants are ignited by a high-energy wire which initiates the deflagration of the propellant. The wire must be pressed against the propellant surface, and then a high current is run through the wire which then gets red hot and subsequently initiates combustion. All experiments were performed using the high-pressure strand burner facility described in more detail by Carro et al. [1]. The new method to ignite the propellants uses a 100 Watt Synrad firestar t100 model laser, which produces a high-purity beam of 2.5 mm diameter and wavelength of 10.6 μm. The laser allows for a more-uniform heating of the propellant surface rather than just the thin surface area of the nickel-chromium (nichrome) wire. Ignition with high-intensity lasers has become common to igniting solid propellants. Applications include the ignition of thermite powders with the ability to measure the energy input to the propellant [2], as well as determining the ignition delay times for propellants with various additives [3]. Presented in this paper is first a background section on the use of lasers to ignite propellant samples, followed by the details of the present experiment.

Cain and Brewster determined that the radiant ignition of AP and HTPB propellants by laser radiation is strongly influenced by the ability to absorb the 10.6-μm wavelength photons. The effect of adding various metal oxides was also found to be minimal for the ignition delay timing [4]. Zanotti and Giuliani first applied a laser to heat up the surface of a solid propellant to its ignition temperature using a 70-W continuous wave CO₂ laser [5]. Aiming the beam down the top of the test apparatus through a zinc selenide (ZnSe) window, the beam ignited the propellant. The ZnSe window was used since is allows the 10.6-μm beam to be optically transmitted through the material at low pressures. Ignition time was determined based on a go/no-go burning criterion which was stated to be the time when combustion was sustained upon interruption of the radiation flux, and not at first light [6]. An electro-mechanical shutter was used to control the delivery of the beam to the propellant surface, and laser power was varied from 60 to 400 W/cm² and was aimed on the top of the propellant surface. The ignition times for the propellant were then plotted [7]. Arkhipov and Korotkikh found that the addition of ultrafine aluminum powder reduced the ignition delay time using the 100-W and the greatest effect on the ignition time was by changing the course-to-fine ratio of the AP [8]. The most effective way to decrease the ignition time is to increase the power output from the laser [4, 8-10]. To ensure that the strength requirements were met for the present high-pressure study, zinc selenide (ZnSe), zinc sulfide (ZnS), and germanium (Ge) window materials were evaluated using the criteria for high strength and optical transmission. The strength was evaluated using thickness correlation for a given diameter and maximum test pressure [11].
2 Experiment

All propellants were produced by hand-mixing techniques developed. The average size of the ammonium perchlorate (AP) particles was found to be 203 µm. A binder of R-45M hydroxyl-terminated polybutadiene (HTPB) was cured by diisocyanate (IPDI). A thorough explanation of the mixing method is provided by Stephens et al. [12, 13]. To ignite the propellant, a nichrome wire is laid across the top surface and a high voltage was applied to the small wire. Future experiments will use high-speed imaging to analyze the flame structure of the propellants, such as shown in Fig. 1.

![Image](image1.png)

Fig. 1 The flame is viewed using high-speed photography showing how the flame is impinged on the electric leads used to initiate combustion (left). Schematic of the control and data acquisition system used at Texas A&M University (right). The illustration includes both ignition systems with the power source and switch for the nichrome wire and the pulse generator to control the laser output.

To evaluate the effectiveness of the new laser ignition system, baseline formulations were ignited using the laser. To effectively control the shutter, a BNC pulse generator was employed to receive a signal from the photodiode to open and close the shutter to ignite the propellant. Initially the shutter was operated manually, but the outcome proved unfavorable, as discussed below. Once the propellant reached self-sustaining combustion, the shutter was closed to prevent excess energy being provided to the propellant surface. Figure 1 is a schematic of the data acquisition system as well as the control system. The power source is only used for the wire ignition experiments, thus, the laser has an independent control switch. Experiments were run with the laser operating at 80 W to reduce the ignition delay time and provide a clearer definition for the light intensity trigger.

3 Results and Analysis

Each propellant when burned produces a pressure trace that is used to calculate the burning rate of the propellant. Knowing that the pressure rises slightly during the test, the test pressure is calculated from the average of the initial and final pressure within the chamber. The burning rate is recorded for various pressures within a set pressure range. Since the relationship of the burning rate is exponential, a conversion to a logarithmic scale is utilized to produce a linear relation. Traditionally, the burning rate \( r \) is given as a function of pressure in the following equation where \( a \) is the leading coefficient, \( P \) is the chamber pressure, and \( n \) is the pressure exponent [1]. The leading coefficient is indicative of the burning rate’s magnitude.

\[
    r = a \ P^n
\]  

Propellants burned using the manual control system resulted in too much energy hitting the surface of the propellant. The amount of excess energy was consistently higher and increased the magnitude of the burning rate when compared to that from the baseline propellants burned using the wire-ignition method. After examining the light trace from the experiment (obtained from the photodiode, Fig. 1), the optimal light emission intensity to close the shutter was determined. That is, the feedback from the photodiode served as the voltage input signal used to
close the shutter. Experiments using the automated shutter produced burning rate data with a magnitude that was measured using the wire-ignition method. The results can be viewed in Fig. 2.

![Burning rate plot of the baseline propellants comparing the initial and final tests using laser ignition. The burning rate is much faster with a manual shutter control (diamonds). After applying a shutter controller, the laser ignition system results (stars and solid line) are the same as for the wire ignition (open circles and dashed line).](image)

The propellant ignited using the manual shutter controls produced burning rates much higher than typical baseline formulations because the amount of time the sample is exposed to the laser light cannot be precisely controlled. Hence, the increased burning rate was due to the excess amount of laser radiation hitting the surface of the propellant.

References


Laminar Flame Speed of Methane with Ethane and Ethylene Addition

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1 Introduction

Ethylene ($C_2H_4$) is an important intermediate species in the oxidation of ethane [1] and higher-order hydrocarbons (HC) used as surrogates for biofuels. Given the hierarchical nature of chemical kinetics mechanisms, blending a higher- and a lower-order HC (alkene and alkane) provides a stringent assessment for identifying model deficiencies. In addition, valuable insights into the fundamental kinetics and combustion behavior of HC’s can be obtained by studying binary mixtures containing $C_2H_4$. All these factors provide the necessary motivation for measurement of flame speeds of alkane-ethylene mixtures.

2 Experimental Setup

Flame speeds of spherically expanding flames were measured using the cylindrical vessel described in Krejci et al. [2]. A z-type schlieren setup was used in conjunction with a high-speed camera to record the flame propagation event. The flame images were processed using a MATLAB-based edge-detection code. The test mixtures were prepared using the method of partial pressures, and all consumable gases were of ultra-high-purity grade.

3 Laminar flame speeds of $CH_4/C_2H_X$ blends and Discussion

Fig. 1 and Fig. 2 show the laminar flame speeds of $CH_4/C_2H_X$ blends at two different mixing ratios, 80/20 and 60/40 by volume. The blending ratios for the $CH_4/C_2H_X$ fuel mixtures were chosen to agree with the blends utilized in the earlier ethane study [3] to perform a comparative assessment on the $C_2H_X$ addition to methane. All experiments were performed at ambient initial conditions. As seen with ethane addition, ethylene addition enhances the flame speeds of methane at all equivalence ratios but at much higher enhancement rates than for $C_2H_6$. The original $CH_4/C_2H_6$ data from Lowry et al. [3] were repeated in a 10 new experiments at the same conditions, and the new data agree with the earlier measurements. The model over predicts the flame speeds at all equivalence ratios for ethane-based mixtures. The agreement is better for $CH_4/C_2H_4$, but improvements are still needed for the fuel-rich cases.

It is of interest to determine whether the difference in the laminar flame speeds for the blends is due to adiabatic flame temperature ($T_{ad}$) effects or due to the chemical kinetics. A mixture...
was formulated so that a fuel blend containing ethylene had the same flame temperatures as a corresponding blend containing ethane. Such a mixture was formulated by adding excess nitrogen to CH\(_4\)/C\(_2\)H\(_4\) such that T\(_{ad}\) of the resulting mixture was within 5 K of that of CH\(_4\)/C\(_2\)H\(_6\) (in air) for the same equivalence and fuel blending ratios. Nitrogen-rich flame speeds of both 80/20 and 60/40 blends of CH\(_4\)/C\(_3\)H\(_4\) were measured over the same range of \(\phi\) of the blends measured earlier using standard air. The measured flame speeds of the ethylene blends in air containing excess nitrogen are also shown in Fig. 1 and Fig. 2. The resulting flame speeds decreased significantly for the diluted blends. Also, the agreement between the measured data and the model predictions improved for these T\(_{ad}\)-matched blends.

From Fig. 1 and Fig. 2, one can see that, as expected, the laminar flame speeds for the blends containing ethylene are higher than those with ethane. It is of interest to determine whether the difference is due to adiabatic flame temperature (T\(_{ad}\)) effects or due to the chemical kinetics. A mixture was formulated so that a fuel blend containing ethylene had the same flame temperatures as a corresponding blend containing ethane. Such a mixture was formulated by adding excess nitrogen to CH\(_4\)/C\(_2\)H\(_4\) such that T\(_{ad}\) of the resulting mixture was within 5 K of that of CH\(_4\)/C\(_2\)H\(_6\) (in air) for the same equivalence and fuel blending ratios. Nitrogen-rich flame speeds of both 80/20 and 60/40 blends of CH\(_4\)/C\(_3\)H\(_4\) were measured over the same range of \(\phi\) of the blends measured earlier using standard air. The measured flame speeds of the ethylene blends in air containing excess nitrogen are also shown in Fig. 1 and Fig. 2. The resulting flame speeds decreased significantly for the diluted blends, for example by 10 cm/s for the 60/40 CH\(_4\)/C\(_3\)H\(_4\) mixtures in Fig. 2. Also, the agreement between the measured data and the model predictions improved for these T\(_{ad}\)-matched blends.

Flame-speed-enhancing effects of C\(_2\)H\(_X\) addition to CH\(_4\) can be categorized into thermal, kinetic, and diffusive effects [4, 5]. The contribution of each effect can be modeled as

\[ S_{L,u}^* \sim (aLe)^{1/2} \exp(-T_a/2T_{ad}) \]  

(1)

The first term on the right-hand side represents the diffusive effect (which is the product of the mixture thermal diffusivity, \(\alpha\), and the Lewis number of the blend). The second term is the Arrhenius factor which represents the combined contribution of the activation temperature (T\(_{ad}\)=E\(_a\)/R; where E\(_a\) is the global activation energy, and R is the universal gas constant) and the adiabatic flame temperature. The two terms represent the kinetic and thermal pathways, respectively. For HC blends, two definitions, namely, heat-release-based values (Le\(_q\)) and a volumetric-weighted-scheme (Le\(_v\)) are typically used, as reviewed by Bouvet et al. [6] (and references therein). However, the overall trends in Le are the same irrespective of the definition (not shown here).

The activation energy E\(_a\) is defined as the slope of the mass burning flux and the inverse adiabatic flame temperature at constant \(\phi\). The mass burning flux can be varied by changing the diluent concentration or by preheating the unburnt gas (or numerically varying unburnt gas temperature in PREMIX as done herein), but the diluent approach also changes the reactant concentration [7]. E\(_a\) for pure ethylene, estimated herein from chemical kinetics simulations, agreed well with the experimentally determined values by Kumar et al. [8] (not shown here).

The vastly different enhancement rates of ethylene when compared to ethane in CH\(_4\)/C\(_2\)H\(_X\) blends were investigated. Equation (1) can be differentiated to determine the sensitivity of each pathway on the overall enhancement or inhibition of flame speeds. Thus,

\[ \frac{1}{S_{L,u}} \frac{dS_{L,u}}{dx} = \frac{1}{2aLe} \frac{d(aLe)}{dx} - \frac{1}{2T_{ad}} \frac{dT_a}{dx} + \frac{T_a}{2T_{ad}^2} \frac{dT_{ad}}{dx} \]  

(2)

where \(x\) is the volume fraction of C\(_2\)H\(_X\) in the fuel blend.

Diffusive effects are represented by the first term on the right of Eq. (2). The kinetic (activation temperature) and the thermal (flame temperature) contributions are the last two terms, respectively. The kinetic and thermal effects are coupled and hence are usually grouped as the Arrhenius effect. Sensitivity analysis was conducted at two different mixture strengths
(Fig. 3 and Fig. 4) over a wide range of blending ratios (10-50% C$_2$H$_x$ in the blend). All three pathways have a positive sensitivity (or enhancing effect) on the flame speeds of CH$_4$/C$_2$H$_x$ blends at $\phi = 0.7$. The diffusion effect, however, has a negative sensitivity (or inhibiting effect) for the fuel-rich mixtures. For CH$_4$/C$_2$H$_x$ mixtures, the dominant mechanism of flame speed enhancement is through the reduction of the activation energy, i.e. the kinetic effect. For lean ethane-based mixtures, the diffusive pathway has a stronger influence on the enhancement rate than the thermal effect. This behavior is consistent with the fact that the T$_{ad}$ of CH$_4$/C$_2$H$_6$ does not increase appreciably with ethane addition. However, for lean ethylene blends, the thermal effect is stronger than the diffusion effect, and the thermal effect becomes comparable to the kinetic effect as the C$_2$H$_4$ concentration is increased (as the activation energy asymptotes to E$_a$ for pure ethylene). Furthermore, the kinetic effect of CH$_4$/C$_2$H$_4$ is higher (lower) than that of C$_2$H$_6$-doped blends for rich (lean) mixtures.

### 4 Conclusions

Two binary fuel blends, 80/20 and 60/40 (by volume), of CH$_4$/C$_2$H$_x$ were measured. Sensitivity analysis showed that the dominant mechanism of flame speed enhancement of the CH$_4$/C$_2$H$_x$ blends was through the reduction of the global activation energy (i.e., a kinetic effect). The diffusion effect had a positive (negative) sensitivity for lean (rich) $\phi$ for the different blends. Flame temperature had a stronger effect than the diffusive pathway for ethylene-containing mixtures, but was comparable to the diffusive effect for ethane-based mixtures.

### References


Influence of Nano-Aluminum on Stoichiometric Methane-O$_2$-N$_2$ Laminar Flame Speed

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1 Introduction

Dust explosions in process industries cause millions of dollars in damage to facilities and incalculable damage to personnel, making the understanding of the mechanisms behind dust explosions a top priority to prevent such disasters. The long-term objective in this study is to establish a method of measuring laminar flame speed of an aerosol mixture to a higher degree of accuracy than has been achieved in previous studies.

In the present study, improvements were made on an existing gas-phase, spherical flame vessel to introduce dust into a controlled environment in a repeatable fashion to measure the flame speed using existing optical methods. As follows is a summary of the experimental facility and the techniques that have been developed thus far for producing a controlled heterogeneous flame speed experiment. The second half of the paper presents results from flame speed experiments involving suspended Al particles in a CH$_4$/O$_2$/N$_2$ mixture.

2 Experiments

The low-pressure laminar flame facility at Texas A&M University is a 28.1-L, 35.6-cm long cylindrical vessel designed to be filled with gas-phase components up to a maximum of 5 atm. Fuel-air mixtures are ignited using a central ignition system, and the resulting propagating flame is captured using a high-speed camera in a Z-type schlieren setup. For information regarding the existing flame speed facility, including equipment, testing procedure and theory, see the earlier work by Lowry et al. [1].

2.1 Dust injection

From exploratory experiments there was loss of mass during transfer of the powder. To minimize the mass loss, a new setup was employed where a section of pipe was removed so that the mass loading is now measured inside the tube section rather than transferred to it. A schematic for this design is shown in Fig.1.

In this experimental design, the entire system is filled to atmosphere with the mixture and then the section between valves 1 and 2 is isolated to remove and fill with dust. The entire system is then vacuumed down to 745 torr. To inject the dust, the volume between valves 2 and 3 is filled to 172.5 psi of nitrogen. The experiment begins the moment valve 2 is opened and the dust is injected.
2.2 Extinction experiments

It is vital to be able to measure the amount of mass as a function of time in these experiments for both repeatability and, most importantly, to know the amount of suspended mass at the time of combustion. The method chosen was a non-intrusive laser extinction diagnostic based on the Beer-Lambert Law which calculates the attenuation of light due to extinction from particles [3]. A standard laser system was installed at the flame speed rig. In this setup, a 632.8-nm, 5-mW Helium-Neon (HeNe) laser is sent through a 50/50 beamsplitter, which splits the laser light and sends roughly half of it to the first photodiode and the rest through the combustion vessel and ultimately onto a second photodiode. Focusing lenses are used to focus the laser for maximum signal and polarizers are used to set $I_0$ and $I$ equal to each other before any dust is introduced.

As mentioned before, these two signals are then combined and used to evaluate the mass of particles in the chamber based on the Beer-Lambert Law shown in Eq. (1) [3].

$$m_{\text{susp}} = \frac{-\pi (d_P)^2 \rho_P d_V^2}{q_{\text{ext}}} \ln \left( \frac{l}{l_0} \right)$$  (1)

where $m_{\text{susp}}$ is the suspended mass, $d_P$ is the average particle diameter, $\rho_P$ is the particle density, $d_V$ is the inner diameter of the vessel, $q_{\text{ext}}$ is the extinction efficiency factor, $l_0$ is the reference signal, and $l$ is the attenuated signal. It is assumed that each particle is a perfect sphere of diameter 100 nm because the chosen dust is a 100-nm nano-aluminum purchased from US Research Nanomaterials, Inc. This dust is used because of the nature of the testing procedure, which can occur over several minutes. The particles must be very small so that they stay suspended long enough for the air to become quiescent, and so they vaporize and react quickly.

2.2 Aerosol combustion experiments

For the present experiments, the nano-aluminum was introduced into a fuel-oxidizer-diluent mixture. In this way, the system under study was therefore one where the flame is initiated in the main fuel-air mixture that contains a seeding of nano-aluminum particles. The mixture used was a stoichiometric CH$_4$/O$_2$/N$_2$ mixture that was oxygen rich, 70% N$_2$/30% O$_2$. The reason for the choice of CH$_4$ is because it is a common and very well-studied fuel, allowing for any results to be attributed to the introduction of the nano-aluminum rather than uncertainties in the fuel’s flame speed. The reason for the oxygen-rich air is because in Vissotski et al. [2] it was suspected that the aluminum would not contribute to the reaction if the adiabatic flame temperature was below about 2300 K (i.e., the melting temperature of aluminum).
3 Results and Discussion

Target suspended masses were set at 1, 6, 8, and 14 mg for combustion experiments. The suspended masses in the combustion experiments nearly match the targeted suspended masses, which bodes well for repeatability. The combustion results are shown in Fig.2, in terms of the laminar flame speed.

![Graph showing laminar flame speed results](image)

In this plot of unburned-unstretched laminar flame speed as a function of suspended mass, there is a noticeable drop in flame speed with the addition of particles of about 5 cm/s, which is above the estimated experimental uncertainty of ±1 cm/s. This conclusion brings up the question of whether or not the aluminum is participating in the reaction at all. This question is partially answered by looking at the raw images from the experiments. It appears that the onset of flame surface instabilities occurs faster with larger levels of suspended mass. This trend indicates that the nano-aluminum does play some part in the combustion process. The current theory is that the decrease in flame speed is caused by some of the heat of combustion being used to melt through the alumina layer that coats all particles and subsequent heating of the aluminum to its vaporization temperature.

4 Results and Discussion

A method of introducing dust into an existing spherical flame speed vessel was refined by increasing the repeatability and ease at which experiments could be performed. Combustion tests were performed and analyzed with optical techniques that allow for visual inspection to determine the onset of flame instability as well as identifying the amount of suspended mass. The resulting flame speed results show that adding nano-aluminum does influence the combustion process by decreasing the flame speed of the CH$_4$/O$_2$/N$_2$ mixture, but it is also contributing because of the quicker onset of flame surface instabilities.

References


Ignition Delay Time and Laminar Flame Speed Measurements of Propene

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1 Introduction

Propene is an important intermediate species in the combustion of larger hydrocarbons, making it important to understand the details of its combustion kinetics. Ignition delay time and flame speed studies have been conducted several times, but there is not agreement amongst the data [1-5]. New experimental measurements are necessary to further develop the sub-mechanism. This study compares experimental results conducted at Texas A\&M University (TAMU), to validate the mechanism developed at National University of Ireland, Galway. The work presented herein represents only part of a larger, multi-institution effort to study the kinetics of propene.

2 Experimental setup

2.1-Shock tube

Ignition delay times were measured in a single-diaphragm, stainless steel shock tube. Further details and schematics on the shock tube are available in Petersen et al. [6] and Aul et al. [7].

2.2 Flame Speed

Flame Speed was measured using the stainless steel constant-volume bomb at TAMU. The design of this vessel is explained in detail in Krejci et al. [8]. The vessel was filled with Research grade Propene (99.5\%) and Primary Standard Air using the partial pressure method. Experiments were conducted over a wide range of equivalence ratios ($\phi$) from 0.7 to 1.7.

3 Results

3.1-Shock tube

Seven mixtures with Ar dilution were investigated in this study. The first two mixtures correspond to undiluted mixtures in air (with Ar replacing N\textsubscript{2}). The results for these two mixtures are visible in Fig. 1. The difference in the equivalence ratio between Mix 1 and Mix 2 does not lead to a large difference between the ignition delay times. The pressure effect was investigated for Mix 2 only. It is visible that there is a very large effect of pressure on ignition delay time. For these mixtures, the model does a good job at predicting the 10-atm data, with only a slight under-prediction of the reactivity with Mix 1. At lower pressure, the model is however not as good, notably for the lowest temperature investigated since a 40\% difference was observed.
For an intermediate dilution level, Mix 3, the pressure effect is still very important (Fig. 2), with a factor of around 3 being observed between data at near 1.75 atm and those near 9.4 atm. The model is predicting well the high-temperature side of the low- and high-pressure data, while an over-prediction of the ignition delay time can be observed for low temperatures.

The Mixtures 4, 5, and 6 share the same O\textsubscript{2} concentration, and the equivalence ratio was varied by changing the amount of propene. As can be seen in Fig. 3, an increase in the equivalence ratio leads to an increase in the ignition delay time, this trend being more prominent at low temperature and pressure. Overall, these data are well predicted by the model.

For the highest dilution level investigated, Fig. 4, the pressure effect is relatively large and uniform over the range of temperature investigated. The model is notably under-reactive for the 10-atm case, with ignition delay times that are too long by 50\% at high temperatures and by a factor of 2.5 on the low-temperature side. For the low-pressure case, data are correctly predicted at high temperature but the model is still under-reactive at low temperature.
3.2 Flame Speed

Flame speed and Markstein Lengths were calculated using both the linear Markstein relation and the nonlinear model as shown by Chen [9]. No appreciable difference in flame speed was found between the two methods. While the experimental data compare very well to the original model, there were some under estimations of flame speed. The updated version of the mechanism compares much better with the experimental results. Experiments proved to be repeatable with a calculated uncertainty as outlined in Krejci et al. [8] and Moffat [10] to be ± 0.58 cm/s.

![Graph showing laminar flame speed of propene in air](image)

**Fig. 5.** Laminar Flame Speed of Propene in Air

4. Conclusion

To improve the sub-mechanism of propene, new ignition delay time and laminar flame speed measurements have been performed. The comparison between the model and the data showed good agreement, although predictions for very dilute mixtures in the shock tube can still be improved. Compared to the original version of the mechanism, the laminar flame speed predictions have been significantly improved. As the mechanism continues to be updated and improved, new experimental results will continue to be used to validate and improve the model.

5. References

Development of a New Drag Model for Spherical and Non-Spherical Particles

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1. Introduction
Due to an abundance of coal available in the United States researchers are trying to find more efficient and less polluting ways to utilize coal for energy production. Use of gas-solid fluidized beds is a technology where coal is reacted with air and steam to produce syngas. Syngas is a fuel that allows for less polluting and more efficient way to extract chemical energy from coal. With the use of large computational facilities researchers have extensively explored ways to model the multiphase fluidization process computationally. In these models the solid particles and the fluid mix inside the gasifier column or bed and create a very complex flow patterns. When the coal is pulverized for use in the gasifier many of the particles are of irregular shape. Up to now literature has provided a large amount of information on the behavior of spherical particles, mainly because of the assumptions one can make about the physics of a symmetrical round particle. In an actual system, however, many non-spherical particles will be present leading to a different set of equations necessary to predict the physics of the flow in the gasifier column. Hilal et al. [1] analyzed the effects of bed diameter, gas distributor, and inserts on minimum fluidization velocity. Sau et al. [2] determined that the total pressure drop increased with the increase of superficial gas velocity. Escudero et al. [3] proposed that the minimum fluidization velocity is influenced by the changes in particle density. Tran-Cong et al [4] proposed an empirical correlation for drag coefficient from experimentally measured data of six different shapes of sphere particles. Therefore, based on the needs in this area to model non-spherical particles, this paper will present a new experimentally derived drag relationship that can be used in computational models of non-spherical particles.

2. Objective
The objective of this paper is to determine the drag and Reynolds number relationship which can predict the drag of particles for spheicity of 0.4 to 1.

3. Experimental setup
To run the experiments a laboratory scale fluidized bed was designed and constructed which was 12.4 cm in diameter and 1.5 m in height and made of Plexiglass. A 53 micron mesh was used at the bottom of the bed to hold the particle and the static bed height was 5 cm. A 3.73 kW blower was used to supply the air through the duct to the test section. To control the flow rate a butterfly valve was used. Honeycomb shape flow distributor
was used to ensure the uniform flow to the bed. For the test 1 mm diameter borosilicate glass beads were used as the test particle.

4. Results & Discussion:
A compilation of data obtained from experiments performed at UTEP and those available in literature [5] was used to determine the relationship between drag coefficient and Reynolds number for particle sphericities from 0.4 to 1.0. The particle sphericity is a non-dimensional unit of measure that determines the roundness of an object, the closer to the value of 1 the more like a sphere the shape approximates. The new drag relationship presented in this paper captures this large range of sphericity values. The main contribution of this paper involves the inclusion of this large range of sphericities which has not been used before. Typically available correlations only have a very small range of sphericities which they capture, a small amount of shapes, or do not consider particle shape in their calculation. By performing a non-linear least squares approximation from the compiled data coefficients were obtained and are shown in Table 1.

Table 1: Non-linear coefficients obtained after curve fitting a wide range of data for spherical and non-spherical particles

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>A</th>
<th>B</th>
<th>C</th>
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<td>0.4261</td>
<td>0.2941</td>
<td>19.5</td>
</tr>
</tbody>
</table>

These coefficients were then fitted to the semi-empirical model first proposed by Haider and Levenspiel. Using this equation drag and pressure drop in a fluidized bed can be used to predict the drag for different Reynolds numbers for sphericity from 0.4 to 1.0. This equation in shown on the next page.
\[
C_D = \frac{24}{R_e} \left[ 1 + \exp \left( -142.7125 + 555.6305\theta - 533.0946\theta^2 \right) R_e^{(-0.57310-0.9510)} \right] \\
+ \frac{\exp \left( -3.7196 - 14.1788\theta - 15.6879\theta^2 - 3.9920\theta^3 \right)}{1 + \exp \left( -870.8 + 4224.9\theta - 6584\theta^2 + 3232.9\theta^3 \right)}
\]

5. Conclusion:
The need for better understanding and prediction of particle behaviors in a gasifier has been established. This paper presents a relationship that can be used in computational models that can improve the prediction of flows in a multiphase flow system. A relationship was derived from experiments and literature that uses the particle Reynolds number for various sphericities. The formula developed in this paper can predict the drag of the particles with the change of Reynolds number for sphericity of 0.4 to 1.

References


Experimental Evaluation of a Stability Map for a Multi-
Tube Fuel Injector

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1. Introduction

According to U.S Energy Information Administration [1], coal is predicted to be the dominant source of power production in the United States until 2035. With fifty percent of the electricity generated in the United States originating from coal, the U.S. produces close to 2 billion tons of CO₂ per year from coal-burning power plants. The Integrated Gasification Combined Cycle (IGCC) offers a cleaner way to generate electricity using coal. IGCC is a process where the feedstock is gasified and converted into syngas (CO-H₂) which can then be used as a fuel source to power energy-generating gas turbines [2]. Compared to other hydrocarbons, high hydrogen content fuels behave differently because of their much higher specific heat, higher diffusivity, flammability limits and higher laminar flame speed [3]. The design of a fuel injector plays a vital role in terms of mixing which impacts flame stability. A stability map of a multi-tube injector is presented in this paper. Stability is of special concern when designing combustion devices and allows the designer to know what the stability regions are and to keep away from flame flashback and flame blowout. In this paper the stability map of a multi-tube injector is investigated. The stability predictions presented are valid for a syngas composition of 30%H₂ and 70%CO by volume at different equivalence ratios at atmospheric conditions.

2. Experimental Setup and Components

The orifice diameter and design for the multi-tube injector was selected to prevent flashback by sizing exit ports to be near or at the quenching diameter of syngas fuel mixtures. Since the orifice ports are smaller, lean blow out due to higher velocities poses a challenge in the design. Using smaller ports also cause higher pressure drops which may be of concern for some combustors. The final design is composed of three different parts: injector head, connecting tube, and the injector base. A grouping was made at the bottom side of the injector head and welded with the connector. The injector base connects to the injector to the front cap of the combustor. The base has a diameter of 0.02 m which accommodates the combustor’s front cap for an easy installation.

The injector was installed in the existing high pressure combustor. The high pressure combustor is designed with a safety factor of 1.7 and is capable of sustaining a maximum temperature of 2400K, a chamber pressure of 1.5 MPa, and a thermal power of 500KW.
3. Experimental Procedure

In order to achieve stability, the flame speed must be equal to the speed of the normal component of the unburned gas at each location [4]. To define the stability map for the multi-tube injector, volumetric flow rates were calculated in order to have the fuel pre-mixed gases exit at the same calculated flame velocity $S_L$. Research grade fuel was delivered to the manifold from pressurized tanks at 2.75 MPa while air was supplied at 2.75 MPa from a compressor. Manual precision metering valves in conjunction with solenoid and proportional valves were used to control fuel and oxidant flow rates. A bank of digital flow meters was used to measure volume flow rates of fuels and oxidants to achieve the desired compositions. A methane pilot flame was used to ignite the main fuel line. Figure 1 depicts a schematic diagram of the experimental setup.

Figure 1. Experimental setup schematic

In order to be able to predict the stability range of the injector, an initial estimate of the velocities at which the flame would be stable was made. A velocity boundary layer profile was defined which was used later to define the flow rates needed. In order to have an anchored flame the fuel’s velocity should be at least equal to the flame speed when sufficiently close to the injector outer wall, in this way boundary layer flashback would be avoided. A sample of a stabilized-near flashback flame is presented in Fig. 2.

Figure 2. Premixed flame emitted from injector near flashback condition
4. Results and Discussion

In order to be able to predict the stability range of the injector an initial estimate of the velocities at which the flame would be stable was made. A velocity boundary layer profile was defined which was later on used to define the flow rates needed. The flashback state of the flame was determined visually as seen in Fig. 2. Figure 3 presents the stability plot obtained for the injector.

![Graph of jet velocity and flame speed](image)

Figure 3. Jet velocity through each injector port and flame speed plotted against equivalence ratio

Any bulk jet velocity below the values presented would induce boundary layer flashback on the tested injector. A ratio of bulk velocity to flame speed of 7 was documented throughout the different equivalence ratios tested. Combustion instabilities were also noted during experimentation which will be a topic of future research.

5. Conclusions

A multi-tube injector was designed and installed on a high pressure combustion facility. The stability of the presented multi-tube injector was determined. It is of particular interest that combustion instabilities were generated during the experimentations which could be a topic of interest for future research.

References

Effect of Metal Foam on Heat Transfer Rates When Applied to Air Cooled Condenser Tubes

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1 Introduction

Air-cooled heat exchangers are used in steam power plants as an alternative to water cooled condensers in order to both cool water-vapor used in the steam turbines and reduce freshwater usage from these types of power plants. In these types of heat exchangers with tube banks, one fluid flows through the tubes while the other passes over the tubes convectively cooling or heating the fluid flowing within the pipe. This study will consider the effect of metal foam consisting of 20 pores per inch (PPI) that is applied to the outer surface of the tubes. The height of the metal foam applied on the tubes is 20 mm and three important parameters are examined including the pressure drop, velocity change, and the overall heat transfer exchange when adding the metal foam to the surface.

2 Objectives

The objective of the current study is to document the performance of an ACC where tubes are wrapped with metal foam and compare it with bare tubes by developing a two-dimensional computational grid with appropriate boundary conditions. These results will be verified with theory and by developing a three-dimensional computational grid.

3 Methodology

3.1 2D Analysis

The 2D simulation consisted of a cross section of a bank of tubes with two rows in the flow direction (\(N_L=2\)) and three columns (\(N_T=3\)). The dimensions are based in the minimum commercially available size which is 0.0508 m in diameter and 4.8768 m in length (Serth, 2007). In this case, the longitudinal pitch, \(S_L\), and the transverse pitch, \(S_T\), are equal in size which is 0.05715 m. Fig. 1 shows the bank of tubes in pre-process.

The initial air properties are taken at standard conditions, 1 atm and 20°C. For the walls of the tubes, they are assumed to be stationary and the no slip condition is selected. The air’s inlet velocity is 5 m/s and the absolute pressure is set to be atmospheric. The air velocity is determined.

![Fig. 1 Tube-bank](image_url)
The conservation of energy principle is used to validate and analyze the temperature changes in both air and water vapor, the conservation of energy used can be seen in the equation below:

\[ m_{air}c_p\Delta T_{air} = m_{vapor}c_p\Delta T_{vapor} \]  

(1)

Before any further analysis, the calculation of Reynolds Number and Nusselt Number is crucial in this analysis. The follow was used to verify the results of the model from a heat exchanger.

\[ Re = \frac{\rho V_D}{\mu} \]  

(2)

\[ Nu = 0.27Re^{0.27}Pr^{0.36}\left(\frac{Pr}{Pr}\right)^{25} \]  

(3)

Therefore, the change in temperature of both air and vapor can be calculated.

### 3.2 3D Analysis

The 3D model uses the same parameters as the 2D model but with a depth of 61 cm. Figure 2 shows the actual 3D model of the heat exchanger. The square enclosed represents the region of air flow and the cylinders inside the tubes that water vapor is flowing through. The tube material is made of aluminum.

![Fig.2 Three-dimensional bank of tubes.](image)

### 4 Results and Discussion

#### 4.1 2D Results

The maximum theoretical velocity over the tube bank is calculated by:

\[ V_{max} = \frac{s_t}{s_{t-D}} \times V \]  

(4)

Which gives, \( V_{max} = 9.0 \) m/s. According to Cengel [1], the maximum velocity of air occurs between the tubes. Figure 3 shows the velocity contour of the air in the inlet and how the maximum velocity is in between the tubes. According to Cengel [1], the maximum velocity of air occurs between the tubes. Figure 3 shows the velocity contour of the air in the inlet and how the maximum velocity is in between the tubes.
4.2 3D Results
For the 3D analysis, the temperature drop of the water vapor is calculated. Using Eq. (3), the total heat transfer from the air to the water is 15.8 kW. Figure 4 shows the temperature drop alongside each tube.

5 Conclusion
Air cooled condensers prove that it is possible to use other fluid than water to condense high temperature water vapor. The cross-flow of air was able to transfer about 15.8 kW from the water-vapor generating a temperature drop of 200 K.

References
Development of a Wireless Temperature Sensor Using a Lithium Niobate Pyroelectric Ceramic

Md Rashedul H Sarker, Salvador Sandoval, Norman Love
Department of Mechanical Engineering, El Paso, TX 79968, USA;

1 Introduction
Combustion and energy production systems in use can gain operational advantages if operational parameters are monitored and controlled properly for better performance. By using information gathered from the power generation unit adjustment of combustion parameters can improve the efficiency, reduce detrimental impact on environment from emission of pollutants, and also minimize the green house effect. There are different key parameters that control energy conversion technologies performance such as temperature, pressure, emission of exhaust gas, flow rate and density [1]. Among all of these, temperature is one of the most important parameters dictating the efficiency of many systems; this is verified by a quick calculation on the Carnot efficiency of a system. Materials used in power generation units are also of concern since these have some practical limits due to high temperature and thermal cycling that can cause catastrophic failure of components [2, 3]. Because of the balance of these constraints, a temperature safety margin is usually maintained between high performance and reliability. The safety margin is met by maintaining temperatures lower than optimal temperature in order to avoid temperature induced fatigue failure. This safety margin becomes larger when operating temperature is not well characterized. However, safety margin can be minimized, allowing for higher optimal temperature ranges thus increasing performance. Hence, this paper presents real time the process of the use of a pyroelectric sensor for wireless temperature measurements. With the development of this technology future power generation units may be able to reduce the operational temperature safety margin and thereby increasing efficiency.

2 Objectives
The proposed work will demonstrate the application of sensor, capable of receiving wireless signal remotely from a pyroelectric ceramic. A correlation between temperature and voltage generated from sensor will also be proposed by calibrating sensor response, temperature change over time

3 Experimental Methodology
To measure the temperature, a Hall Effect sensor working principle will be used to detect magnetic flux from the pyroelectric ceramic. Lithium Niobate (LiNbO$_3$) ceramic will be used as test material to detect temperature. Lithium niobate ceramic provide charge while experiencing temperature change over time. This charge will be carried out by a winding coil which will produce a magnetic flux and will be detected by the presence of Hall Effect sensor remotely. The Hall Effect sensor produces a voltage which is perpendicular to current and magnetic field and proportional to current and voltage.

\[ V_H \alpha I \times B \]
At the beginning of the project, external power supply was used to provide current in winding coil to produce magnetic field in order to demonstrate the working capability of wireless sensing method. Figure 1 shows Hall Effect Sensor and circuit diagram.

![Figure 1: Hall Effect Sensing Device and its Circuit Diagram](image)

The Hall Effect sensor device was also used to measure generated voltage from a commercial thermoelectric device while maintaining a temperature gradient on it with the help of water-cooled heat sink and electronically controlled heater. Generated current from thermoelectric device due to temperature gradient connected to a winded coil for current loop. The winded coil with current loop produced a magnetic field detected by the Hall Effect device. To determine signal loss due to obstacles between the magnetic flux source and wireless sensing device, an aluminum plate with a 0.3 cm thickness was placed between magnetic coil and Hall Effect sensor. In this experiment, current was supplied to the magnetic coil from the external power source up to 2 amps. Figure 2 shows experimental setup using thermoelectric device and 0.3 cm aluminum block between the coil and Hall Effect sensor.

![Figure 2: Experimental Setup using Thermoelectric Device and Aluminum Block (3 mm)](image)

The lithium niobate pyroelectric ceramic sample has also been made with the help of laboratory facilities. The pyroelectric has dimensions of 2x2 inches and 0.079 inch thickness which can be cured at 150°C for 2 hours. Sample will be sintered and SEM result will be acquired. As a future work this sample will be used as test materials to produce a current when exposed to a temperature which will generate a magnetic flux in the attached coil.

### 3 Results & Discussion

Figure 3 shows a relationship between Hall Effect sensor output voltage fluctuation and increasing and decreasing temperature gradient in Thermoelectric Generator. Current (I) supply in the winded coil from thermoelectric generator produced magnetic field which is
detected by the Hall Effect sensor. Voltage fluctuation in Hall Effect sensor was measured to be as high as 3.5 mV.

![Figure 3: Voltage vs. Temperature Relationship](image)

Figure 4 shows the results when the aluminum block was placed between the Hall Effect sensor and magnetic flux generating coil. From the results, the voltage fluctuation from the Hall Effect sensor was higher when using block than without any block.

![Figure 4: Signal loss comparison with/without aluminum block](image)

4 Conclusion

A novel experimental setup was developed using the magnetic flux generated from a thermoelectric and pyroelectric temperature sensor. The signal from the sensors was transmitted wirelessly and measured for a variety of conditions. Future goals of this project include the measurement from within a high temperature environment using a lithium niobate ceramic pyroelectric material.

References

Study of Tungsten-Yttrium Based Coatings for Nuclear Applications

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1. Introduction

In the previous report it was investigated the fundamental structure-property evaluation of Tungsten-Yttrium (W-Y) nanostructure variable with dependent sputtering pressure $P_{Ar}$. It was found that the sputtering pressure can tailor the phase structure of the film. A transformation from body centered cubic ($\alpha$-W) was favored at sputtering pressures greater than 0.63E-2 mbar whereas a metastable A15 phase ($\beta$-W) was favored when sputtering pressures of 0.46E-2 or lower were used. It was also investigated the incorporation of Y atoms into the lattice using the Rutherford backscattering technique and established that Y content in the film is less than 5wt. % the film will behave similar as pure W would under variable pressure. In order to achieve an isotropic, crack-resistant material, mechanical W-Y allow a fundamental understanding of mechanical and electrical properties must be investigated. This quarter was devoted to grow comparable W-Y samples with a variable content of Y in the lattice and its electrical and mechanical properties were compared to pure W, W 95 –Y 5 wt. % and W 90 –Y 10 wt. %.

It is well known that the mechanical properties of nanocrystalline metals apparently differ from those of the conventional polycrystalline materials [1,5]. In the case of hard metal films, some studies have reported that the very high hardness of Ta[6] and Mo[7] films were obtained as 11.6 and 11.8 GPa, respectively, which are much higher than those of bulk Ta and Mo. Tungsten (W) and W-based alloyed films possess many attractive properties, such as high melting temperature, high mechanical strength, and good metal barrier performance [8,9]. Taking account of the fact that bulk W is harder than corresponding Ta and Mo, W films is anticipated to be of great scientific and technological interest. In this work, W films were prepared by magnetron sputtering onto Si (100) substrates. In order to improve the adhesion properties between W films and Si substrates, 30 nm Cr sticking layers was deposited prior to the W deposition for a set of samples. Nano-indentation was used to characterize the hardness and modulus of W films. Surprisingly, the ultrahigh hardness (24.5 GPa, 21.3 GPa) which are significantly higher than
that of coarse-grained W in bulk form (3.92 GPa[10]) are obtained for the deposited and annealed W films with the average grain size of about 26.9 and 32.5 nm, respectively. The relationship between hardness enhancement and the microstructure features is discussed.

2. Experimental Methodology

Nanocrystalline tungsten coatings with a thickness in the range of 600 nm were deposited onto Silicon (100) and Sapphire (C-plane) using radio frequency (RF) sputtering technique. Tungsten-Yttrium samples with variable content of Yttrium were fabricated using the same deposition parameters described in previous reports; please refer to report Sep-Dec 2013 for details. The new target used was W 90 – Y 10 wt. % and depositions were carried out pressure dependent and substrate temperature dependent. Table number 1 depicts the deposition parameters as well as the variables during each experiment.

2.1 Microstructure Characterization of the films

Depending on the growth conditions, W thin films are usually made up of either the stable a phase (bcc lattice), the metastable B phase (A15 cubic lattice), or a mixture of both phases [12]. As it can be appreciated in plot 1A corresponding to pure W samples with variable deposition pressure, all the peaks in XRD data can be correlated to either bcc α or A15 β structure. The occurrence of dominant β(210) is observed at sample W-Y 1 as highly crystalline with a mixture of α(200) phase at P_{Ar} =0.46x10^2 mbar. As the deposition pressure increases to P_{Ar} =0.63x10^2 the dominant peak corresponds to a phase change in α(110) and also a mixture with α(200) plane. For the samples W-Y 3-6 the phase changes to a dominant α(110) with different intensities of the peak. In plot 1B obviously, the effect of Yttrium content in the lattice affects the crystallite size making bigger crystals when compared to pure tungsten. Overall phase change can be considered the same for both when increasing the deposition pressure, the behavior is the same. Therefore it is concluded that the desired phase with less than 5% of Y wt. % can be tailored with the sputtering pressure as the appearance of the metastable β-W phase is related to the lowered deposition flux of W atoms, increased film porosity and correspondingly to the higher probability of oxygen incorporation all this related to sputtering pressure. This same behavior was previously observed by K. Salomon et al in pure W films prepared by magnetron sputtered films.

3.0 Electrical Conduction Mechanisms

The sheet resistance was calculated to the pure W and W-Y deposited films. Sheet resistance is a measure of resistance in thin films that are nominally with the same thickness. This states that the sample is taken as if it was only measured in 2D. The resistivity can be used for comparative purposes and microstructural effects on electrical properties of a
particular set of samples. Deposition of A-15 and bcc W thin films was achieved by varying the sputtering pressures from 0.43 to 3.4 $\text{E}^{-2}$ mbar.

### 4.0 Figures

<table>
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<tr>
<th>Deposition Parameter</th>
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<th>Variable Parameter</th>
<th>Variable Parameter</th>
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<tr>
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<td>200°C</td>
<td>W95-Y5 wt. %</td>
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Table 1. Specific constant deposition parameters and variable dependent parameters.

![Figure 2. GIXRD diffraction patterns for: A) Pure Tungsten B) W, Y 95-5 wt. % and All plotted with increasing sputtering pressure and grown on Si (100) substrate.](image)

### 5.0 References


Selective-Area Growth of CdTe/ZnTe on Micro Patterned-
SiO₂/CdS/ITO/Glass Wafers

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Abstract

Pseudomorphic selective growth of CdTe on ZnTe on micro-patterned CdS/ITO/glass substrates was performed using a multisource close space sublimation reactor using powdered CdTe and ZnTe as source material. The procedure and structural characterization of the CdTe solar cells are reported.

I. Introduction

Cadmium telluride photovoltaics have a predicted maximum theoretical efficiency of ~29% due to its near-optimal direct bandgap of 1.5 eV and large optical absorption. However, laboratory CdTe based solar cells have been able to reach efficiencies only as high ~16%. The difference between the theoretical and laboratory cells efficiencies are attributed to the high defect densities which in turn is due to the large lattice mismatch between the CdS and CdTe (~10%) and the non-uniformity of grains in the layers. One way to reduce the defect densities is to add a ZnTe layer. Furthermore, implementing micro and nano-enabled pseudomorphic selective growth of CdₓZn(1-x)Te will increase the efficiency of CdTe modules. In this work, we report the selective-area growth of CdTe/ZnTe islands on micro patterned-SiO₂/CdS/ITO/glass wafers using a multisource close spaced sublimation reactor as shown in Figure 1. The experimental procedure is discussed followed by the structural characterization materials.

Fig. 1. Schematic representation of the growth sequence layers of the CdTe solar cells.
II. Growth Procedure

The selective-area growth of ZnTe/CdTe on patterned CdS was performed using a close space sublimation (CSS) reactor. Close space sublimation is a physical vapor deposition method in which the source and substrate are separated by only a 1 – 5 mm and the pressure is held between 1 to 10 Torr. In this experiment, separation was 3mm, the base pressure was 0.05 Torr, and 50 sccm of helium gas flowed during deposition. In order to achieve selective-area growth, a layer of SiO$_2$ was deposited and patterned on a CdS/ITO/glass substrate leaving windows in the SiO$_2$ which expose the CdS. The ZnTe and CdTe deposited selectively only on the CdS and not on the SiO$_2$ due to much larger surface diffusion length on the SiO$_2$. The temperatures used for selective growth of ZnTe were 550°C and 665°C for the substrate and source, respectively; while the temperatures used for selective growth of CdTe were 540°C and 565°C for the substrate and source, respectively.

The ZnTe was deposited first, followed by the CdTe. However, in one case vacuum was broken between growths to analyze the ZnTe via SEM prior to depositing CdTe: This is known as the interrupted process. In a second case, ZnTe and CdTe are deposited in a single run without breaking vacuum: This is known as the uninterrupted process.

III. Results and Analysis

Uniform growth selectivity was observed with SEM in both the interrupted and uninterrupted cases, as shown in Figure 2. The CdTe/ZnTe islands measured 1 micro meter in diameter. However differences were observed in island microstructure. The uninterrupted process revealed larger grains while the interrupted sample demonstrated smaller grains.

![Fig.2. SEM of selectively deposited CdTe/ZnTe on patterned SiO$_2$/CdS/ITO/glass via the (left panel) interrupted and (right panel) uninterrupted process.](image)

X-ray diffraction (XRD) was performed on both samples as shown in Figure 3. The XRD trace from the interrupted sample showed two peaks clearly corresponding to ZnTe and CdTe (Figure 3). However, the XRD trace from the uninterrupted sample showed only one peak near CdTe(111) reflection angle. The peak is asymmetric with a very steep rise on the left side, while the right side contains a much broader shoulder. This indicates that the broadening of the peak is attributed to systematic change in the lattice parameter and not a high defect density. If the broadening was due to a high defect density, the broadening of the peak would be more symmetric. Instead the broadening on the right size is attributed to intermixing between ZnTe
and CdTe to create Cd$_x$Zn$_{1-x}$Te. This is further corroborated by the lack of a ZnTe peak. Figure 4 shows a schematic representation of the possible structure Cd$_x$Zn$_{1-x}$Te obtained by the intermixing of ZnTe and CdTe in the uninterrupted process. Future work will consist of performing atom probe tomography to investigate the atomic-scale chemistry of individual CdTe/ZnTe islands.

![Figure 3. XRD patterns of the Cd(x)Zn(1-x)Te islands using the two different processes.](image3)

![Figure 4. Schematic representation of the possible structure obtained by the uninterrupted process.](image4)

IV. Acknowledgments
This work was supported in part by the following grants: NSF/PREM: DMR-1205302 and DOE/BRIDGE: DE-EE0005958. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

V. References

Modeling the Interfacial Stresses in Thermal Barrier Coatings

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Abstract

A finite element model for interfacial stresses in the thermal barrier coating (TBC) system is presented. A multi-layered model was developed for TBC’s with different top coat materials using HYPERMESH and ABAQUS. The models were subjected to numerous thermal cycles at a temperature of 1200 °C and the resulting stresses at the interface were compared. One set of models were incorporated with oxide layer which grows volumetrically during the cycling process. The material properties and oxide layer growth were found to have a profound influence on the stress distribution in the TBC systems.

1. Introduction

The current gas turbine technology that operates at high temperatures are coated with thermal barrier coatings (TBCs), which are mainly used for protecting the components from high temperature, corrosion and improve the overall thermal efficiency. The TBC system is mainly made up of base metal, bond coat (BC), thermally grown oxide (TGO) and a ceramic top coat (TC). The base metal is usually a Ni based superalloy which has superior creep strength. The BC which is made up of MCrAlY (where M = Ni, Co, Fe) is deposited on the surface of the super alloy to provide good adhesion and also acts as reservoir for Al to form the oxide layer to protect the base metal from oxidation due to the diffusion of oxygen through the top coat. The TGO is a layer of alumina which is formed on top of the bond coat during operation which results in discontinuities of material properties across the thickness of the coating.\[1\] The traditional top coat is made up of 6-8% Yttria Stabilized Zirconia (YSZ) which has a maximum temperature tolerance of 1200 °C for long time operation.

The commercially available YSZ coatings undergo a phase change at 1200 °C which makes it unsafe to operate at higher cycling temperatures since failure mechanisms like spalling take over and expose the base metal leading to a complete failure of the system. Hafnia (HfO\(_2\)) which has similar crystalline structure like Zirconia was found to be a viable replacement due to its higher melting point (2900 °C) and lower thermal conductivity. Hafnia based coatings have proven to withstand higher temperatures with increased thermal durability up to 1400 °C in comparison with YSZ coatings.\[2\] Finite element modeling has provided a great capability to simulate the stress distribution in the muti-layered coating systems. Numerous studies were performed on understanding the stress distribution in TBC’s.\[3,4,5\] These studies were mainly focused on the YSZ based coatings. No reports exist at this time towards understanding the stress distribution in Yttria stabilized Hafnia (YSH) coatings using finite element modeling. To fill this gap and contribute towards understanding of the YSH system for TBC applications, in the current work, a finite element model was developed to study and compare the stresses and mechanics of degradation of YSH and YSZ top coat as a result of thermal cycling.
2. Simulation Scheme

A two layer model (Fig.1) consisting of TC and BC and a three layer model (Fig. 2) consisting of the TC, TGO and BC were modeled using HYPERMESH. The TC was treated as an elastic material, while the TGO and BC were considered as elastic-plastic materials. The model was meshed using 4 node continuum plane stress elements (CPS4R). The mesh was very refined at the TGO and the interfaces while gradually becoming coarse as moves away from the interface. The initial size of the TGO was set to one micron. Its growth has been simulated using a time-dependent volumetric expansion model called SWELLING available in ABAQUS, by which its thickness reaches three microns by the end of the cycling process.

Fig.1. Two layer model                                                   Fig.2. Three layer model

2.1 Thermal cycle

Each cycle (Fig. 3) in the thermal cycling process has three steps. The first is a heating step where the temperature is ramped from room temperature to 1200 °C in 5 min. In the second step, the temperature was held at 1200 °C for a duration of 10 min. The third step is a cooling phase where the temperature is dropped from 1200 °C to room temperature in 5 min. The system is run through 75 cycles during the thermal cycling process.

Fig.3. Thermal Cycle
3. Results

Thermal cycling of the layered models of YSZ and YSH were simulated using ABAQUS. Comparing the stresses at the interface between the YSZ-bond coat and YSH-bond coat from Fig. 4, it can be noted that there are higher stresses developed in the YSH interface than at the YSZ interface. This can attributed to the fact that YSH has a higher modulus of elasticity when compared to YSZ. This has been confirmed from the work done by He et al\textsuperscript{[6]} where an increase in modulus of elasticity leads to higher stresses. The oxide layer grows from one micron during the first cycle to three microns by the end of the 75\textsuperscript{th} cycle, during which higher stresses are developed due to the volumetric expansion.

Fig.4. Stresses in (a) YSZ and (b) YSH after thermal cycling

4. Conclusions

Finite element models of YSZ and YSH coatings were developed with and without the presence of the thermally grown oxide layer. High temperature thermal cycling was simulated in these models and it was found that the YSH coatings have higher interfacial stresses due to the influence of the modulus of elasticity when compared to the YSZ coatings. Also, the volumetric expansion of the TGO has applied additional stresses at the interface.

5. References

Experimental Study of Structure and Dielectric Properties of Gadolinium (Gd\textsuperscript{3+}) Incorporated Cobalt Ferrite

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1 Introduction

Spinel ferrites are very important group of materials and have been subjected to numerous investigations for many years due to their fundamental scientific research and technological applications in various fields such as of electronics, optoelectronics, magnetics, magneto-electronics, electrochemistry and biotechnology[1-3]. Among spinel ferrites family, cobalt ferrite CoFe\textsubscript{2}O\textsubscript{4} (CFO) has attracted remarkable attention and widely studied because of their large magneto-crystalline anisotropy, high coercivity, moderate saturation magnetization, large magnetostrictive coefficient, chemical stability and mechanical hardness [2]. The structure and dielectric properties of cobalt ferrite (CFO) plays a key role in designing the magnetic, electronic, microwave and electrochemical devices [2]. In the engineering of advanced functional materials, doping with different rare-earth (RE) ions is a well-known straightforward and versatile way to tune their desirable physical properties [3]. The work reported in this paper is, therefore, focused on the synthesis of CoFe\textsubscript{2-x}Gd\textsubscript{x}O\textsubscript{4} (x=0.0 to 0.4) ceramic materials and evaluation of their structure and dielectric properties.

2 Experimental Method

The Gd substituted polycrystalline compounds were prepared from 99.99\% pure CoO, Fe\textsubscript{2}O\textsubscript{3}, and Gd\textsubscript{2}O\textsubscript{3} by the solid state reaction method. Powders of the starting materials were grinded in a agate mortar and pestle for 2 hr in a ethanol medium and the mixtures were heat treated at 1200°C for 12 hr employing controllable furnace with a ramp rate of 10°C/min for both heating and cooling. Phase identification and crystal structure of the materials were investigated using X-ray diffraction (XRD) measurements employing a Bruker D8 Discover X-ray diffractometer. Measurements were made at room temperature using CuK\alpha radiation (λ=1.5406Å). Morphology and composition were examined by scanning electron microscopy (SEM). Each batch of pellets for dielectric measurement was pressed in a Carver press at 4.5 tons and sintered at 1300°C for 12 hours. The pellet diameter and thickness was roughly 7.9mm and 1.5mm respectively. For dielectric measurements, the surfaces of the samples were well polished, rubbed with silver paste as the electrode for the electrical measurements and then cured in a furnace at 93°C for 2 hr in order to get the best performance. The temperature dependent dielectric data was collected for 1KHz, 10KHz, 100KHz and 1 MHz.
3 Result and Discussion

XRD patterns for CFO and Gd substituted CFO are shown in Fig. 1. XRD data indicate that the synthesized CFO and Gd substituted CFO material crystallizes in the inverse spinel phase. The lattice constant of CFO determined from XRD is 8.373 Å which agrees with the reported value for CoFe$_2$O$_4$ [4]. For $x=0.1$ to 0.4 concentration the lattice constants are 8.397 Å, 8.385 Å, 8.394 Å, and 8.422 Å respectively. It is obvious that when some Fe$^{3+}$ ions are substituted by Gd$^{3+}$ ions, the lattice parameters are changed. The lattice parameters may increase or decrease depending upon the result of two effects. Having large ionic radius than Fe$^{3+}$, Gd$^{3+}$ tries to increase the lattice parameter or did not substitute the iron in the cubic structure but formed another distorted phase, resulting in lower degrees of alignment of lattice fringes. As a result the lattice parameter decreases [4, 5]. The morphology of CFO (Fig.1b) and CFO-Gd ($x=0.40$) (Fig.1c) are compared by high resolution SEM images in Fig. 1. The presence of smooth grain boundaries for CFO-Gd ($x=0.40$) can be seen in Fig. 1(c).

Fig. 1. XRD patterns of the CoFe$_{2-x}$Gd$_x$O$_4$ ferrites as a function of x (a). SEM image for x=0.0 (b) and 0.4 (c).

Fig. 2 shows the temperature dependent dielectric constant $\varepsilon'$ of CFO and Gd-substituted CFO for a given frequency. Even though it is evident that $\varepsilon'$ increases as Gd content increases the highest value found for $x=0.30$. It is observed that for $f = 1$MHz the rate of increase of $\varepsilon'$ becomes constant at higher temperature. For pure CFO plot $\varepsilon'$ indicates two dielectric relaxations in the frequency range of 1-10 KHz whereas other composition shows only single relaxation at 1 KHz.

Fig. 2. The temperature dependent dielectric constant $\varepsilon'$ of Gd-substituted CFO for a given frequency are shown.
Fig. 3. shows the variation of $\tan \delta$ with the temperature at different frequency. It is evident from the profiles that the dielectric loss decreases with increasing frequency for all samples. The data exhibits well-defined peaks for all the compositions. The shift in loss tangent edge for $x = 0.0$ to $x = 0.4$ compositions indicates that hopping mechanism is operative in this process.

Fig. 3. The temperature dependent dielectric energy loss ($\tan \delta$) of CFO and Gd-substituted CFO for a given frequency are shown.

4 Conclusion

Pure cobalt ferrite and Gd$^{3+}$ substituted cobalt ferrite were synthesized by solid state reaction method varying Gd concentration from 0 to 40%. XRD analysis indicates that Gd substituted cobalt ferrites crystallize in the inverse cubic spinel phase which was expected. From the SEM it was found that the grains of substituted CFO were roughly spherical, uniformly distributed and the average crystallite size decreases with the increase in dopant amount. The magnitude of $\varepsilon'$ increases as the Gd content increases and the highest value found for $x=0.30$ composition. For $f = 1\text{MHz}$ the rate of increase of $\varepsilon'$ becomes constant at higher temperature and dielectric energy loss decreases with increasing frequency.

References

Effect of Tungsten Incorporation on Thermal Stability of Gallium Oxide Thin Films

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Introduction:

The constant threats to the environment caused by the energy harvesting and production from fossil fuels is a present, and future concern for the human kind. The effect on the optimization of the combustion processes for energy production, will not only improve the health on earth population, but it also has a great impact in the economics point of view. It was estimated that in 2006 a yearly saving of $409 million dollars could be achieved if an optimization on the combustion process inside fire-coal power plants is realized [1]. The combustion optimization process can be performed by the control and measurement of three main products ($O_2$, $NO_x$, and $CO$), where $O_2$ and $CO$ are the two products that provide the information about the completeness of the combustion, and $NO_x$ in the main controllable pollutant from the combustion process [2].

In this work, the focus is toward the fabrication of a high temperature oxygen sensor capable of tolerating temperature higher than the ones reported for energy systems oxygen sensors (>700 °C) [1]. Several types of oxygen sensors have been investigated, being in our case metal oxide semiconductor sensors, which offer many advantages during manufacturing process and cost [3]. One promising material for this application is Gallium Oxide (Ga$_2$O$_3$), which has proven to be sensible to oxygen at temperature higher than 600 °C, at the same time, its highly stable phase β (monoclinic) is capable of tolerate temperatures of 1725 °C without any structural change. The sensing properties of Ga$_2$O$_3$ have been previously reported. However, it has been demonstrated that plenty of work can be performed in this material in order to improve their response and performance [4]. In the case of gallium oxide, the method of sensing oxygen is by changing its conductivity values in the presence of oxygen, the conductivity gradient, and the time to finalize the change in behavior can be tune by the addition of a doping agent. In our case the introduction of tungsten ions, by co-sputtering deposition technique, into gallium oxide lattice is studied to enhance the sensor performance. One important aspect to understand is the behavior of gallium oxide and W-doped Ga$_2$O$_3$ under extreme temperatures (>700 °C), and the repeatability of the behavior without any change in surface morphology, and crystal structure. This work presents a study of the properties suitable to change under intense heat environments similar to the ones encounter in fossil fuels energy systems.

Experimental:

Pure Gallium oxide and W-doped Ga$_2$O$_3$ films were deposited onto silicon (Si) wafers and quartz substrates by radio frequency magnetron sputtering. Gallium oxide and Tungsten targets (Plasmaterials, Inc.) of 2 in. diameter and 99.999% purity were employed for sputtering.
A sputtering power of 40 W was initially applied to the targets while introducing high-purity argon (Ar) into the chamber to ignite the plasma. Once the plasma was ignited the power was increased to 100 W for reactive deposition for Ga$_2$O$_3$ target, while in the case of W was varied from 50 to 100 W to vary the tungsten content in the film. The flow of the Ar was controlled using an MKS mass flow meter, in addition high purity O2 was pump inside the chamber in order to avoid the metallic behavior of pure tungsten target. The deposition was carried out for 30 min. Substrate rotation is maintained during the entire deposition time to ensure uniform coverage on the substrate surface. The first set of samples was deposited at a constant substrate temperature (Ts) of 500 °C, while the sputtering power for the W target was varied. Furthermore, second set of samples was deposited at variable Ts (500 °C to 800 °C) and W-power was kept at 50W for the depositions. Ga$_2$O$_3$ films were characterized by performing structural and optical measurements. X-ray diffraction (XRD) measurements on pure Ga$_2$O$_3$ and W-doped Ga$_2$O$_3$ films grown on Si were performed using a Bruker D8 Advance X-ray diffractometer. Surface imaging analysis was performed using a high-performance and ultra-high-resolution scanning electron microscope (Hitachi S-4800). The characterization was performed as the samples were deposited, and after the heat treatment process. The high temperature exposure was performed at a CM high temperature furnace, for several cycles at 900 °C.

Discussion:

The crystal structure analyses of both pure Ga$_2$O$_3$ and W-doped films demonstrated that the presence of tungsten into the matrix of gallium oxide does not affect the crystal structure inside the material. Only β-phase Ga$_2$O$_3$ is present in the XRD patterns for as-deposited film with variable sputtering power. Similar behavior is encountered in the sample deposited with variable T$_s$ (deposition temperature), where only β-phase was present in all the films. The existence of only one phase for all films is primordial in order to understand the sensor behavior of the material, due to the fact that the presence of WO$_3$ inclusions in the film will generate uncertainties in the outcome. Different behavior is shown when we examined the surface morphology of as deposited films; in the case of power dependent samples, only pure Ga$_2$O$_3$ film showed presence of nanocrystallites at the surface, and segregated presence of surface granular structures when tungsten was co-sputtered, suggesting that W ions provide a crystallization barrier requiring more energy to finalize crystallization. For films deposited with temperature dependence we noted that surface nano-crystallites start to interact with each other, finalizing crystallization at 800 °C. Nevertheless, the grain structures at the surface of the films are different in both films fully crystalline, in the case of pure Ga$_2$O$_3$ the grains are uniform throughout the film, but for W-doped the grain are completely different in size one from the other, suggesting that tungsten allows non uniform expansion of their grain boundaries.

The films were heat treated, after primary characterization of as-deposited samples, at 900 °C for different time periods. The time sequence was followed starting by increment of 1 hour for the first 3 hours, then an increment of 2 hours to reach 5 hours of exposure, and ending with 5 hours to achieve a total of 5 hours of exposure. The morphology change due to the heat process is shown in Figure 1, where it is clear that the transformation that the W-doped films followed. Pure Gallium Oxide film does not showed any effect due to the high temperature exposure. A complete analysis of the thermal stability will be shown including the effect of the chemistry percentage and crystal structure of the films will be presented for all films.
Fig 1. Heat treatment effect in the surface morphology of Pure Ga$_2$O$_3$ and W-doped Ga$_2$O$_3$ films; a) Pure Gallium Oxide, b) 500 °C: 50W-W and 100W - Ga$_2$O$_3$, c) 800 °C: 50W-W and 100W - Ga$_2$O$_3$.

References:

Fabrication and Characterization of Nanocrystalline Hafnium Oxide Thin Films

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I. Introduction

Hafnium oxide (HfO\(_2\)) has been the subject of intense research in the past few years due to its unique properties and phenomena. Specifically, the structural, mechanical, optical and electrical properties of HfO\(_2\) low dimensional structures have been receiving significant attention in recent years due to the possible options for tailoring the structure-property relationships at the reduced dimensions \([1,2]\). Relatively high band gap \((E_g > 5 \text{ eV})\) and index of refraction \((n \approx 2)\) make HfO\(_2\)-based thin films and coatings interesting for optical applications such as optical filters, ultraviolet (UV) heat mirrors, antireflection coatings and scintillation materials \([1-4]\). The optical constants, namely the refractive index \((n)\) and extinction coefficient \((k)\), of HfO\(_2\) play a critical role in designing the optical and electro-optic devices. Structural, electronic, and optoelectronic properties are a function of the surface/interface structure, morphology, and chemistry, which are all dependent on the processing conditions and post-fabrication treatments. Moreover, it is important to characterize and obtain a correlation between microstructure and optical properties in nanocrystalline HfO\(_2\) films as a function of growth conditions. The impetus for the present work, is therefore to derive a crystal structure, density and optical property correlation, which suggest that the optical quality of HfO\(_2\) films can be tuned by tuning the processing conditions and microstructure.

II. Experimental

HfO\(_2\) films were deposited onto silicon (100) wafers substrates by radio frequency magnetron sputtering. The power applied to the target was 100 W. The ratio of Ar to O\(_2\) was kept at 70:30. The total gas flow was maintained at 40 sccm. Deposition times were selected in order to obtain films with a thickness of \(\sim 40 \text{ nm}\). Growth temperature \((T_g)\) was varied in the range of room temperature \((RT) - 700 \text{ °C}\), while keeping the other variables constant. Grazing incidence X-ray diffraction (GIXRD) measurements on HfO\(_2\) films grown on Si were performed using a Bruker D8 Advance X-ray diffractometer. GIXRD patterns were recorded using CuKa radiation \((\lambda = 1.54056 \text{ Å})\) at room temperature. High resolution scans were also performed on the most intense peak observed. X-ray reflectometry (XRR) measurements were performed on a Rigaku Smartlab X-ray diffractometer. Experimental data was then fit with the software package GlobalFit associated with Rigaku Smartlab diffractometer. Optical properties were evaluated using spectroscopic ellipsometry (SE) measurements. The SE measurements were performed ex-situ on the films grown on silicon wafers by utilizing a J. A. Woollam W-VASE instrument.
III. Results & Discussion

X-ray diffraction patterns of HfO$_2$ films are shown in Fig. 1 as a function of $T_s$. The XRD patterns of HfO$_2$ films grown at $T_s \geq 200 \, ^\circ C$ indicate that these films are crystalline and textured along (111), designating a crystallization temperature of 200 °C. In monoclinic HfO$_2$ films, the (111) crystal planes will primarily populate as they exhibit the lowest surface energy, and as evidenced the films exhibit a strong (111) texture, which is expected based on phase-stability considerations.

Simulation of the XRR experimental data using appropriate models can provide physio-chemical information of HfO$_2$ films. Specifically, the surface and interface roughness, thickness and density of the HfO$_2$ films can be obtained from XRR spectra. The surface and interface roughness were also considered in order to accurately fit the experimental XRR spectra of HfO$_2$ films. A positive shift of the critical edge noted from XRR spectra indicates that the film density increases with $T_s$; further analysis was made with SE measurements.

Optical constants of the HfO$_2$ films were primarily probed by SE, which measures the relative changes in the amplitude and phase of the linearly polarized, monochromatic incident light upon oblique reflection from the sample surface. The experimental parameters obtained by SE are the angles $\Psi$ (azimuth) and $\Delta$ (phase change), which are related to the microstructure and optical properties. After which, the $\Psi$ and $\Delta$ curves were modelled with a conventional Cauchy dispersion model, because the films are transparent in the visible region the Cauchy model is optimal. The dispersion profiles of $n(\lambda)$ determined from SE data for the HfO$_2$ films is shown in Fig. 2a. The $n(\lambda)$ curves also indicate a sharp increase at shorter wavelengths corresponding to fundamental absorption of energy across the band gap. However, the effect of $T_s$ is evident in the $n(\lambda)$ profiles, where there is an increase in ‘$n$’ values with increasing $T_s$. It is well known that the refractive index is closely related to the physical properties and density of the films. Thus, the observed increase in ‘$n$’ values when HfO$_2$ films grown at higher $T_s$ can be attributed to the improved packing density of the films coupled with improved structural order. In order to further confirm the proposed physics, the relative density of the film is also approximated using the Lorentz-Lorenz relation employing ‘$n$’ values measured at 550 nm. The functional dependence of the relative density of HfO$_2$ films on $T_s$ is shown in Fig. 2b [5]. The density measured for amorphous HfO$_2$ films at $T_s$=RT is only 7.4 g/cm$^3$. However, the density increases to 9.1 g/cm$^3$ for nanocrystalline HfO$_2$ films deposited at $T_s$=300-700 °C. XRR density measurements commensurate with the values derived from Lorentz-Lorenz relation as seen for the crystalline samples in the inset within Fig. 2b.

![Fig. 1](image-url) (a) GIXRD patterns of the HfO$_2$ films grown as a function of temperature; monoclinic HfO$_2$ crystallizes preferentially in (-111) orientation.
V. Results & Discussion

Summarizing the results, HfO$_2$ films were fabricated using sputter-deposition and demonstrated a functional relationship between growth conditions, microstructure and optical properties. HfO$_2$ films grown at T$_s \geq 200 \, ^\circ$C were nanocrystalline, monoclinic structured with (111) texturing. The film density increases with increasing T$_s$ as evidenced in XRR data and Lorentz-Lorentz modeling of the SE data. The remarkable effect of film quality is reflected in ‘n’ values, which are significantly higher for films with improved structural order and density. A direct T$_s$-$\rho$-$n$ relationship observed suggests that tailoring the optical quality is HfO$_2$ films can be tailored by tuning the growth conditions and microstructure.

References

Modeling Progressive Damage and Failure for Polymer-Matrix Composites

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Abstract

A model to predict the damage evolution and failure of unidirectional fiber-reinforced polymer-matrix composites (PMC) is developed using CCM-Schapery-Crack Band theory. Polymer matrix progressive damage is modeled using Schapery Theory (ST), which is later extended up to failure in order to account for more catastrophic failure mechanisms. The degrading elastic parameters of the fiber-reinforced PMC are obtained as a function of damage to finally determine the amount of damage associated with a PMC under uniaxial, biaxial, multiaxial and combined axial-shear loading.

1 Introduction

In the last two decades, the advancement of composite materials has been generating technological and economic improvements. Advanced composite materials have been used in aircrafts, automobiles, industrial machinery, sporting goods and in many other applications. To assure the efficiency of these composite materials, a progressive damage and failure analysis has to be performed. The purpose of this paper is to model progressive damage and failure to determine the amount of damage associated with a unidirectional fiber-reinforced PMC under any load configuration. To predict the progressive damage of the PMC, this model is based on a thermodynamically-based work potential theory developed by Schapery [3]. The progressive damage in PMC is accounted by matrix microdamage, which yields to more severe failure mechanisms. Therefore, ST has been extended up to failure in order to account for the maximum strain and amount of damage at which the fiber-reinforced PMC completely fails.

2 Methodology

2.1 Progressive damage

Failure initiation in the PMC is given by the critical strains, which are obtained by physical experiments of a small-scale PMC. Elastic properties of the fiber and matrix, as well as the fiber volume fraction and matrix Poisson’s ratio are known variables of the model. Plastic deformation, viscous effects and axial compressive loads are not taken into account in this model. The fiber and polymer matrix elastic properties are obtained from Prabhakar and Waas [2]. Progressive damage is represented as the region before the critical strain, where micro-structural damage causes non-linearity in the stress-strain response of the PMC. The progressive damage mechanisms in PMC are accounted by matrix microdamage, i.e. microcracks, transverse cracks, voids, fissures, shear bands, kink band and delamination. The CCM model is used to determine the upscaled PMC mechanical properties, utilizing only the basic constituent properties, as explained in the article by Prabhakar and Waas [2].
2.2 Schapery Theory

According to ST, the total work potential, \( W_T \), is equal to the sum of the recoverable work potential (elastic), \( W \), and the dissipated energy, \( S \) [3]. A fiber-reinforced PMC undergoes structural changes (damage) when subjected to a load, affecting its mechanical properties. On the contrary, the recovered energy is obtained once the material is unloaded and it follows the elastic path. Moreover, the fiber-reinforced PMC is considered to be a transversely isotropic material and from the stress-stress relation \( \{\sigma\} = [C]\{\varepsilon\} \) or simply \( \sigma_i = C_{ij}\varepsilon_j \) for \( i,j = 1,2,3...6 \), the elastic strain energy equation given by Schapery [3] can be differentiated with respect to \( S \) and related to the elastic constants \( C_{ij} \).

2.3 Extended Schapery Theory

More catastrophic failure mechanisms due structural changes occur once the critical strain of the PMC is reached and the PMC stiffness decreases drastically until the PMC completely fails. The Crack Band model is used to manifest these failure mechanisms. The fracture toughness and characteristic length are assumed to be constant throughout the model to overcome pathological mesh dependency.

3 Results and Discussion

The stress–strain response for the homogenized lamina of PMC are obtained by the CCM model and the nonlinearity of \( E_{22}, G_{12} \) and \( G_{23} \) is verified and it is attributed to progressive damage of the polymer matrix. It is important to state that the response of the PMC in the axial direction is linear since it depends only on the axial stiffness of the fibers, which is very high compared to the stiffness of the polymer matrix. Then, the ST has been extended up to the failure state, at which the maximum strain supported by the PMC is reached and it completely fails, as seen in Fig. 1 (a) and (b). Since the stiffness in the 1 direction is much higher compared to the other directions, Fig. 1 (b) reproduces a better view of the nonlinear stress-strain responses.

The elastic constants \( C_{ij} \) are plotted against the amount of damage (S), as shown in Fig. 2. (b) black curves, while the fitted curves are colored. It can be observed in Fig. 2. (a) that the elastic constant in the 1 direction has much higher values than the other constants. Then, to better visualize these other constants, the plot is zoomed and shown in Fig. 2 (b). Similarly, Table 1, shows the results obtained for different configurations of strain loading, i.e. uniaxial, biaxial, multiaxial and combined transverse-shear loading.

![Fig. 1. Stress-strain responses of a homogenized lamina up to failure. (a) Complete representation of the responses (b) Zoomed plot to visualize nonlinearity.](image-url)
Fig. 2. Elastic constants ($C_{ij}$) vs amount of damage ($S$). (a) Complete representation (b) Zoomed plot to visualize a comparison of original plots and approximated curves.

<table>
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<th>Strain Configuration</th>
<th>Strain ($\epsilon$)</th>
<th>Amount of Damage ($S$)</th>
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<td><strong>Uniaxial Strain ($\epsilon$)</strong></td>
<td>$\epsilon_{22}=.05$</td>
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<td><strong>Shear Strain ($\epsilon$)</strong></td>
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<td><strong>Combined Axial-Shear Strain ($\epsilon$)</strong></td>
<td>$\epsilon_{11}=.02$, $\epsilon_{22}=.05$, $\epsilon_{33}=.06$, $\epsilon_{12}=.07$, $\epsilon_{23}=.08$, $\epsilon_{13}=.06$</td>
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<td>$\epsilon_{11}=.015$, $\epsilon_{22}=.06$, $\epsilon_{33}=.06$, $\epsilon_{12}=.08$, $\epsilon_{23}=.07$, $\epsilon_{13}=.05$</td>
<td>5.558e6</td>
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</table>

Table 1. Results obtained for amount of damage ($S$) for different configurations of strain applied.

4 Conclusion

It is concluded that the amount of damage is bigger for multiaxial and combined axial-shear strain loading configuration. For uniaxial and biaxial strain, the amount of damage is small if this value is less than the critical strain of the PMC in the corresponding direction. However, damage increases drastically once the critical strain is reached. A finite element computational model can be developed to verify these results, which is currently being studied.

References

Prediction of Damage due to Compaction during Manufacturing of Textile Composites

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1 Introduction
Textile composites are finding extensive use in the aerospace and automobile industry due to their high stiffness to volume ratio, easy formability and drapability[1]. For a rapid development of these materials in terms of high strength and durability, there is a need for a thorough understanding of the material state, and the influence of processing on the material response in subsequent service applications. Therefore, along with design aspects, like geometrical design and weaving, manufacturing induced defects have to be accounted for. These defects act as global failure initiation points within the composite. Therefore, in order to minimize any premature failure in the final composite manufactured, it is crucial to investigate the process induced defect in these composites.

In this paper, the influence of the compaction on woven glass fabric during the VARTM process is investigated. In this context, the tensile response of the woven composite subjected to varying compaction is computationally studied. As a first approach, compaction on fabric layer during manufacturing and tension on the final composite was considered in this paper. Stresses developed during the curing process of resin is not considered in this paper which is under consideration as a next step. Mesoscale models of 4 layers of the woven glass composite are considered.

2 Computational Modeling
The computational modeling approach is divided into two parts: 1) Compaction of the fiber tows with uncured resin, and 2) Tensile response of the post-cured composite with damaging capability included in the matrix. Four layers of glass fabric (as reinforcement) and Epon 638 with Epikure (as matrix) was used in the paper. Fig. 1 shows the RVE with woven fiber tows and matrix. The dimensions of the RVE in x, y and z directions are 4.4, 4.4 and 0.44 mm respectively. The fiber tows are elliptical in shape with a major dimension of 0.8 mm and minor dimension is 0.01 mm. The in-plane spacing between two successive yarns is approximately 0.3 mm. Geometry of the RVE was modeled with Texgen software, which is specially designed to model textile composites. The geometry of the model was then exported to ABAQUS (commercially available software) to perform the finite element analysis.

In the compaction step, the RVE shown in Fig. 1 was used. The properties of the glass fiber used in this model are \( E_f = 85 \text{ GPa} \) and \( \nu_f = 0.22 \). For the compaction model, it was assumed that the liquid resin fills the entire space between the dry fabrics. Therefore, prior to solidification of the resin, it was considered that 5 % of the resin has already cured. The matrix properties at this stage are \( E_m=0.081 \text{ GPa} \) and \( \nu_m = 0.48 \)[2]. The homogenized tow properties were calculated using these properties of fiber and matrix using the concentric cylinder model[3]. Table 1 shows the homogenized properties of tows in the uncured state. The boundary conditions used in the compaction modeling are shown in Fig. 2(a). Displacement of the bottom surface was restricted in the z-direction, and a displacement condition simulating a compaction was applied on the top surface. All other faces were maintained to be flat, i.e. the faces all allowed to breathe while
remaining flat. Five different compactions, i.e. 5%, 7.5%, 10%, 30% and 50% of the thickness of composite were considered to study the effect of compaction of the final composite.

![RVE of the woven composite](image1)

Fig. 1. RVE of the woven composite.

![Boundary Conditions](image2)

Fig. 2. Boundary Conditions (a) Compaction Modeling and (b) Tension Modeling.

Table 1: Homogenized Tow Properties with 5% cured Matrix.

<table>
<thead>
<tr>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22} = E_{33}$ (GPa)</th>
<th>$\nu_{12} = \nu_{13}$</th>
<th>$\nu_{23}$</th>
<th>$G_{12} = G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>51.034</td>
<td>0.254</td>
<td>0.307</td>
<td>0.2142</td>
<td>0.111</td>
<td>0.105</td>
</tr>
</tbody>
</table>

The models corresponding to the different compaction values were subjected to tensile loading. As mentioned above, the curing process is not modeled in this paper. Therefore, the cured matrix properties were considered for the tensile loading step. That is, the cured matrix properties are $E_m = 4.95$ GPa and $\nu_m = 0.375$ [2]. Table 2 shows the corresponding homogenized tow properties. Boundary conditions for this case is shown in Fig. 3(b). Flat boundary conditions mentioned used for the compaction step was used for free surfaces in this current step as well. Crack Band theory (CBM)[4] was implemented into the matrix properties to introduce damage in the matrix. This theory was introduced in the model by means of a user subroutine compatible with ABAQUS.
Table 2: Homogenized Tow Properties of Final Composite.

<table>
<thead>
<tr>
<th>E₁₁ (GPa)</th>
<th>E₂₂ = E₃₃ (GPa)</th>
<th>ν₁₂ = ν₁₃</th>
<th>ν₂₃</th>
<th>G₁₂ = G₁₃ (GPa)</th>
<th>G₂₃ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>53.01</td>
<td>13.67</td>
<td>0.375</td>
<td>0.251</td>
<td>6.044</td>
<td>5.468</td>
</tr>
</tbody>
</table>

Only damage in the matrix was considered in this study. The inputs to the CBM are the cohesive law for the matrix. Fracture toughness (G_c) and critical strengths (σ_c) are the two inputs to the cohesive law. The value of G_c used in this model was 0.8 N/mm and four different values of σ_c i.e. 45, 60, 75 and 90 MPa were used for parametric study.

3 Results and Discussions

Fig. 3 shows the load displacement diagrams for tensile test of 10% and 50% compaction and different critical stress (σ_c) for the matrix. The initial stiffness for different σ_c is almost same for a particular compaction. But, the maximum load carrying capacity of the compacted models varies with compaction. It was observed that the onset of damage is premature for larger values of compaction due to higher stresses in the matrix regions between the tows. So, the amount of compaction plays an important role in the quality of the final composite.

Fig. 3. Load displacement response for (a) 10% and (b) 50% compactions.

References

Numerical Prediction of Collection Efficiency of a Personal Sampler Based on Cyclone Principle

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1 Introduction

Cyclone separators are extensively used in hospitals, schools, offices, industries and agronomical poultry farms to maintain indoor and outdoor air quality as the air quality may degrade due to various microbial agents. These microbial agents may cause several health issues like allergic reactions, toxic effects, and infectious diseases. Due to minimal operational costs, relatively simple geometry, absence of moving parts and high reliability, cyclones are widely used in industries. This study is focused on the microbial agent fungi. A high moisture level in surrounding is favorable for fungal growth. Fungal spores are also acknowledged for asthma risk factor in indoor environments.

A conventional method used to detect and quantifying fungal aerosols and airborne particles is called short-term area grab samples. A considerable number of researchers have promoted techniques for detecting specific or “total” indoor fungal species [1]. So, they developed a bioaerosol sampler that permits sample analysis without the requirement for a sample transfer step. As a big difference from industrial cyclone separators, the bio-aerosol samplers do not require high temperature, high pressure loadings, thus it is highly effective to collect airborne aerosol particles/droplets including various microbial species and airborne microorganisms. This type of bio-aerosol samplers can be directly used to supplement computational fluid dynamics (CFD) simulation of airborne particles transport. The objective of the present work is to use 3D full order high-fidelity CFD tool to simulate the particle flow inside a bio-aerosol cyclone sampler to evaluate different design options for optimization of the collection efficiency of particles and different surface roughness of the collection tube inner wall through CFD simulations.

2 Cyclone Design and Modelling

2.1 Design of Cyclone

The present study deals with the cyclone bioaerosol sampler with different inlet tube as shown in Figure 1. The cyclone bio-aerosol sampler comprised with a microcentrifuge tube and a cyclone attachment. These tubes are mainly used for sample sonicating, homogenizing, separating and sample transferring in molecular analysis. To enhance the particle collection in the tube and initialize the particle impaction onto the wall, instead of placing tangentially, the cyclone inlet makes an inclined angle (of 40°, 30°, 45° and 60°) with the horizontal axis.
Fig. 1: The cyclone bioaerosol sampler geometry created in this project for angle (a) 30°, (b) 40°, (c) 45° and (d) 60°

The collection efficiency was calculated based on the following equations, which is known as Lapple model equations.

\[
(d_{p50\%}) = \sqrt{\frac{9\mu b}{2\pi N_e V_i \rho_p}}
\]  

(1)

Where, \( b=0.25D; \) \( N_e=\frac{H+0.5Z}{D_{i}}; \) \( V_i = \) velocity at inlet = 20 m/s

Collection efficiency \( n \) can be written as follows:

\[
n = \frac{1}{1+(\frac{(d_{p50\%})}{d_p})^2}
\]  

(2)

2.2 CFD simulation

A commercially available CFD code, FLUENT is used to solve the discretized equations (conservation of mass, momentum and energy equations) by finite volume formulation. Air was considered as continuous phase material and water-liquid was as dispersed phase material in this study. The Eulerian-Lagrangian approach has been employed to simulate the cyclone separator. In this investigation, a velocity inlet boundary condition was implemented at inlet, outflow boundary condition (BC) at overflow and no slip BC at the walls. As k-\( \varepsilon \) model has some limitations to swirling turbulent flow, Reynolds stress turbulence model (RSTM) was used to simulate the cyclone-based bioaerosol sampler. The fluctuating gas velocities can be determined by using a discrete random walk (DRW) model which is based on the stochastic tracking scheme.

3 Results

The RSM used in this study described the turbulence model and DPM described the dispersed phase. RSM model is very effective to comprehend the flow field of cyclone separator. The contours plots of different parameters using RSM and particle or droplet trajectories using DPM are shown in Figure 2 (a) and (b), respectively. Continuous phase model validates the flow individualizations with different velocity fluctuation profiles.
Fig 2: Contour plots for (a) at (i) Static pressure, (ii) Tangential velocity and (iii) Radial velocity and dispersed particle trajectories plots of (b) at (i) particle residence time, (ii) particle velocity magnitude and (iii) particle y velocity using DPM.

Dimensionless radial velocity profiles were measured along the x-axis at different stations of the cyclone separator. Figure 3 (a) shows the mean tangential velocity profiles at z/D=1 of the cyclone separator. Also, the collection efficiency curve at a flow rate of Q= 4 L/min is shown in Figure 3 (b). It can be deduced from the figure that the measured collection efficiency curve shows the ‘S’ shape pattern and goes well with the automated scheme used for analyzing dispersed phase equations.

Fig. 3: (a) The mean tangential velocity profiles for cyclone separator at z/D=1, (b) Collection efficiency curve with the particle diameter at flow rate of Q= 4 L/min

4 Conclusion

This research project introduces the particle motion and particle-air interaction in a personal bio-aerosol sampler. The results show that the inlet angle of 40° leads to a better collection efficiency which is 99.99%. Therefore, this study demonstrates the fluid flow of the cyclone sampler with different inlet angle and flow velocity with corresponding velocity fluctuation profiles of axial, radial and tangential components.

References

Numerical Investigation of Wet Compression

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1 Introduction

It is known that an increase in inlet temperature of a gas turbine system will cause a series of problems with the system. Initially, there is a rapid decrease in the density of fluid due to elevated temperatures; which mainly reduces the power output of the system. In past years, to counteract this effect, fog cooling and wet compression has been implemented into systems to reduce the inlet temperature at the compressor \cite{1}. Fog cooling is the process of cooling the continuous phase until it reaches 100\% relative humidity; hence no droplets are present in once the compression begins. \cite{1} Wet compression on the other hand, is the process in which droplets are injected directly into the continuous phase associated with continuous evaporation of droplets during the compression process; this process is often referred to contain overspray \cite{1}.

Previous research \cite{1-3} has investigated the effects that droplets have on the compressor. It is found by Tomita \cite{2} that injections increase the stagnation pressure which coincides with \cite{1, 3}, in turn it will increase the power generated. In those numerical investigations, the blades and droplets have only contained one interaction; either stick or rebound. The expansion of a droplet after impinging on the blade may have an important effect on mass exchange between droplets and continuous phase air as well as the blade temperature. To investigate this, first blade boundary condition of rebound is investigated using full order high-fidelity computational fluid dynamics (CFD) simulation. This will allow a future comparison to the effects of overall heat transfer rate changes experienced by wall film formation.

2 Numerical Model

2.1 Geometrical Domain

The domain was generated in two dimensions and contains three zones: inlet, rotor, and stator/outlet zones; as depicted in Figure 1. This configuration allows simulating movement of the rotor section between the inlet and stator zone through sliding mesh theory. The model measures 243 mm in length and 42mm in height. The geometries of the rotor and stator blades were obtained from Hsu \cite{4}. The blades had a chord length of 60 mm, pitch of 42 mm, and a distance of 6 mm between blades, as positioned by Khan \cite{4}. The rotor blade was split into two being placed on the top and bottom of the rotor zone; the rotor will move in the +y direction. Four droplet injection locations will be positioned on the left side of the inlet zone. The boundaries along the rotational direction will be assigned periodic boundary condition.

![Figure 1: Schematic of the computational domain for a single stage rotor-stator layout with injection locations](image-url)
2.2 Governing Equations

In this model the 2D Navier-Stokes equations are solved as well as the equations for conservation of mass, momentum, and energy equations. Contributions of water vapor mass, droplet forces and evaporation energy are taken into account. Species transport equation is also modeled taking into account three components in the continuous flow: water vapor (H$_2$O), oxygen (O$_2$) and nitrogen (N$_2$). The turbulence model standard k-epsilon is implemented due to its better stability and 10-15% less CPU time required when compared to the RNG model, and 50-60% less CPU time per iteration compared to the RSM model [5]. Additional enhancements are applied in the k-epsilon model to capture flow near wall interaction; mainly enhanced wall function [5]. The discrete phase model (DPM) is enabled with droplet coalescence and droplet breakup. Droplet coalescence is predicted using the O’Rourke model and droplet break-up uses the Taylor Analogy Breakup (TAB) theory [5]. Stochastic tracking is implemented to simulate droplet movement in turbulent environment.

2.3 Boundary Conditions

Boundary conditions for the continuous phase were obtained from Khan and Wang [4] for validation purposes. For the inlet boundary condition a constant mass flow rate of 2.9kg/s at a temperature of 300K and the turbulent intensity was assigned to be 1%. Additionally, the continuous flow was specified to have relative humidity of 60% at the inlet. The walls in the domain have a no slip condition, adiabatic. The outlet was assigned as a pressure outlet and included a target mass flow rate. No values were assigned to these properties, so as the calculation was done throughout the domain by the software including the density change; backflow was assigned to be 310K. Two categories of cases were generated, one in which there are no droplets injected (base case) and another where injections are made (overspray case). For the overspray case droplets were injected at a temperature of 294.2 K in four different locations equally apart from the next; as seen in Figure 1 (blue dashes). Each droplet had an initial velocity of 5 m/s, a diameter of 0.01 mm and mass flow rate of 0.029 kg/s. The DPM boundary condition for the rotor and stator blades was set to rebound. In order to simulate the compressor with 3600 RPM, the inlet and stator/outlet zones are kept stationary, while the rotor zone is assigned a translational velocity of 94.72 m/s in the +y direction.

2.4 Numerical Method

The software used was Fluent (Version 13) from ANSYS, Inc. The simulation used a pressure-based segregated algorithm in which the individual governing equations are solved sequentially and are decoupled from each other [5]. The pressure and velocity was coupled using the SIMPLE algorithm. All of the spatial discretization terms were assigned second order upwind scheme. Mesh generated contains 182050 cells. It also included a boundary layer around the blades, and the rest of the domain contained triangular elements with the exception of the inlet, which contains coarser and quadrilateral elements.

3 Results

3.1 Model Validation

The current model was compared to the model generated by Khan [4] and results were within acceptable values, Table 1 contains a comparison of pressure ratio (P.R.) and change in temperature.

<table>
<thead>
<tr>
<th></th>
<th>P.R.</th>
<th>Δ T (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current model</td>
<td>1.065</td>
<td>6.17</td>
</tr>
<tr>
<td>Percent error</td>
<td>.95%</td>
<td>11.2%</td>
</tr>
</tbody>
</table>

Table 1: Model validation in comparison to [4]
3.2 Baseline Case vs. Overspray Case

Two cases were simulated both with inlet conditions at 300K and 60% RH. From looking at the pressure and temperature contours in Figure 2, we can observe that in both cases there is an increase in pressure and temperature. In the baseline case a P.R. was calculated to be 1.065, in the overspray model the P.R. was found to be 1.068. In the baseline case, we can see the distribution of temperature is increased where the maximum temperature experienced in the domain is 305.86K. This is slightly decreased in the overspray contours to a maximum of 305.37. Even though this is a slight decrease, it is also appreciable that the overall contours are lower due to the droplet absorption of heat. Using the Fluent Software, the total heat transfer rate was extracted for the whole domain and droplets absorbed 12160.7 W.

![Figure 2: Pressure (a) and Temperature (b) contours with inlet temperature of 300K and RH of 60% and Pressure (c) and Temperature (d) contours with overspray.](image)

4 Conclusion

With these results obtained we can appreciate that wet compression has a positive overall reduction in temperature in the domain and an increase in the pressure ratio. Even though the changes were relatively small, it must be considered that this simulation is of a single stage, compressors, and a compressor can have 4 or more stages. With these results it is possible to aid in the investigation of wall film formation in the blades and if this addition of complexity really changes the overall heat transfer coefficient.

References


ABSTRACT

In this paper, we examine the impact of wind power generation on electricity market prices considering the case studies of two electricity markets, Nord Pool spot market and ERCOT.

1. Introduction

The development of wind electricity generation has rapidly progressed over the last decade and wind power is now a maturing renewable energy technology for electricity generation. The U.S department of energy has analyzed that wind power is estimated to meet approximately 20% of the U.S electricity demand by 2030. Despite various benefits of the wind power, with the growth in its popularity as a commercially viable renewable energy resource, a number of problems arise with integration of that resource into existing power systems and electricity markets [1]. Since the wind power produced by a wind farm depends critically on the stochastic nature of wind speed, unexpected variations of a wind power output may increase operating costs for the electricity system.

2. Addressing the Impact of Wind Generation on Electricity Prices

A. Case-1: Nord Pool’s Western Danish Price Area

Denmark and Germany are the leading nations in the design; production and harnessing of wind power with an aggregated sum of 21GW annually, contributing around a total of 15% and 5% individually to their electricity production annually [1], [2]. When the generation of wind power is taken into account, there are many external factors that directly impact the spot prices. In Fig.1, we can see the effect of wind power penetration on spot prices for the considered span of the data set. It can be observed that the average spot price generally decreases with an increase in wind power in the system. Also, according to the distribution analysis performed by Tryggvi Jonsson [4] using histograms for different levels of forecasted wind power penetration, the probabilities of extreme high prices and wind power penetration were found to be inversely proportional. However, the impact of wind also depends upon the time of the day.

B. Case-2: ERCOT

A case study of ERCOT is selected based on the fact that Texas is the highest wind power generator in United States. Fig. 2 shows the scatter plots depicting the effects of wind generation on zonal market prices. As we can see that though there are negative but weak correlations between wind generation and electricity prices, but they have a significant statistical relation.
can also be observed that these two variables are inversely related. We can also figure out that positive price difference has a more probability of occurrence with relative high wind generation.

![Fig. 1. Spot prices based on wind penetration in DK-1: 1/4/2006-10/31/2007 [3].]

![Fig. 2. Impact of Wind generation on Zonal market prices [5].]

3. Sensitivity Analysis

In order to determine the most appropriate variable which influences the behavior of spot price variance, a sensitivity analysis is performed on Texas (Houston, North, South and West zonal markets) based on the framework provided by Woo et al. [6] on all the input factors considered. This analysis was based on the 15 min dataset for a 12 month period of June 2009 to May 2010 as identified in the respective case study. Figure 3 presents the results of our analysis. We can see that the scalar Ø, the variable that determines the percentage increase in wind power generation, has the most significant impact on the variance of electricity spot prices, based on which we can conclude that wind power energy capacity and electricity spot prices are highly correlated.

![Fig. 3. Sensitivity Analysis.]

4. Proposed Framework

The analysis performed in this paper suggested that there is a direct correlation between the variation of wind generation capacity and the electricity spot prices. Based on the literature
survey, we observed that there is not enough analysis on the effects of operational costs, ancillary services, wind penetration levels, transmission congestion and risk mitigation strategies along with the potential effects of transmission charges on the overall cost of generating electricity through the increased use of wind energy to understand the behavior of electricity prices based on wind power generation. We propose a framework illustrated in Fig. 4 that will help the analysts to visualize, quantify and address the effects of these factors on the overall cost of generating electricity and to understand the behavior of electricity prices based on wind power generation.

Fig. 4. Proposed framework to improve price forecasting accuracy based on wind power prediction.

5. Conclusion
In this paper we investigate the volatile nature of wind which has a profound impact on the operating procedures of markets and thereby having a significant influence on economic dispatch to consumers. Based on the analysis, a high level framework has been suggested which addresses the stochastic factors to increase efforts towards better price forecasting based on wind power prediction.

References
Optimal Placement of Wind Turbines on Non-flat Terrain using Cluster Identification and Multi-objective Genetic Algorithm

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1. Introduction
Currently, wind energy is receiving considerable attention as an emission-free, low cost alternative to traditional energy sources. For large grid-connected arrays of turbines, they are becoming an increasingly important source of wind power-produced commercial electricity. In this paper, a method entitled Cluster Identification Algorithm (CIA) and an optimization approach called a Multi-Objective Genetic Algorithm (MOGA) \cite{1} are integrated and developed to solve the problem of determining the optimal wind farm layout \cite{2} on non-flat terrain and at the same time it maximize wind power, the efficiency of wind power affected by the aerodynamic losses and minimizes cost due to the size and quantity of wind turbines installed in the wind farms.

2. Methodology
Figure 1 demonstrates a conceptual framework of the proposed methodology, and Figure 2 describes more detailed steps in the methodology.

2.1 Methodology and strategy
The rows and columns of the generated matrices are used as input and output data and they are based on terrain reference coordinates of integers and represent only the coordinates of the terrain. The coordinates represent a normal row and column sequence (i.e., left to right and top to bottom). Also, as a constraint in this methodology, it is considered that the wind direction goes in one direction.

2.2 Objective functions
The main objective of this paper is to determine the optimal positioning of wind turbines \cite{3-5} that will maximize wind power generation, maximize wind power efficiency and minimize the cost by using the genetic algorithm in a non-flat terrain application. It can be summarized in the next optimization statement:
Efficiency of wind power that the wind farm is exposed to:

$$\text{Max} \left\{ \sum_{i=1}^{n} \sum_{j=1}^{m} 1/2(\rho U_{ij}^3 X_{ij} A_{ij}) \right\} / \left\{ \sum_{i=1}^{n} \sum_{j=1}^{m} \rho_{\text{avg}} \left( \frac{Y_{\text{avg}} + LK}{H_0} \right)^{3+\alpha} X_{ij} A_{ij} \right\}$$

(2)

Wind power that the wind farm is exposed to:

$$ax \left\{ \sum_{i=1}^{n} \sum_{j=1}^{m} 1/2\rho U_{ij}^3 X_{ij} A_{ij} \right\}$$

(3)

Cost

$$\text{Min} \sum_{i=1}^{n} \sum_{j=1}^{m} X_{ij} \text{(Unit cost)} \quad \forall i = 1,2,3 \ldots n, j = 1,2, \ldots m$$

(4)

Constraints:

- \(a \leq \sum X_{ij} \leq b\), \(\forall i,j\) where \(i=\{1,2,3\ldots\}, j=\{1,2,3\ldots m\}\) and where \(a\) and \(b\) are the minimum and maximum number of turbines.
- \(\sum X_{ij} \leq b_1, \sum X_{ij} \leq b_2, \sum X_{ij} \leq b_3, \sum X_{ij} \leq b_4\) where \(b_1, b_2, b_3\) and \(b_4\) are the maximum number of turbines by type.
- \(X_{ij} = 0, 1 \forall i,j\)

2.3 Description of the proposed algorithm

**The proposed algorithm:**

Step 0. Divide the terrain (Area) in sections of 5D X 5D, where D is the average of the diameters of the rotors of the wind turbines available and plug in the average terrain height. Following is the representation of Matrix ‘A’ (see Table 4).

<table>
<thead>
<tr>
<th>Position</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>. . .</th>
<th>m</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Y11</td>
<td>Y12</td>
<td>Y13</td>
<td>Y14</td>
<td>Y15</td>
<td>Y16</td>
<td>Y17</td>
<td>. . .</td>
<td>Y1m</td>
</tr>
<tr>
<td>2</td>
<td>Y21</td>
<td>Y22</td>
<td>Y23</td>
<td>Y24</td>
<td>Y25</td>
<td>Y26</td>
<td>Y27</td>
<td>. . .</td>
<td>Y2m</td>
</tr>
<tr>
<td>n</td>
<td>Yi1</td>
<td>Yi2</td>
<td>Yi3</td>
<td>Yi4</td>
<td>Yi5</td>
<td>Yi6</td>
<td>Yi7</td>
<td>. . .</td>
<td>Yij</td>
</tr>
</tbody>
</table>

Step 1. Determine the minimum and maximum height value \(Y_{\text{min}}, Y_{\text{max}}\) of Matrix ‘A’.

Step 2. Obtain the increment of the limits.

Step 3. To establish the limits of each column position of Matrix A, create a set of limits using the next equation for all positions:

Lower and Upper Limits of Column 1: \(LL_1 = Y_{\text{min}}, UL_1 = Y_{\text{min}} + \text{Increment}\)

Limits of remaining columns: \(LL_j = Y_{\text{min}} + \text{Increment} \times \text{Column position} j, UL_j = LL_j + \text{Increment}\)

Step 4. Once the limits are created for each column it is necessary to classify each \(Y_{ij}\) value as 1 or 0. If \(LL_j < Y_{ij} < UL_j\) then place a ‘1’ in the Matrix B in the ‘ij’ position if not enter a ‘0’.

Step 5. Once created the Matrix B of 1’s and 0’s, apply the Cluster Identification Algorithm (CIA).

**Cluster Identification Algorithm (CIA)**

Step 5.0. Set iteration number \(k = 1\).

Step 5.1. Select row ‘i’ of incidence matrix \([a_{ij}]\)(k) and draw a horizontal line \(h_i\) through it.

Step 5.2. For each entry of ‘1’ crossed by the horizontal line \(h_i\) draw a Vertical line \(v_j\).

Step 5.3. For each entry of ‘1’ crossed once by the vertical line ‘\(v_j\)’ draw a horizontal line \(h_k\).

Step 5.4. Repeat steps 2 and 3 until there are no more crossed-once entries of ‘1’ in \([a_{ij}]\)(k). All crossed-twice entries ‘1’ in \([a_{ij}]\)(k) form row cluster RC-k and column cluster CC-k .

Step 5.5. Transform the incidence matrix \([a_{ij}]\)(k) into \([a_{ij}]\)(k+1) by removing rows and columns corresponding to the horizontal and vertical lines drawn in steps 5.1 through 5.4.

Step 5.6. If matrix \([a_{ij}]\)(k+1) = 0 (empty matrix), stop; otherwise set \(k = k + 1\) and go to step 5.1.

Step 6. From the final decomposition result, pick the cluster matrix according to the selection criteria:
• Search for the well form arrangements, not the non-shaped arrangements.
• Look the matrix that fitter the wind farm size or turbines available.
• If similar cluster matrices, pick the one where the optimal wind turbine positions are in the highest side.
• Select the terrain with higher population of optimal positions.

Step 7. The matrix pick from step 6 will be the Height Matrix input (subset of matrix ‘A’) used in the Genetic algorithm methodology that will be called Matrix ‘a’.

Step 8. Use Matrix ‘a’ and apply MOGA to get a set of non-dominated local optimal solutions.

2.4 The proposed MOGA for the wind farm

Step 1: Generate a random population of ‘n’ chromosomes. Each chromosome represents a layout.
Step 2: Objective function values evaluation. Evaluate efficiency, power, and cost.
Step 3: Pareto dominance evaluation. The initially created solutions are checked based on Pareto dominance criterion.
Step 4: Fitness evaluation. Evaluate the fitness functions of each chromosome ‘x’ in the population.
Fitness metric 1- Distance-based \( f_1(i) \): It is intended for maintaining population diversity.
Fitness metric 2- Dominance Count-based \( f_2(i) \): Select those individuals which are more dominating.
Aggregated Fitness metric –Fitness metric 1 + fitness metric 2, \( f_a(i) = f_1(i) + f_2(i) \).
Step 5: Selection. Every non-dominated individual is ranked in descending order based on the aggregated fitness values.
Step 6: Elitism. Select most elite members with a given % of elitism to prevent lost of best solutions.
Step 7: Crossover. Pre-define crossover rate and crossover the parents to form new offspring.
Step 8: Mutation. Pre-defined mutation probability, mutate new offspring at a random position in the chromosome.
Step 9: Replace. Use the new generated population for a further generation of the algorithm.

3. Conclusion

In this study, a methodology was developed and presented for 3 dimensional terrain cases and it was validated through a cases study. The presented work is referred to the MOGA in order to solve the problem of the optimal position of wind turbines on a non-flat terrain (mountainous area) and concurrently maximize wind power that the wind farm is exposed to, efficiency of wind power and minimized cost. The function of CIA is to determine a cluster of possible suitable positions from a large-scale mountainous region that follows a path of heights from lower to higher according to the direction of the wind with the help of a previous classification of height using limit bins, and finally come up with a subset of positions.

4. References
SMART ELECTRICITY MARKET PLANNING AND OPERATION IN A DEMAND RESPONSIVE ENVIRONMENT
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ABSTRACT

This paper presents a smart grid framework for an efficient integration of electricity market forecasting problems incorporating renewable generation in a demand responsive environment into smart grid planning and operation paradigm. This paper also presents the importance of demand response (DR), the role of plug-in hybrid electric vehicles (PHEVs), and smart scheduling/dispatch are collectively addressed and presented in the proposed smart grid framework.

1. Introduction

The electric power grid is going through an unprecedented transformation in the current times of the energy crises. The increasing emphasis to integrate environmentally friendly and/or variable renewable energy resources (VERs) such as solar and wind power has made the planning and operation of electricity markets even more complex and daunting. The inherent unpredictability and variability in wind/solar output power generation poses several technical and techno-commercial challenges [1]. In electricity markets, another challenging issue is the complex and volatile nature of electricity prices originating from causes such as anti-gaming policies, transmission constraint, and inelastic demand. Another related issue facing the current electricity market is the consumers’ demand that is their relative inability to alter their usages in response to factors such as prices and loads, which is important to manage the load in accordance with system constraints and to maintain security of the power systems. This includes robust mechanisms that are necessary for smart dispatch and commitment of resources to cope with increasing system uncertainties. Given increasing penetration of VERs and more price-responsive load, a new challenge to the unit commitment (UC) process has emerged especially in the independent system operator (ISO) managed electricity markets [2]. Therefore, it is necessary for the ISOs to have an effective methodology that produces optimal UC decisions and ensures system reliability and security in the presence of increasing real-time uncertainty. Additionally, accurate forecasting of electricity price, load demand and VERs are essential planning tools to predict system needs by assisting decision-makers to plan more efficiently for the future.

2. Demand Response in a Smart Grid Environment

Demand response (DR) is defined as changes in consumers’ electric usage from their normal consumption patterns in response to changes in the price of electricity over time, as a result, can be effective by reducing carbon footprint and improve VERs usage such as wind and solar. Consumers can take advantage of DR by abiding with DR programs, in return, receive incentives [3]. These programs are developed by ISOs/regional transmission organizations and proposed by the Federal Energy Regulatory Commission (FERC) and department of energy (DOE) [4].
Respectively, consumers have the option to plan ahead to change the time of day when their electricity is being used or decrease the amount that is being used, usually during a peak demand period.

More progressively, the smart grid is a two-way interface where data and electricity can be exchanged between the supplier and consumer through newly added technology by providing a more efficient power grid [5]. The efforts for development of smart grids are increasing, and the projected goal for renewable energy should be to make sustainable energy the dominant source of electricity generation in the smart grid integration. As a result of this intelligent infrastructure, dependable and cost efficient energy can optimize the use of renewable energy such as wind and solar power.

The integration of renewable energy forecasting and price forecasting in a demand responsive smart grid environment will be beneficial to make efficient market operations in electric power systems. While consumers use electricity in smart grids, information of what is being used, how much, and when it’s used will be relayed to the utility company. Based on the consumption, ISOs can understand the behavior of the users’ pattern. The ISOs can determine prices ahead of time, notify the consumers, and then consumers can utilize the DR program effectively. This will facilitate the market operations in becoming more predictable and efficient with the improved forecasting information and by providing reliable and affordable energy to the consumers.

![Diagram of Proposed Smart Grid Framework](image)

Fig. 1. Proposed smart grid framework for planning and operations of electricity markets.

3. Proposed Framework

The smart grid framework as proposed in this paper is shown in Fig. 1, which encompasses VERs forecasting, price forecasting, DR, and scheduling/dispatching. The output of the VERs forecasting will be considered as input information to the ISO forecasting system, especially to the short-term price forecasting (STPF) model. The forecasted price signal is then available from the ISO to the residential consumer. Based on the predicted price (and price uncertainty), the consumer is allowed to choose his hourly day-ahead consumption for the period of 24 hours and adjust accordingly. A rolling window model can be implemented here which will transmit the forecasted electricity consumption of the consumer back to the ISO or supplier. Note that the price uncertainty that is pertaining to 24-\(t\) hours following the current one for the next day (actual day) could be considered via robust optimization model as they are particularly suited to address uncertainty and bounded parameters [6]. Since the forecasted demand of the consumer is already available with the ISO, the GENCO could take advantage of this situation while performing its price-based unit commitment (PBUC), security-constrained unit commitment (SCUC), and bid
scheduling process. In the proposed smart grid framework, the SCUC and PBUC models also consider uncertainties associated with VERs and DR. In addition, the proposed model attains reliability of the power system by balancing generation and demand through the bid/load scheduling process between the GENCO and ISO. Now, the load bids that are finalized by the ISO will be delivered to the respective consumers, but with some price fluctuations when compared to the forecasted price signal due to the VERs intermittent nature and could affect the consumption behavior of the consumer depending on the price. Therefore, the proposed model considers plug-in hybrid electric vehicles (PHEVs) as part of the consumer load because they provide efficient storage facility through which it can solve the problem of large peak demand and allows the consumer to participate in market operations directly [7]. Consumers having access to smart meters and smart charging infrastructure for PHEVs can take advantage of low electricity prices during off peak hours as they could charge their vehicles during that period and use them as a backup during peak periods with high electricity prices or they could also send it back to the grid.

Finally, this type of DR model in real-time would cause a transition of a centralized functioning of the grid to a smart grid and also contributes a wholesale purchase benefit to system operations.

4. Conclusions

This paper proposed a smart grid framework that will be beneficial to enhance the planning and operation of the restructured electricity markets by reducing uncertainties while increasing security and reliability. Through accurate VERs/price forecasts and price based DR model, smart planning and operation of electricity markets can be efficiently attained. This objective can also be achieved through the compliant consumers’ response and structured implementation of their planning. The paper also discussed about PHEVs and their advantages as energy storage facility and allowing the consumers to participate in market operations.

Minimization of the system operating cost while meeting various constraints, such as power balance, generation capacity limits, system spinning reserve requirements, minimum ON/OFF time limits, ramping up/down limits are other major concerns in electricity markets. The proposed smart grid model also provides an intelligent way for dispatching the units using SCUC model that considers VERs and DR uncertainties. This will help coordinate a feasible, secure and economic generation pattern for the day-ahead electricity market.

5. References

Challenges in the Collection and Analysis of Cyber Security Data to improve Cyber Security in Operational Technology for Energy-Dependent Sectors

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1 Introduction

Critical energy-dependent sectors in the United States such as energy utilities, military bases, health institutions, and educational institutions, sometimes rely on outdated legacy equipment to generate and distribute energy to their infrastructures to conduct day-to-day operations. When such sectors fail to effectively generate and distribute the energy, an economic impact occurs. For instance, the total annual loses to the United State’s economy from power outages and disturbances total from $75 billion to $180 billion [1]. Modernizing the Operational Technology (OT) that generates and distributes energy to critical infrastructures by including more cyber assets improves the efficiency, reliability, and cost-effectiveness of such infrastructures. Operational Technology refers to the equipment, hardware and software that detects or causes a change through the direct monitoring or control of physical devices, automation and communication, processes and events in enterprises [2]. However, such cyber updates to the OT also make the infrastructure prone to cyber-attacks. A cyber-attack on the OT of an energy infrastructure can have an economic impact similar to equipment malfunction because in both cases economic disruption is produced due to lack of energy.

A way to improve the cyber security of the OT is to constantly evaluate the cyber risk associated with OT critical assets by calculating the impact and likelihood of threats exploiting one or more vulnerabilities on such assets. In this context, a critical asset is defined as an infrastructure component that is of interest to the stakeholder due to its value. Impact is an unexpected effect of a change on a critical asset. A threat is any circumstance or event with the potential to exercise vulnerabilities. A vulnerability is an inherent weakness in the critical asset’s criticality path, i.e. group of individual components that if compromise can directly affects the critical asset of interest [3].

The Vulnerability Assessment and Risk Management (VARM) [3] process identifies, prioritizes, and quantitatively estimates risks for OT critical assets. The VARM identifies operational areas that are most vulnerable to threats and suggests areas of added protection, which if appropriately addressed by the infrastructure’s owner, help reduce the possibility, and ultimately cost, of operational disruptions due to cyber-attacks. This work describes some of the challenges encountered through the collection and analysis of cyber security data associated with near real time risk assessments such as the VARM. The challenges described in this work are applicable to most cyber vulnerability assessment methodologies.

2 Data Collection and Analysis Challenges

2.1 Overview

The VARM process relies on data collection and analysis to calculate the cyber risk associated with OT critical assets. The following subsections describe the theoretical and
practical data challenges that have been addressed through the development and conduction of VARM processes.

2.2 Pre-Assessment

As part of the VARM pre-assessment, a group of individuals with expertise on the organization’s infrastructure being assessed is assembled for a pre-assessment interview. In particular, the interviewed group includes a person with expertise on the OT infrastructure, a person with expertise on the IT infrastructure, and a supervisor to the IT and OT individuals that can enforce decisions taken in the pre-assessment interview and ensure information exchange among the participants. The main challenge in the pre-assessment stage is the lack of data sharing among the parties of interest and with the VARM team. The organization’s personnel is sometimes hesitant to share the required data because the data does not exist, internal institutional procedures prevent employees from sharing data to external entities, the misconception that being compliant with some standard ensures being secured, or due to personal conflict of interest. Thus, it is difficult to achieve a complete understanding of the enterprise until the involved parties share the data. In addition, data collected through the VARM process, including the pre-assessment, might be of different formats and sizes, so it is a challenge to extract the required information and to capture it using a single exchange format.

2.3 Critical Assets Identification

This step identifies the criticality paths in the energy infrastructure. A criticality path is a group of individual components in different planes of an infrastructure, which if compromised, can directly affect a critical asset of interest. The initial challenge in building the criticality paths is to determine what is critical in an infrastructure. Critical assets are initially identified at the enterprise level, i.e. assets of high value due to their importance to day-to-day operations or monetary, safety, or sector specific factors. In order to customize the criticality factors, several types and volumes of data have to be collected and correlated using equations specific to every sector, given that each sector have different criticality priorities depending on their mission or business.

Once the group of enterprise assets is identified, a list of critical OT assets used to support energy generation and distribution to the critical enterprise assets is compiled. Given that some OT assets might serve possibly large numbers of enterprise assets, it is a challenge to prioritize the interconnections of OT assets to the critical enterprise assets and to other OT assets. Critical OT assets are typically accessed through Human Machine Interfaces (HMI) and computer terminals that might be remotely accessible. Such access points, along with the associated communication channels, have to be analyzed as well. The combination of identified critical assets at the different levels captures the criticality paths. A challenge that derives from the criticality assessment process is the analysis of the data generated by all the possible combination of the different critical assets at the different levels.

2.4 Vulnerability Assessment

Cyber vulnerability data associated with each critical asset in the infrastructure layers, except for the enterprise layer, is collected from different sources such as online repositories and results from penetration tests. The challenge is how to calculate a quantitative vulnerability value from data generated from a possible large number of critical assets with a large number
of vulnerabilities. A separate challenge is that part of the vulnerability assessment depends on third party vulnerability repositories, which if compromised, can prevent the vulnerability assessment from taking place or might provide incorrect results due to lack of data. A side effect of such challenge is the requirement for back-up copies of such repositories to be maintained or new proprietary vulnerability repositories to be created.

Also, when conducting resilience analyses as part of the vulnerability assessment on the critical assets, it is a challenge to quantify how physical and cyber resilience measures put in place to protect a critical asset as a whole, protect specific cyber vulnerabilities. For example, it is difficult to quantify how a physical lock used to restrict physical access to an Internet accessible electrical panel can protect the panel from a cyber attack.

2.5 Threat Assessment

The threat assessment quantitatively estimates the likelihood of threats on critical assets. A challenge is how to use theoretical and historical threat data stored in data repositories to determine the likelihood of a threat at near real time. Furthermore, specific threats are also identified at near real time for every recognized vulnerabilities, thus, it becomes a challenge to instantly analyze and cross-reference all the possible combinations of threats and vulnerabilities. In addition, the threat assessment uses near real time threat data to evaluate the likelihood of threats, so it becomes a challenge to process the larger amount of near real time data and to cross-reference them with the data retrieved from the theoretical and historical data repositories.

2.6 Risk Analysis

Once the various steps of the VARM are conducted, all of the results have to be aggregated using reducing equations. A major challenge is the reduction and combination, at near real time, of all of the data collected on the previous steps. Also, once the risk data is evaluated, the results have to be provided to an operator. The challenges associated with risk information presentation to the operator include addressing information overloading, risk data presentation for multiple types of users, ranking of large lists of critical assets based on risk levels, and enabling operators to respond to risk emergencies in a timely manner.

3 Summary

The modernization of Operation Technology (OT) of energy-dependent sectors helps prevent operational disruptions due to lack of energy, but also makes the sectors prone to cyber attacks. The VARM and other similar processes can be used to reduce the risk of operational disruptions due to cyber attacks by identifying vulnerabilities and threats. Various cyber security data collection and analysis challenges are encountered and have to be overcome in order to accurately conduct risk analyses at near real time. This work provides an overview of some of the data collection and analysis challenges that the VARM process addresses to help mitigate data overloading associated with such risk management processes.

4 References

Design of a Supercritical Carbon Dioxide External Tubular Superheater for Solar Power Towers

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1 Abstract
Supercritical CO₂ Brayton power cycles that can produce ~1 MW of electricity are being investigated. Closed-loop sCO₂ Brayton cycles are considered higher energy-density systems when compared to the equivalent super-heated steam Rankine cycles. A computational fluid dynamics (CFD) model was developed to further analyze the behavior and thermal efficiency of a direct tubular receivers using sCO₂ as a heat transfer fluid as opposed to super-heated steam. The tubular receiver consists of an arrangement of tubes and manifolds that help reduce the pressure losses while efficiently transferring the concentrated heat in a single-pass flow system. In an effort to strive for higher efficiencies (~50%), the outlet temperature of the receiver will have to be at least 700°C while sustaining a working pressure of 20 MPa (200 bar).

2 Introduction
As the demand of energy grows rapidly, scientists and engineers are looking for new ways to generate it while ensuring a sustainable future. Due to the limitations of non-renewable resources such as fossil fuels, renewable technologies to harvest solar energy have become a very attractive alternative. Concentrating solar power (CSP) has become a potential solution for a sustainable source of energy. CSP plants operate on the same fashion as coal/gas plants do. The main difference is the energy source that produces steam and/or high temperature gases that drive the turbine. Power cycles with higher efficiencies are being pursued to reduce the levelized cost of energy from CSP technologies [1]. The supercritical carbon dioxide (sCO₂) Brayton requires higher temperatures than those currently being used. Current central receiver technologies employ either steam or molten nitrate salt as a heat transfer medium and steam as working fluid in a subcritical Rankine power cycle. The average thermal-to-electric conversion efficiency of these cycles is typically between 30 and 40% at turbine inlet temperatures < 600 °C [2, 3].

Thermodynamic efficiencies above 50% at achievable concentration ratios and temperatures make sCO2 Brayton cycles a potential system for concentrating solar [4]. With this interest increase, sCO2 has been proposed for use as a heat transfer fluid in CSP systems [5, 6].

3 Background
More recent designs and tests have been conducted by direct liquid receiver (DLR) for a solar-hybrid micro turbine system operating in a central receiver for applications on the order of 100 kW – 1 MW. The thermal efficiency of the tubular design has increased up to 80-85% theoretical (simulations) [7]. A supercritical carbon dioxide Brayton cycle has the potential to replace steam-driven Rankine cycle turbines, which have lower efficiency, are corrosive at high temperature, and occupy 30 times as much space because of the need for large turbines and
condensers to dispose of excess steam. The Brayton cycle could yield 20 MW of electricity from a package with a volume as small as four cubic meters [8].

4 Objective
The goal of this work is to develop various potential receiver designs (i.e. dimensions, configuration, material) to compare and obtain the best possible arrangement, and maximize absorptance, minimize heat loss, and maintain a high structural stability at high temperatures.

5 Theory
The concentrated sunrays coming from the heliostat field will be heating the pipe; however, there will be some losses. Figure 1 shows the heat transfer that will occur at the tube surface. From the total solar radiation \( \dot{Q}_{sun} \), there will be re-emittance, reflective and convective losses. The absorbed energy will be the difference between the total solar radiation and the losses. The absorbed energy will heat the supercritical carbon dioxide, which will drive the turbine in order to generate electricity. It is well known that a higher temperature and pressure, more electricity will be produced. The Super critical carbon dioxide Brayton cycle does not have a heat exchanger as the common cycles used to produce electricity. The heat exchanger was eliminated in order to keep the high temperature and pressure of the super critical carbon dioxide.

![Fig.1. Solar radiation on a pipe (losses and absorbed energy).](image)

6 Problem Description

6.1 Methodology
The models were created using NX 7.5 which is a computer-aided design (CAD) software package used to design and to perform FEA. [9] The models were also done on ANSYS Workbench™ which has a computer-aided design (CAD) software package widely used to design and perform FEA (finite element analysis). It also provides the capability to perform computational fluid analysis (CFD). [10].

6.2 Assumption
- The distributor will be fixed at the top and the bottom.
- Pressure applied is 20,000 MPa.
- Gravitational effects are considered.
- The material used is Incoloy Alloy 800.
Mass flow rate = 1 kg/s
The factor of safety is 2.

Variable heat flux $q^\prime = 400,000 \frac{W}{m^2}$

6.3 Results
Figure 2 and 3 shows the results obtained from the contours of temperature and pressure.

The outlet temperatures obtained from the simulation was approximately the theoretical temperature (973 K). The pressure drop across the pipe was only 0.01 MPa. The pressure is considered constant through the whole distributor, so there will not be pressure loss and more electricity will be produced.

Future Work
- Continue working on a more efficient receiver.
- Generate FEA models to assure that piping (pipes, manifolds) and joints will withstand the stress using a SOF => 2.

References
A Heterogeneous Multiscale Method for an Elliptic Reaction Diffusion Equation

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1 Introduction

A recent approach to multiscale poroelasticity [1] decouples the operators into individual elliptic flow and deformation problems and resolves the multiscale nature individually [2, 3]. The decoupled flow problem is multiscale reaction diffusion equation which is not efficiently resolved by conventional numerical methods. In this paper, we develop and test a multiscale method for the reaction diffusion problem using distinct models at the micro and macro scales iteratively coupled by a linear flux assumption.

2 Model Problem

The decoupled multiscale flow problem[1] is a reaction diffusion equation of the form

\[ -\nabla \cdot (k(x)\nabla P) + c^* P = S, \]

where P denotes the fluid pressure, k(x) the mobility, and S the source term. It was shown in [1] that the convergence of the operator splitting approach is improved by increasing the step size \( \Delta t \); effectively reducing the impact of the reaction term. In order to achieve higher accuracy, we test a multiscale method to obtain better accuracy when the reaction term dominates.

3 Multiscale Method

We propose a heterogeneous multiscale method [4] similar to [1–3, 5, 6] using an incomplete macroscopic model based on finite volume method. At the continuum scale, the finite volume method discretizes the domain into finitely many control volumes and imposes the divergence theorem within each volume. Using an equispaced grid, the one dimensional case results in:

\[ F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} + c^* P_i \Delta x = S_i \Delta x, \]

where \( \Delta x \) is the length of the control volume and \( F_{i+\frac{1}{2}} \) is the flux through control volume boundaries. The microscale model is a modified pore network model with additional reaction terms given by:

\[ \sum_{j \in K_i} q_{ij} + c^* p_i L = s_i L, \]
where \( q_{ij} \) is the volumetric flux, \( L \) the length of the throats, and \( s_i \) the micro source term. We use the linear Hagen Poiseuille Flux law between pores. To couple the scale models together, we impose the linear flux assumption from [1, 2, 5, 6]. The microscopic flux is iteratively coupled to the macroscopic pressures by

\[
-D^+ \left( f_{i+\frac{1}{2}} \left( P_i^n, P_{i+1}^n \right) \right) D^+ P_i^{n+1} + c^* P_i^{n+1} = S_i,
\]

where the flux term \( f_{i+\frac{1}{2}} \) is determined by interpolating macroscopic pressures onto dirichlet boundaries of the microscale model and solving the microscale equations.

4 Numerical Experiments

We study the convergence of the multiscale method for the model problem on a domain \( \Omega=[0,1] \) with Dirichlet boundary conditions. We compare our multiscale method to a fully coupled microscale model consisting of \( N=4096 \) throats. The multiscale method samples the mobility coefficients from the fully microscale model over \( N_s \) subdomains of length \( \delta=N_c \cdot L \) for an integer \( N_c \) such that \( N_c \cdot N_s \leq N \). Assuming uniform randomly distributed \( k(x) \in [1,1000] \), we calculate the average error in the relative \( L^\infty \) norm for pressure and flux for each \( (N_s, N_c) \) pair over 100 simulations. We consider reaction-limited and reaction-dominated cases with \( c^*=1 \) and \( c^*=100 \), respectively.

5 Results

Fig. 1 & 2 show the convergence behaviors for the reaction-limited and reaction-dominated cases, respectively. Relative pressure and flux errors monotonically decrease holding \( N_s \) constant while increasing \( N_c \) and vice versa in the reaction-limited case. For the reaction-dominated flow case, errors monotonically decrease only while holding \( N_c \) constant and increasing \( N_s \). Errors increase as \( N_c \) is held constant and \( N_s \) increases until subdomains are sampled within a sharp boundary layer near \( x=0 \). When \( N_s \) increases beyond this point, errors monotonically decrease.

6 Conclusions & Future Work

The numerical experiments above verify the convergence of our multiscale method for a reaction diffusion equation. We demonstrated that our method achieves monotonically decreasing errors in pressure and flux in the reaction-limited case. In the reaction-dominated case, increasing sampling subdomains improves convergence only when subproblems are solved within the existing boundary layer. This suggests that the optimal convergence strategy for this multiscale method involves using a non-uniform grid with control volumes clustered densely near the boundary layer. A computationally expensive adaptive grid refinement may be required in the case of general source terms, since the size and location of this boundary layer can be unpredictable. In our future work, we will explore an alternative approach to capture the effects of the boundary layer on a uniform grid by enriching the microscale model with residual free bubble functions.
Fig. 1: Convergence of multiscale method for $c^*=1$.

Fig. 2: Convergence of multiscale method for $c^*=1000$.

References


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1 Introduction

With the demand of growing energy, Concentrating Solar Power has become an important technology in solar energy harvesting. CSP technologies are facilitating with the solar energy storing accessibility in the form of thermal energy. Inclusive all the CSP technologies, Direct solar thermal energy storage technology is more conducive and cost effective technology compare to Indirect solar TES technologies. Direct solar TES technology can be implemented to meet the energy demand i.e. power supply during night time, peak hour or any changes in solar irradiation (e.g. winter season, cloudy day). Combination of CSP and TES technology is a complete system could overcome the intermittency of renewable power generation alone and can contribute to making electricity with conventional sources and cost competitive way.

Among of all three technologies, Single tank TES system has more potential on large scale heat storage aptitude [1]. HTF is the crucial part in TES system, as it is the only medium for storing thermal energy in the CSP plant. Synthetic high temperature (2930c-3930c) oil Caloria® was used as the HTF in SEGS (Solar Electric Generating System) plants. But the limitation with this synthetic oil was it cannot go beyond 4000C. Solar salt, HITEC®, HITEC XL are the potential molten salt candidates to be used as HTF [2]. Molten salt properties allow operating at higher temperature with low melting point (about 2200C-6000C) and high heat storage capacity.

TES shows significant intensification of thermal behavior while adding nanoparticle to the HTF. If the value of thermal diffusivity increases with nano HTF, it will disrupt the thermocline region; will increase the non-useable energy area resulting diminishing in efficiency of the system. So it is crucial to preserve this thermocline region with less thermal diffusivity and uniform velocity distribution of the HTF.

2 Problem Description

A cylindrical tank is designed such that the hot fluid comes through the inlet pipe disposed at the top of the tank and cold fluid takes exit through the outlet pipe disposed at the bottom of the tank. During discharging cycle the thermal storage fluid flows to adverse direction. The thermocline zone is stationed at the horizontal surface so we need to interject the flow such an action which can retain the zone with less destruction. If the fluid is heading with a jet stream it will perturb the thermocline zone by mixing the hot fluid with cold fluid.

Following schematic diagram in Figure 1 showed a single tank thermocline TES system with pipe flow distributor.
The dimension of the single tank is $12 \times 12 \text{ m}$. The inlet and outlet diameter of the tank is $d_{\text{in}} = d_{\text{out}} = 0.05d_{t} = 0.6\text{ m}$. The main pipe, diameter is $d_{m} = 0.8\text{ m}$. Diameter of the distributor pipes is $d_{\text{dist}} = 0.6\text{ m}$, diameter of hole is $d_{h} = 0.025d_{t} = 0.3\text{ m}$. We assume total charging period is 6 hours i.e. operating time from 10:00 am to 4:00 pm. The inlet velocity is calculated as $0.2 \text{ m/s}$.

To increase the storage capacity with available facility we blend nanoparticle with the existing Hitec® molten salt. Hitec® is a tertiary nitrate based salt with the composition of potassium nitrate (53% by wt), sodium nitrite (40% by wt) and sodium nitrate (7% by wt). The physical and thermal properties of this salt eutectic are density $1870\text{ kg/m}^{3}$, viscosity $(\mu)$ $0.0032 \text{ kg/m} \cdot \text{s}$, thermal conductivity $(k)$ $0.398 \text{ W/m} \cdot \text{K}$, specific heat capacity $(C_p)$ $1553.3\text{ J/kg} \cdot \text{K}$ at $300\text{ K}$ [3].

Five different types of nanoparticles ($\text{SiO}_2$, $\text{Fe}_3\text{O}_4$, $\text{Al}_2\text{O}_3$, $\text{ZnO}$, $\text{Ag}$) have been used with three different concentrations i.e. 1%, 5% & 10% by volume fraction assuming that after adding the nanoparticles into the eutectic salt the operating temperature range will be from 300 $\text{K}$ to 773 $\text{K}$.

### 3 Numerical Discretization Method

The numerical calculation is obtained by finite volume analysis following by the Navier-Stokes equation with the commercial software Fluent 6.3. The new value of $k$ and $C_p$ for the nanofluids are called $k_{\text{eff}}$ and $C_{\text{peff}}$. Here, $k_{\text{eff}}$ is calculated by using the following formula,

$$k_{\text{eff}} = \frac{k_{p} + 2k_{bf} + 2(k_{p} - k_{bf})\phi_{v}}{k_{p} + 2k_{bf} + (k_{p} - k_{bf})\phi_{v}} \quad (1)$$

$C_{\text{peff}}$ is calculated by using the following formula [20],

$$C_{\text{peff}} = \phi_{m}C_{np} + (1 - \phi_{m})C_{pbf} \quad (2)$$

The conservation of mass equation, the conservation of momentum equation, energy equation are used to calculate the velocity and total energy of the system.

To analyze the flow distribution and the thermal distribution the tank domain is discretized into smaller volumes using triangular mesh. Boundary condition for the outer tank wall is assumed adiabatic condition as the heat transfer loss is negligible. The heat transfer across the outer wall of the pipe flow distributor is also disregarded as the heat flow by convection is
very little. Pressure velocity coupling is calculated by SIMPLE algorithm and for momentum first order upwind discretization method is used. By using the pressure based solver, velocity and thermal distribution is calculated for unsteady-state, non-iterative method for 6 hours charging period considering uniform flow distribution.

4 Result and Conclusion
The doping of nanoparticles results in higher thermal conductivity and heat capacity, compared to the base fluid. Higher heat capacity is expected to improve the thermal storage capacity but higher value of thermal conductivity is expected to increase the thermal diffusivity, thereby affecting the performance of the thermocline. Similarly, higher value of viscosity reduces the flow disturbances but a higher value of density increases the flow disturbances which can cause thermocline perturbations and hence reduction in the useful energy storage. So, to balance of the effective properties to improve thermal storage performance, total energy storage capacity is then checked by finite volume based computational fluid dynamics software. The simulation shows how the performance of the nanofluid changes at different concentrations in a single tank TES system during its charging-discharging cycle. From Figure 3(b), the graphical representation of percentage of energy increase along with the volume concentration shows the improvement of the TES system.

Fig. 2. (a) Velocity contour of nanofluid at 5% volume fraction (b) Temperature contour of nanofluid at 5% volume fraction

Fig. 3. (a) Temperature contour of Hitec® Molten salt on a plane at different instances (b) Volume concentration vs. Energy increase

References
Meta-modeling on Building Energy Consumption

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1 Introduction
According to EIA (U.S. Energy Information Administration), nearly 40% of the total U.S. energy consumption in 2012 was consumed in residential and commercial buildings. As a result, research on designing building energy models and improving energy efficiency is of great importance. Model-based simulation of building design and operation is typically used and coupled with an optimizer for energy efficient building operation decisions. However, it is reported the model-based simulation suffers from long cycle iteration time when a large number of different design scenarios are desired. To alleviate computational cost, an analytical meta-model generated from physics-based model on which a number of points representing different design scenarios are sampled is fit to the data. Thus, a cost efficient surrogate model, rather than the original expensive simulation model, can be applied in an optimization process in which thousands or even millions of evaluations are obtained with less computational effort. Meta-modeling is much more computationally efficient than physics-based modeling due to its simplified black-box model form. Despite its simplistic form, meta-modeling still maintains good accuracy. A case study is presented using real data of an existing building located on Drexel University’s campus in Philadelphia, Pennsylvania as a demo of the implementation of the above approach. The result shows that meta-modeling is indeed a promising approach for building energy consumption simulation for achieving both accuracy and computational efficiency.

2 Meta-models
A meta-model is a surrogate model that approximates the simulation model used to study a system. Extensive research has been done investigating the performance of different meta-modeling techniques in terms of accuracy and/or robustness. Results showed the performance of the techniques vary depending on the problem constructs. Based on the literature review, three metamodelling techniques are of interests in this research: Kriging[1], Support Vector Regression (SVR)[2] and Radial Basis Function (RBF)[3]. Each of them is briefly reviewed in this section. In addition, an ensemble model is also discussed.

2.1 Kriging
Kriging (also known as Gaussian process regression), which gives the best linear unbiased prediction of the intermediate values, is a method of interpolation for which the interpolated values are modeled by a Gaussian process. It generates the prediction in the form of a combination of a global model with local random noise. Kriging is one of the most intensively studied meta-models because it is flexible with a number of correlation functions from which to choose. It is generally acknowledged that the Kriging model outperforms other meta-models on nonlinear problems. However, it is not easy to develop due to the time consumed by Maximum Likelihood Estimation, which is a multi-dimensional optimization problem.

2.2 SVR
SVR is analogous to support vector classification. The goal of the technique attempts to maximize the distance between two classes of data by selecting two hyperplanes in such a way that they separate the training data with no points between them. It is interesting to note that research has demonstrated SVR performs well on a number of problems, and even outperforms Kriging for some cases. However, most studies have been empirical.

2.3 RBF

RBF is used to develop interpolation on scattered multivariate data. A RBF is a linear combination of a real-valued radially symmetric functions based on distance from the origin. Fang et al. [4] found RBF performs well on highly nonlinear problems.

2.4 Ensemble

Ensemble is a technique combining multiple models in order to create a stronger overall representation of the studied system. In general, a weighted average surrogate model is:

\[ \hat{y}_{avg}(x) = \sum_{i=1}^{M} \omega_i(x) \hat{y}_i(x) \]

where \( \hat{y}_{avg}(x) \) is the ensemble response prediction by the weighted sum of each surrogate model response prediction \( \hat{y}_i(x) \), \( \omega_i(x) \) is the weight corresponding to the \( i^{th} \) surrogate, and \( M \) is the number of surrogate models. Acar and Rais-Rohani [5] propose a weight selection approach by solving an optimization problem on identifying the weight for each surrogate that would minimize a selected error metric (e.g., root mean square error). That is,

Minimize \( \varepsilon_e = \text{Err}\{\hat{y}_e(\omega_i, \hat{y}_i(x_j), y(x_j))\}, j = 1, \ldots, M\}

subject to \( \sum_{i=1}^{N} \omega_i = 1 \)

where \( \text{Err}\{\} \) is the error metric of the built ensemble predicted response. Accuracy metric reflects the degree of closeness of measurements of the meta-model outputs \( \hat{y} \) to true output \( y \). One global measurement on accuracy is Normalized Root Mean Square Error (NRMSE)

\[ \text{NRMSE} = \sqrt{\frac{\sum_{t=1}^{n}(y_t - \hat{y}_t)^2}{n}} / (y_{max} - y_{min}) \]

Based on the literature review, we conclude no consensus is reached on the performance of the various surrogate models. Therefore, in this research, we conduct comprehensive experiments to evaluate the performance of the models on a real world building case which is a highly dynamic nonlinear system.

3 Design of Experiment

From May 1st to July 31st, 2011, the energy data was collected every half an hour from sensors and meters of a building on Drexel University’s campus. Data is divided into two groups: 37 occupied (5:30-23:30) and 11 unoccupied (23:30-5:30 next day) data points. Each data record has 11 variables, time (t), setpoint (spt), zone temperature (rat), humidity (oah), outdoor temperature (oat),
oat_{t-2}) and 1 response variable, load (electricity load). Based on our understanding of building energy studies, we include both the current time stamp and the immediate two previous time stamp data to capture the dynamics of the system. 4414 data records were collected, in which 110 occupied and 50 unoccupied data points were trained with 2-fold cross validation with three meta-models, and 1000 data points that exclude the training data records were tested. Parameter settings can significantly affect the meta-model’s performance. Thus a grid search that produces an ergodic exploration over the entire parameter space is chosen to obtain the optimal parameter settings which give the minimum error on the cross-validation. Finally, when all of the three optimal meta-models are trained, an ensemble is built.

4 Results

Table 1 shows the NRMSE of three meta-models and their ensemble on occupied and unoccupied data. It indicates RBF outperforms Kriging and SVR, with SVR underperforming in both cases. Ensemble, which is built based on error minimization, is at least as good as the best performer. It is noticeable that the accuracy of the resulting model is restricted to the one we selected if only one of the three meta-modeling techniques was adopted. Nevertheless, an ensemble is able to combine and make the best of all three models to achieve an optimal solution. As observed from Table 1, the overall ensemble performance is within 90% of accuracy.

Table 1 NRMSE of Meta-models and Ensemble

<table>
<thead>
<tr>
<th>NRMSE</th>
<th>Occupied</th>
<th>Unoccupied</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kriging</td>
<td>0.128</td>
<td>0.119</td>
</tr>
<tr>
<td>SVR</td>
<td>0.159</td>
<td>0.129</td>
</tr>
<tr>
<td>RBF</td>
<td>0.106</td>
<td>0.093</td>
</tr>
<tr>
<td>Ensemble</td>
<td>0.105</td>
<td>0.093</td>
</tr>
</tbody>
</table>

5 Conclusions

Experiments of three meta-modeling techniques and their ensemble are conducted for the prediction of real building energy data. The results show that RBF and Kriging outperform, while SVR underperforms. However, a stand-alone model is restricted to its own performance, thus an ensemble is further built to learn from each technique’s strengths. The resulting model proves to be better than or equally good as the best stand-alone model. Moreover, the computational cost is much lower than a physics-based simulation model, as the training and testing process only takes a few seconds. The minimal time expense will be of great help when a large number of simulation evaluations are needed for design optimization.

References

Fabrication and Preliminary Testing of Metamaterial Based Passive Wireless Temperature Sensors

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1 Introduction  
The continuous advancement in energy conversion systems such as gas turbines, coal based and more recently oxy-fuel combustion power plants has lead to an increasing interest in the further innovation of sensing technologies for processing parameters. Among these parameters, continuous and precise temperature monitoring is of main concern in order to improve the combustion process leading to higher thermal efficiencies and the reduction of pollutants released to the ambient. Furthermore, constant temperature sensing is necessary to ensure the structural integrity of these systems [1]. The presence of high temperature, high pressure and corrosive atmosphere conditions require sensing technologies to be able to maintain effective and reliable operation. Nevertheless, the adverse conditions aforementioned comprised of temperatures up to 1300°C [2] have rendered current solutions unreliable due to existence of semi-conductor materials and energy storage devices in their configuration [3]. This has emphasized the need for affordable and reliable passive, wireless temperature sensors for harsh environment applications. Among the possible technologies, metamaterials are a feasible solution for wireless sensor solutions with the needed characteristics.

Metamaterials are man-made materials that present characteristics normally absent in natural occurring materials [4]. Among the available metamaterials, Split Ring Resonators (SRRs) are one of the most commonly found structures to date. Previous research efforts have focused on characterizing and applying the metamaterial concept to sensing technologies. Aydin, et. al. focused on characterizing the magnetic resonance for different designs of SRRs with varying parameters [5]. Moreover, Ekmekci proposed and proved the feasibility of metamaterial based sensors for pressure, temperature and humidity employing a “V” shaped and broadside-coupled split ring resonator (BC-SRR) structures [6]. This project focuses on the fabrication and preliminary testing of a low cost, passive wireless temperature sensor for harsh environment applications using a Closed Ring Resonator (CRR) structure. The proposed sensor can be modeled as an LC circuit and temperature sensitivity will be achieved by the variation of the dielectric constant on the ceramic with the change in temperature, affecting the capacitance and hence the resonant frequency of the system.

2 Experimental Procedure  
2.1 Sensor Fabrication  
Sensors were fabricated using the traditional powder compression method using a 1-inch and
2.75-inch in outer diameter cylindrical dies and a 2-inch square die. For this process, barium titanate (BaTiO$_3$) nanopowders with an average particle size of 700 nm were used as the dielectric ceramic and different commercially available copper and aluminum washers were employed as the conductive metal rings. Additionally, polyvinyl alcohol (PVA) was used as binding material to achieve better cohesion in the ceramic substrate. For the fabrication, BaTiO$_3$ nanopowders were placed in a mortar with 7.5% wt. of PVA. The mixture was ground until uniform distribution of the PVA in the ceramic was achieved. After that, the ceramic mixture and two rings were placed inside of the compression die as shown in Figure 1 (a). Manual compression was performed in each layer to prevent misalignment between the rings. The die was then placed in a Carver hydraulic pressing machine and was compressed to 3 metric tons for 5 minutes to compact the ceramic, as seen in Figure 1 (b). Additionally, binder curing was performed for the 1-inch samples by placing them in a furnace at 150°C for 90 minutes, utilizing a 5°C/min ramp in order to improve sample rigidity.

Fig. 1: (a) Schematic of sensor fabrication, (b) Die placed inside of the pressing machine, prior to compression

2.2 Free Space Testing

The 2.75-inch samples were tested using the free space measurement configuration consisting of two Mr. Bean Gaussian beam antennas and a vector network analyzer. For this setup, two chambers were utilized. One of the antennas was placed in the bottom chamber with aluminum walls. Additionally an aluminum plate with an iris was used as a perfect electric conductor. The receiving antenna was placed on the top chamber, directly aligned with the bottom one. Finally, the sample was placed on top of the iris to prevent signal dissipation and noise.

3 Results

The sample fabrication was successfully performed. Different configurations were achieved for wireless temperature sensors using the CRR architecture. Figure 2 (a) shows a 2.75 – inch OD sample with copper washers and a thickness of 0.75 inches while Figure 2 (b) shows an arrangement of 4 square samples with aluminum washers and a thickness of 0.25 inches.

Fig. 2: (a) 2.75-inch sample with copper washers, (b) Arrangement of square samples with aluminum washers
The results for the preliminary testing for the free space testing of the 2.75-inch sample can be seen in Figure 3. From these results, resonance peaks can be observed in the available frequency range. The first peak is observed at around 5 GHz, the second one is located around 9 GHz. Finally, the last one is observed at around 13 GHz. The second peak can be used for sensing purposes since it displays the highest intensity.

![Transmission response for the 2.75 cylindrical sample for a frequency range of 2 to 18 GHz](image)

**Fig. 3:** Transmission response for the 2.75 cylindrical sample for a frequency range of 2 to 18 GHz

### 3 Conclusion

This research project presents the fabrication and preliminary testing of metamaterial based wireless temperature sensors for high temperature applications. Samples were successfully fabricated using BaTiO$_3$ nanopowders and commercially available copper and titanium washers. Preliminary testing was performed for the 2.75-inch sample, portraying three resonant frequencies, the most prominent one located at around 9 GHz. Further sample characterization and high temperature testing needs to be performed in order to prove the feasibility of the sensor in harsh environments.

### References


A Double Inclusion Model for Multiphase Piezoelectric Composites

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1 Introduction

Recently a novel active piezoelectric structural fiber was introduced that can be placed in a composite material to perform sensing and actuation, as well as having a load bearing functionality. In order to fully understand the electroelastic properties of the material, this paper will introduce a three-dimensional micromechanics model for estimating the effective electroelastic properties of the multifunctional composites with different design parameters [1].

2 Micromechanics Model

Current literature has shown the double inclusion model to be a powerful method to predict the effective elastic properties of composites with multiphase inclusions. Consider a transversely isotropic piezoelectric material, where the linear constitutive equations that describe the coupled interaction between the electrical and mechanical variables can be expressed as

\[
\sigma_{ij} = C_{ijmn} \epsilon_{mn} - e_{nj} E_n
\]

\[
D_i = e_{imn} \epsilon_{mn} + k_{in} E_n
\]

where \( \sigma_{ij}, \epsilon_{mn}, E_n \) and \( D_i \) are the stress, strain, electric field and electric displacement tensors, respectively, and the \( C_{ijmn}, e_{nj} \) and \( k_{in} \) are elastic, piezoelectric field stress and dielectric tensors, respectively. Combining the mechanical and electrical variables such that the two equations can be expressed in a single constitutive equation [3], which matrix form can be expressed as

\[
\begin{bmatrix}
\sigma_{11} & C_{11} & C_{12} & C_{13} & 0 & 0 & 0 & 0 & 0 & -e_{31} & \epsilon_{11} \\
\sigma_{22} & C_{12} & C_{22} & C_{23} & 0 & 0 & 0 & 0 & 0 & -e_{32} & \epsilon_{22} \\
\sigma_{33} & C_{13} & C_{32} & C_{33} & 0 & 0 & 0 & 0 & 0 & -e_{33} & \epsilon_{33} \\
\sigma_{23} & 0 & 0 & C_{44} & 0 & 0 & 0 & -e_{15} & 0 & y_{23} \\
\sigma_{13} & 0 & 0 & 0 & C_{55} & 0 & -e_{15} & 0 & 0 & y_{13} \\
\sigma_{12} & 0 & 0 & 0 & 0 & C_{66} & 0 & 0 & 0 & y_{12} \\
D_1 & 0 & 0 & 0 & e_{15} & 0 & k_1 & 0 & 0 & E_1 \\
D_2 & 0 & 0 & 0 & e_{15} & 0 & 0 & k_2 & 0 & E_2 \\
D_3 & e_{31} & e_{32} & e_{33} & 0 & 0 & 0 & 0 & k_3 & E_3
\end{bmatrix}
\]

The overall electroelastic modulus predicted by the double inclusion model can be expressed as

\[
E = E_1 + \sum_{r=2}^{N} c_r (E_r - E_1) A_r
\]

where \( c \) is the volume fraction, and the subscript \( r \) represents the phase of the composites (i.e. 1= matrix phase). \( E \) is the extended electroelastic matrix, and \( A \) is the concentration tensor (function of the Eshelby’s tensor and the electroelastic properties of each phase), it can be defined as
where the S is the Eshelby’s tensor (function of the inclusion geometry as well as the electroelastic properties of the matrix), Φ is the fourth order tensor (function of the Eshelby’s tensor and the electroelastic properties of each phase). The expression of Φ is given by

\[ \Phi = -\Delta S + S_2 + F_2 - S_3 \frac{c_3}{c_2} \Delta S + F_3 -1 \times S_3 - \frac{c_3}{c_2} \Delta S + F_2 -1 \]

where F and ΔS are expressed as

\[ F_2 = (E_2 - E_1)^{-1} E_1 \]
\[ F_3 = (E_3 - E_1)^{-1} E_1 \]
\[ \Delta S = S_3 - S_2 \]

The geometry of the ASF for the multifunctional composite is shown in figure 1 with the coordinate system adopted here [1].

3 Results

Figure 2.1. shows that longitudinal Young’s modulus Y3, increases linearly with volume fraction while the transverse Young’s modulus Y1=Y2, increases exponentially; this due to the fact that increasing the aspect ratio leads to a larger fraction of piezoelectric material. Therefore, the overall longitudinal and transverse moduli decrease and increase with the increasing aspect ratio, respectively. Figure 2.2 show that the longitudinal shear G23=G13 modulus is highly dependent on the volume fraction and fairly insensitive to the aspect ratio. The transverse shear modulus G12 has a larger dependence on the aspect ratio and increases with volume fraction. Because the piezoelectric has the highest dielectric constant of all 3 constituents, the longitudinal dielectric constant increases with increasing volume fraction and aspect ratio as shown in figure 2.3. The transverse dielectric constants also increase with the increasing aspect ratio and volume fraction.
fraction. The results presented in figure 2.4 indicate that using higher aspect ratio leads to higher coupling ratio due to its higher fraction of piezoelectric. Also, the longitudinal and transverse piezoelectric coupling coefficient increase at a very high rate for low volume fractions then increase at nearly linear rate above a volume fraction of 0.2. They also both increase with higher aspect ratio and fiber volume fraction. The model indicates that with proper design parameters (aspect ratio and fiber volume fraction), the piezoelectric coupling coefficient of the structural composites laminate could reach as high as 70% of the active constituent. Multifunctional composites with this level of electromechanical coupling properties would have a strong potential for embedded sensing, actuation, vibration control, and structural health monitoring.

Fig.2.1. Effective Young’s Modulus with respect to ASF volume fraction, (straight line) longitudinal, (dotted line) transverse.

Fig.2.2. Effective shear modulus with respect to ASF volume fraction, (dotted line) longitudinal, (straight line) transverse.

Fig.2.3. Effective dielectric constant with respect to ASF volume fraction, (straight line) longitudinal, (dotted line) transverse.

Fig.2.4. Effective piezoelectric coupling ratio with respect to ASF volume fraction, (dotted line) longitudinal, (straight line) transverse.

References


Concept and Model of a Metamaterial Based Passive Wireless Temperature Sensor

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1 Introduction

The Metamaterials are man-made materials, which can display properties that are otherwise absent in nature. The materials are usually arranged periodically to duplicate the structure of an atom. Depending on the shape, size, orientation, and arrangement, metamaterials can show different exclusive properties such as negative refractive index [1], cloaking [2], and reverse Doppler effect [3]. Because of these unique properties metamaterials have opened a new horizon of possibilities. The potential applications of metamaterials are remote sensing, remote aerospace applications, solar power improvement, communications, improving ultrasonic sensors and shielding structures etc. [4].

Wireless passive sensors are getting more and more attentions in the industries. These sensors are really convenient as they are wireless and do not need any additional power supply. Optical based wireless sensors were developed but the accuracy of these sensors was not satisfactory [5]. SiC and Si\(_3\)N\(_4\) based micro-sensors have been introduced in harsh chemical environment at high temperature, but the complexity of the fabrication process makes it costly [6]. Metamaterials were introduced to remove these limitations. Arbabi et al. [7] proposed a metamaterials based SPR sensor in Terahertz region. Several approaches were made to develop wireless passive temperature sensors capable of sustaining high temperature and harsh environments. Ekmekci et al. [8] demonstrated the feasibility of different types of SRR structures for different types of sensors. They suggested broadside-coupled SRR structure for temperature, humidity and concentration sensor application. Scott and Peroulis [9] presented a slot antenna with an embedded temperature sensor which can sense up to 300°C. The objective of this paper is to propose a metamaterial-based temperature sensor that can sense temperature up to 1000 °C, is able to work in harsh environments such as combustion chambers and will be cheap and easy to replace.

2 Modeling the sensor

The proposed sensor has two closed metal ring resonators embedded in a dielectric material matrix, which separates the two resonators as depicted in Figure 1(a). The dielectric matrix surrounding the metal rings helps protect the metals from harsh and corrosive environments. The whole structure acts as an LC resonance circuit. The equivalent circuit is also suggested in Figure 1(b). Determination for the capacitance (C) and inductance (L) terms can be found elsewhere [10,11]. The resonance frequency of the structure can be expressed as:

\[
f = \frac{1}{2\pi\sqrt{LC}}
\]

where, \(f\) is resonance frequency. The simplest expression for capacitance can be given as:
where, $\varepsilon_0$ is the relative permittivity of vacuum, $\varepsilon_r$ is the relative permittivity of the dielectric matrix, $A$ is the area of one ring resonator and $d$ is the distance between the two resonators. Since, $\varepsilon_0$, $A$, and $d$ are constant for a certain sample, the capacitance depends on the value of $\varepsilon_r$ which is dependent on the temperature. Therefore, any change in temperature changes the relative permittivity of the dielectric matrix and hence changes the capacitance and the resonance frequency of the structure.

To validate the feasibility of the sensor and to determine the geometry and configuration, finite element based modeling was performed using Ansys Ansoft HFSS (High Frequency Structural Solver) 15.0, which is a full wave electromagnetic solver. The length if the matrix = width = 6 mm, and thickness = 3 mm. The outer diameter, width and thickness of the rings are 4 mm, 0.3 mm and 0.03 mm respectively. PEC (Perfect Electric Conductor) and PMC (Perfect magnetic Conductor) boundary conditions were used on the surfaces perpendicular to the $z$-axes and $x$-axes respectively while $y$-axis was chosen as the direction of propagation.

### 3 Effect of relative permittivity ($\varepsilon_r$) on the resonance frequency

To evaluate the temperature sensitivity of the sensor structures, the standard dielectric constant of LiNbO$_3$ from 450 °C to 800 °C was taken into account [12], which varies from 52 to 145 within this temperature range. Using the dielectric constant of 52, 55, 65, 70, 76, 87, 110 and 145 at temperatures 450 °C, 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, 750 °C and 800 °C, respectively. It was observed that with the increase of dielectric constant value, the resonance frequency of the structure decreases, which is expected as the capacitance of the structure increases with the increase of dielectric constant.
4 Conclusion
A metamaterial-based temperature sensor was suggested using a ceramic substrate, which has a dielectric constant that changes with temperature and shifts the resonance frequency of the sensor under a magnetic excitation. Modeling and simulations were done using HFSS and the effect of temperature change on the resonance frequency of the structure was evaluated. The proposed CRR structure displays a good sensitivity of 7.286/°C and in addition, the use of CRR structures makes the sensor fabrication process simple and low cost as well.

References
Enhanced Energy Storage of Dielectric Nanocomposites at Elevated Temperatures
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Abstract
With the development of modern technology, the demand of high energy density dielectric capacitor devices is increasing for its significant role in stationary power systems, mobile devices, and pulse power applications. Enhancing the performance of dielectric capacitors especially towards higher energy density and higher operation temperatures are of special interest. Therefore, in this investigation, research effort has been dedicated to the fabrication and characterization of nanocomposites for enhance the energy density and the performance at elevated temperatures. The dielectric capacitors are fabricated using nanocomposites of BaTiO3/PI (Polyimide) that combines the capacitance achieved by ceramic materials and the breakdown strength from the polymeric matrix. Dielectric properties and energy densities were measured on samples, and properties were studied by varying the volume ratio (0-20%) of the nanocomposites, the operating frequency (20Hz-1MHz), and temperature (20-120°C).

This paper will focus on the characterization of the energy storage properties of PI nanocomposites with different volume fraction of BaTiO3 nanoparticles and the influence of temperatures on dielectric properties. The highest value of energy density was found in the nanocomposites at 1 kH, the nanocomposites with 20% volume fraction showed the highest values of energy density starting at 20°C with 9.64 J/cm³ up to 100°C with 6.83 J/cm³.

Results and Discussion
To measure the capacitance of all the samples, an LCR meter (HP 4284A) was used at different frequency levels ranging from 20Hz to 1MHz. The capacitance of a dielectric capacitor was influenced by the volume fractions of ceramic filler materials and frequency. The nanocomposites with 20% volume fraction of BaTiO3 nanoparticles showed the highest capacitance of 95.59 (pF) at 20 Hz frequency and 84.26 (pF) at 1 MHz, the change in capacitance from 20 Hz to 1 MHz frequency was 13.44%. All the samples with different volume fractions - 0%, 5%, 10%, 15% and 20% of BaTiO3 displayed the same trend of change in capacitance with change in frequency.

To investigate the temperature influence on capacitance, all the samples were also tested at different temperature- 20°C, 50°C, 75°C, 100°C and 120°C, maintaining the same level of frequency of 1kHz, the test results are shown in Figure 1. For each temperature, capacitance for was calculated considering the average capacitance tested from 20Hz to 1MHz.

By using the test results for capacitance, the dielectric constant for all the parallel plate dielectric capacitors were calculated at the same frequency ranges from 20Hz to 1MHz and

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temperature of 20°C, 50°C, 75°C, 100°C and 120°C. The following equation was used to calculate the dielectric constant

\[
\varepsilon_r = \frac{Cd}{\varepsilon_0 A}
\]

(1)

here \( \varepsilon_r \) is the relative dielectric constant of the dielectric, \( C \) is the measured capacitance in Farads (F) by the inductance-capacitance-resistance (LCR) meter, \( d \) is the thickness of the capacitor measured in meters (m), \( \varepsilon_0 \) is the permittivity of the vacuum \((8.854 \times 10^{-12} \text{ F/m})\) and \( A \) is the effective surface area of the electrode of capacitor calculated in \( \text{m}^2 \). All the samples with different volume fractions of BaTiO\(_3\) showed their highest relative dielectric permittivity at low frequency due to improved interfacial polarization, but at high frequency, there was significant drop in relative dielectric permittivity of dielectric capacitor due to unstable molecular polarization of the polymer, which resulted in less contribution to its relative dielectric permittivity [2]. The highest relative dielectric permittivity was calculated as 34.55 at 20 Hz for samples with 20% volume fraction of BaTiO\(_3\) and it decreased by 13.46% at 1MHz.

A dielectric capacitor’s dielectric properties are strongly influenced by temperature. With increasing temperature, the relative dielectric permittivity of dielectric capacitor also increases due to rapid molecular movement caused by high temperatures. For all the samples, higher dielectric constant was calculated at elevated temperatures. Among the different samples, those with 20% volume fraction of ceramic filler materials displayed higher relative dielectric permittivity at all the tested temperatures and there was significant improvement in relative dielectric permittivity from 20°C to 120°C. At 120°C, highest relative dielectric permittivity was obtained, a value of 51.66 was calculated for sample with 20% volume fraction at 20Hz, which was 52.97% higher than relative dielectric permittivity at 1MHz.

Following the dielectric capacitance testing, the breakdown strengths of dielectric capacitors were also measured under higher voltage ranges and elevated temperature for all the samples with different volume fraction of ceramic filler materials. The breakdown voltages were measured according to the ASTM D149-09 standard [1] and using the following equation:

\[
E_{bd} = \frac{V_{bd}}{d}
\]

(2)

where \( E_{bd} \) is the breakdown strength of the material measured in MV/m, \( V_{bd} \) is the breakdown voltage and \( d \) is the thickness of the capacitor. For breakdown strength testing of dielectric capacitors, test setup included a 30 kV high voltage power supply (Acopian PO3HP2), digital oscilloscope (Rigol DS1102E), 20 MHz function/arbitrary waveform generator (Agilent 33220A) and a digital multimeter (FLUKE 16 Multimeter).

The breakdown strength testing was carried out at different temperatures from 20°C to 120°C for all the samples; results are shown in Figure 1.

Lastly, the energy density of the dielectric capacitors were calculated by using the calculated dielectric constants and breakdown strengths of the samples:

\[
W = \frac{1}{2} \varepsilon_r \varepsilon_0 E_{bd}^2
\]

(3)

where \( W \) is the energy density measured in J/cm\(^3\), \( E_{bd} \) is the breakdown strength of the dielectric capacitor, \( \varepsilon_r \) is the dielectric constant of the dielectric materials and \( \varepsilon_0 \) the dielectric constant of
vacuum. Energy density was calculated for all the samples with different volume fraction of ceramic filler materials at different temperatures ranging from 20°C to 120°C shown in Figure 1. Energy density is proportional to the dielectric constant and breakdown strength of the dielectric capacitor. Improved dielectric constant and breakdown strength greatly influence the energy density of the capacitor.

![Graphs showing Breakdown strength and Energy density vs. temperature for BaTiO$_3$/PI nanocomposites with different volume fractions.]

**Figure 1**: Breakdown strength (left) and energy density (right) of BaTiO$_3$/PI nanocomposites for 0% to 20% volume fraction of BaTiO$_3$ at different temperature.

For all the samples tested, the minimum breakdown strength occurred at 20%, 120°C, with 200 MV/m and 6.88 J/cm$^3$; at 50°C with 249 MV/m and 9.63 J/cm$^3$. The maximum energy densities occurred at 10%, 100°C and 20 Hz with 14.39 J/cm$^3$ and 279 MV/m; at 1 kHz, 20%, up to 75°C with at least 9.05 J/cm$^3$ and 235MV/m. This represents an overall improvement of breakdown strengths for nanocomposites incorporating a high dielectric filler ceramic/polymer capacitor, since reported values do not exceed 250 MV/m [3]. Additionally, at 1kHz the results did not exceed reported values of PVDF with 10.4 J/cm$^3$, the decrease is 7.5%, but is 7025% greater than the 1.2 J/cm$^3$ energy density at 640 MV/m for commercial BOPP [3].

**References**


A Basic Introduction To Graphene And Its Application In Graphene Composites

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Abstract: Graphene, a single layer of carbon atoms, has received great and increasing attention in the science and engineering community over the past few years. The reason is because of graphene’s unmatchable mechanical strength, electrical and thermal conductivity. There is great desire to utilize graphene’s properties in practical applications, thus graphene materials, such as graphene composites, are being fabricated and studied. Graphene is typically produced in low yielding amounts, but chemical means offer the ability to produce relatively large amounts of graphene oxide, which can be reduced into graphene, thus making graphene a more accessible, and feasible engineering material. A main challenge of fabricating graphene composites is achieving even dispersion of the graphene throughout the composite. A solution to this challenge comes from the use of a stabilizer polymer, polyvinylpyrrolidone (PVP), which allows for the successful implementation of graphene in graphene/epoxy composites. The main motivation and goal of the authors is to use a high-yielding chemical method to produce graphene oxide, which is further reduced to graphene, and utilize the graphene in the fabrication of graphene composites.

Keywords: graphene, graphene oxide (GO), graphene composites.

Introduction

Graphene is one of the many physical forms (allotropes) of elemental carbon. It is a planar monolayer of carbon atoms arranged into a tightly packed two-dimensional honeycomb lattice, and it is the basic building block for graphitic materials of all other dimensions. Graphene can adsorb and desorb various atoms and molecules, thus creating an existence of graphitic derivatives [1]. The particular structure of graphene contributes to its particular and extraordinary characteristics. Electrons in graphene behave like massless relativistic particles which contribute to graphene’s peculiar properties such as an anomalous quantum Hall effect and the absence of (electron) localization [2]. Additionally, the structure of graphene gives it phenomenal mechanical, electrical and thermal properties as well as other interesting properties (such as the quantum Hall effect) that are outside the scope of this paper. Electrically, graphene is more conductive than any other substance known, its mechanical strength is 200 times greater than that of steel at a sixth of the weight, and its thermal conductivity is greater than that of diamond [3].

What constitutes graphene as a true 2-dimensional material? It has been shown through research that the electronic structure of graphene rapidly evolves with the number of layers, thus, this criterion would establish a 3-dimensional limit of 10 layers, by which then, graphene would be considered a thin graphite film [4]. Only graphene, and to a good approximation, its bilayer has simple electronic spectra: they are both zero-gap semiconductors (they can also be referred to as zero-overlap semimetals) with one type of electron and one type of hole [4]. For three or more layers, the spectra become increasingly complicated: several charge carriers appear, and the conduction and valence bands start to notably overlap [4].

Properties

The investigation of pristine graphene has brought about incredible property discoveries. An extremely high charge mobility of 230,000 cm²/Vs has been reported [2]. Graphene’s charge carriers exhibit giant intrinsic mobility, have zero effective mass, and can travel for micrometers without scattering (at room temperature); graphene can sustain current densities six orders of magnitude higher than that of copper [1]. Estimated experimental thermal conductivity of single-layer (pure defect free) graphene is a record high of ~3000 W/mK to ~5000 W/mK [2]. After carbon nanotubes, graphene has been reported to have the highest elastic modulus and strength [2]. Researchers have determined the intrinsic mechanical properties of single, bilayer, and multiple layers of graphene. A single, defect free graphene layer is predicted to show the highest intrinsic tensile strength: E~1 TPa, and σ~130 GPa [2]. Due to these amazing properties, pristine graphene has obtained...
a great deal of attention, especially for its conducting capabilities which give graphene great potential in electronics and heat-dissipation applications. However, the low yield production of pristine graphene makes it unfeasible for large yield and budget production of practical graphitic derived components. Graphene Oxide (GO) can be produced in relatively large quantities at a lower cost, while its properties still showing potential for practical applications especially upon reduction, which produces Reduce Graphene Oxide (RGO). As fabricated, GO is found to be insulating due to the presence of oxidized functional groups [2]. The controlled reduction (thermal or chemical) process results in the removal of oxidized groups causing GO to regain most of its electrical conductivity, however, not all of the oxidized groups will be removed and the remaining groups will still limit the electron transport properties of RGO. Depending on the level of reduction, the conductivity of RGO can vary from 0.05 to 500 S/cm [2].

**Fabrication**

Researchers have found many ways to fabricate graphitic material. Few, and single-layer transferable graphene nanosheets were first obtained by mechanical exfoliation ("Scotch-tape" method) of bulk graphite, and by epitaxial chemical vapor deposition [5]. The approaches mentioned are preferred for the high quality graphene produced, but yield very small amounts. Chemical means provide the ability for bulk-scale production of graphene materials. The authors’ goal is to further advance the status of graphene a feasible engineering material so that is not hopelessly scarce and expand its utilization for practical applications. Thus a chemical fabrication approach that can yield higher amounts of graphene is preferred here. A chemical approach to graphite exfoliation uses strong oxidizing agents to yield graphene oxide (GO), a nonconductive hydrophilic carbon material; upon reduction, GO can be transformed back into a conductive graphitic material. The chemical approach followed here is the Improved Hummer’s method (the most common method used today) developed by Marcano et al [5]. Advantages of the improved method are a higher yield, a simpler fabrication procedure, no toxic gas evolution during preparation, and equivalent conductivity upon reduction [5]. Once reduced, the graphene oxide resembles a black powder. This form will allow the authors to utilize the graphene for the production of graphene based composites.

**Composites & Applications**

As previously stated, the mechanical exfoliation of graphene is not suitable for large scale production, while chemical oxidation of graphite into graphite oxide offers an easy path to obtain graphene oxide in large quantities that can be reduced chemically, electrochemically or thermally into graphene [2]. The bulk production of GO and RGO thus allows research to be conducted on graphene based composites. Graphene shows promise in the use as filler for polymer matrix composites. Its reinforcement can offer exceptional properties in composites and applications in the fields of electronics, aerospace, automotive, and green energy [2]. Graphene aids in the increase of mechanical properties of a composite, due to the effective load transfer between graphene and polymer, however the most appealing property enhancements that graphene contributes to composites is the increase of electrical and thermal conductivity in otherwise insulating polymer matrix materials. When used as fillers in an insulating polymer matrix material, graphene may greatly enhance the electrical conductivity of the composite; these composite materials can be used for electromagnetic shielding, photovoltaic devices, sensors, and conducting paint [2]. The use of graphene to increase a polymer composite’s thermal conductivity may open the opportunity of that composite for applications in electronic circuit boards, heat sinks, and light weight high performance thermal management systems [2]. Despite graphene’s amazing thermal conductivity, the thermal conductivity increase of graphene composites is not as high as that of the electrical conductivity increase; typically an increase of the thermal conductivity is of the order of 4, whereas the increase in electrical conductivity is in the order of 15-19 [2]. Overall, the increase in mechanical, thermal, and electrical properties that graphene gives to composites allows for potential graphene composite applications in high-strength, light-weight structural polymer composites for automobile, aerospace, and thermally conductive support in the electronic industry for thermal management, as well as applications of graphene/polymer composites in energy storage, electrically conductive polymers, antistatic coatings and electromagnetic interference shielding [2].

Probably the biggest challenge in graphene composites is the effective and even dispersion of graphene. Graphene tends to agglomerate in solvents and composites mainly due to the strong van der Waals forces.
Agglomeration is a problem because as the graphene clumps up with itself, it begins to lose its special properties that separate it from graphite. To counter this, researchers such as Green et al have used a wide range of solvents using a stabilizing polymer [3,6]. Green et al has made the use of polyvinylpyrrolidone (PVP) as a stabilizing polymer. PVP plays an effective role in graphene/PVP/epoxy composites. It successfully stabilizes graphene and acts as a means for efficient load transfer between the graphene and the epoxy matrix [6]. PVP-stabilized graphene is aggregation-resistant and allows for excellent dispersion in both the resin and final composites [6]. The superior dispersion quality resulted in excellent nanofiller/matrix load transfer with a 38% increase in strength and a 37% improvement in modulus for a 0.46% graphene loading while the electric conductivity increased seven orders of magnitude when compared to the baseline epoxy sample (a highest electrical conductivity value of $10^{-5}$ S/m was reported) [6].

Green et al used pristine graphene in their experiments, the motivation of the authors is to be able to produce substantial amounts of RGO, and incorporate a method similar to Green et al in order to produce and test graphene-composites whose end-purpose will be practical engineering applications.

Fig. 1. Reduced graphene oxide obtained from Hummer’s Improved Method.

Fig. 2. Graphene hexagonal honeycomb structure. Image from: http://www.ewels.info/img/science/graphite/graphene.gif.

References

Flexible Super-capacitor for Energy Storage Application

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1 Introduction

Electrochemical super-capacitors have become one of the most important topics in both academia and industry as novel energy storage devices because of their high power density, long life cycles, and high charge/discharge efficiency. Recently, there has been an increasing interest in the development of multifunctional structural energy storage devices such as structural super-capacitors for applications in aerospace, automobiles and portable electronics [1-3]. These multifunctional structural super-capacitors provide lighter structures combining energy storage and load bearing functionalities. Due to their superior materials properties, carbon fiber composites have been widely used in structural applications for aerospace and automotive industries. Besides, carbon fiber has good electrical conductivity which will provide lower equivalent series resistance; therefore, it can be an excellent candidate for structural energy storage applications [2]. Hence, this paper is focused on performing a pilot study for using nanowire/carbon fiber hybrids as building materials for structural energy storage materials; aiming at enhancing the charge/discharge rate and energy density. This hybrid material combines the high specific surface area of carbon fiber and pseudo-capacitive effect of metal oxide nanowires which were grown hydrothermally in an aligned fashion on carbon fibers. The aligned nanowire array could provide a higher specific surface area that leads to high electrode-electrolyte contact area and fast ion diffusion rates. Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD) measurements were used for the initial characterization of this nanowire/carbon fiber hybrid material system. Electrochemical testing has been performed using a potentiogalvanostat. The results show that gold sputtered nanowire hybrid carbon fiber provides 65.9% better performance than bare carbon fiber cloth as super-capacitor.

2 Experimental Procedure

2.1 Carbon fiber/Zinc oxide nanowire hybrids Synthesis

The ZnO nanowire growth is a two-step hydrothermal growth method including seeding and nanowire growth. Briefly, ZnO nanoparticle seeds were first synthesized in an organic solution, and then the seeding process was performed to coat ZnO nanoparticles onto carbon fiber cloth. The seeded carbon cloth was transferred to ZnO nanowire hydrothermal growth solution at elevated temperature and atmospheric pressure. After the nanowire growth, the nanowire/carbon fiber was rinsed extensively and dried in air for super-capacitor assembly.

ZnO seed particles

Carbon cloth (made of carbon fiber, diameter ~7 µm) of 50 mm X 30 mm was glued (Devcon, 5 minutes epoxy) on the edges. Then carbon cloth was first cleaned in bath sonication (Branson, 2510). Acetone, Deionized water (DI) and ethanol were used as cleaning solvent. Carbon cloth was placed in a beaker with cleaning solvent and bath sonication was performed for 10 minutes using each solvent. Then carbon cloth was dried at ambient temperature in open air. The clean carbon cloth was taken on a glass petri dish to
soak in the nanoparticle solution for 10 minutes and subsequently annealed on a hot plate at 150 °C for 10 minutes to enhance adhesion between the substrates and nanoparticles. This soaking and annealing was repeated two more times to ensure the mass coating of ZnO nanoparticle all over the carbon fibers.

**ZnO nanowires**

After seeding, hydrothermal growth of ZnO nanowires was performed using a low temperature hydrothermal method detailed elsewhere. Briefly, an aqueous solution of 25 mM zinc nitrate hexahydrate (Zn(NO$_3$)$_2$•6H$_2$O, 99.9% purity, Sigma-Aldrich), 25 mM hexamethylenetetramine (HMTA) (C$_6$H$_12$N$_4$, 99.9% purity, Sigma-Aldrich) and 5-7 mM Polyethylenemine (PEI, Branched) were prepared at room temperature. Carbon fiber cloth was immerged in growth solution when the temperature was at 85 °C. The time duration of this growth was 2 hours for all the carbon fiber samples. After the reaction had been completed, carbon fiber samples were taken out of the solution and rinsed with DI water and dried at 100 °C on a hot plate for 2 hours.

**2.2 Super-capacitor fabrication**

A two electrode testing set up was prepared because it provides most accurate measure for an electrode’s performance for electrochemical capacitors. Both bare carbon fiber (CF) and ZnO NWs on carbon fiber samples were sputtered with gold (Au) for 120 seconds to prepare four kinds of electrodes, i.e., a) carbon fiber (CF), b) carbon fiber coated with Au (CF-Au), c) ZnO nanowires on carbon fiber (ZnO-CF), and d) ZnO nanowires on carbon fiber coated with Au (ZnO-CF-Au). An aqueous solution of 5.5 M KOH was prepared for electrolyte and Celgard 3501 was used as separator.

**3 Results**

The morphology of zinc oxide nanowires grown on carbon cloth was analyzed with scanning electron microscope as shown in figure 1A. As indicated by the figure, ZnO nanowires were grown uniformly throughout the carbon fiber. The nanowires had a length between 1 to 3.14 µm and diameter between 40 to 110 nm. No residue or flower was found.

The XRD scan results of the ZnO nanowires on carbon cloth are shown in figure 1. The asterisk (*) mark peak represent carbon of rhombohedral crystal structure. The scan result matches with the standard card JCPDS (01-075-0444) and has lattice parameters of
a=2.29597, b=2.29597 and c=10.15404. The rest of the peaks other than the asterisk marked represent zinc oxide which match with the standard card JCPDS (01-070-8070). The lattice parameters for hexagonal zinc oxide are a=3.24890, b=3.24890 and c=5.20490. No other peaks are found which indicates the sample has only zinc oxide and carbon. The sharp peaks with good intensity assure high quality crystals.

Figure 2. Typical cyclic voltammograms of (a) CF (b) CF-Au (c) CF-ZnO (d) CF-ZnO-Au electrode supercapacitor & galvanostatic charge discharge curve at 56 μA within a voltage window of 0-0.5 V for (e) CF (f) CF-Au (g) CF-ZnO (h) CF-ZnO-Au electrode super-capacitor.

The performance of the super-capacitor was analyzed using constant current charge discharge curve (CC curve) and cyclic voltammetry (CV) plot for four types of samples which were prepared. Specific capacitance was calculated from the discharge slope (dV/dt) of CC curve. Equation 1 was used for calculating the specific capacitance.

\[ C_s = \frac{\Delta I}{\Delta t} \frac{m}{\Delta V} \]  

Carbon fiber coated with gold (CF-Au) has a specific capacitance value of 2.35 F/g which is about 7% higher than that of bare carbon fiber (CF) (2.2 F/g). ZnO NWs on carbon fiber could provide more surface area for the pseudo-capacitance of the electrodes, therefore, provided 16% higher specific capacitance (2.55 F/g) than CF. Highest specific capacitance value was obtained from ZnO NWs on carbon fiber coated with gold which showed about 65.9% higher value (3.65 F/g) than CF.

4 Conclusion

Carbon fiber coated with ZnO nanowire electrode was successfully synthesized for supercapacitor application which shows better performance than bare carbon fiber. Future works need to be done for lowering the ESR which will enhance the capacitance value.

References

Conceptual Design to Fabricate Smart Parts for High Efficiency Energy System Using Electron Beam Melting

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1 Abstract

The energy system components with embedded piezoceramic sensor or altogether “smart parts” can provide real time performance feedback, and can assess risk factors in running condition of the system. The fabrication of “smart parts” using electron beam melting technology (EBM) provides the added benefit of making complex geometries without or little post-process (e.g. machining). The main focus of this paper is the conceptual methodology necessary to fabricate “smart parts” in multiple steps by using the EBM process. Registration challenges related to the multi-step EBM process are addressed in this paper as well. The multi-step EBM process will enable the possibility of fabricating complex Ti-6Al-4V parts with embedded piezoceramic sensors.

2 Introduction

The “smart parts”, with embedded piezoceramic sensors, is a novel approach to fabricate energy system components (e.g. gas turbine blades, exhaust tubes, drills in oil exploration, etc.) using EBM technology. EBM technology uses electron beam to fabricate parts in layer by layer fashion. During the building process, an interruption has to be done to insert the piezoceramic sensors along with wiring system, and then, fabrication continues to finalize the “smart parts”.

Previously, several researchers worked on pausing different additive manufacturing technologies. Some of the works were related to either multi-material system, or electronic components insertion during pause. Terrazas et al. [1] introduced a fabrication method of multi-material parts (cylinders) built with Ti-6Al-4V and copper in both Z, and X directions using EBM technology. A mask plate was machined, and undersized 13\textmu m compared to the previously built Ti-6Al-4V cylinders and those cylinders were press fit into the mask plate. After that, the part made of copper was built on top of Ti-6Al-4V cylinders. An average misalignment of ~70\textmu m was found for the center of copper cylinder from that of Ti-6Al-4V cylinder. It was reported that the centering of the electron beam during the copper fabrication was one of the reasons for misalignment. Two sets of samples were prepared: 1) as-fabricated and 2) EBM fabricated, and HIPed. The microstructure showed a bonded interface within Ti-6Al-4V and copper. HIPing showed an increase of the transition zone between the two joined materials. Hardness measurements showed higher values for the HIPed specimen when compared to the as-fabricated part. In addition, higher hardness for Ti-6Al-4V and lower hardness for copper were found when compared to standard EBM fabrication of those materials. Aguilera et al. [2] described the fabrication of an electromechanical device (a motor) with process interruption for manual insertion of components during the building. A material extrusion based machine, uPrint Plus (Stratasys Inc., Eden Prairie, MN) was used for fabrication.
EBM fabrication implies the continuous and complete build of parts without interrupting the process. Nonetheless, the fabrication of “smart parts” needs to be done in multiple steps in order to insert the piezoceramic sensor, and wiring system. Based on previous work done by various authors, preliminary concept design can be depicted as follows. First, the initial build of the cavity needs to be fabricated and paused afterwards. Then, piezoceramic sensor along with electrical wiring system would be inserted into the cavity. Finally, the build would be resumed to fabricate the entire part. The entire process can be referred as a “stop and go” process and will be discussed in section 3.3. The multi-step or “stop and go” process by EBM will make possible the fabrication of “smart parts”, to acquire information or data from the piezoceramic sensor.

3 Materials and Methods

3.1 Materials

The entire part will be built with Ti-6Al-4V, commonly used material in EBM system. Two types of build plates will be used: regular stainless steel (SS) start plate and CNC machined SS mask plate.

3.2 EBM system

EBM, an additive manufacturing (AM) process, uses a high energy electron beam operating at 60 KeV to fabricate parts in layer by layer fashion. Each layer undergoes preheating followed by melting, according to the geometry of computer aided design (CAD) model of that particular layer. After finishing up this layer, a new layer of powder (layer thickness of 70 µm) is placed using raking mechanism installed inside the build chamber of the EBM system. This process continues until the part is finished. The entire process is performed under vacuum (~10^-4 Torr) to avoid deflection of the electron beam [3, 4].

3.3 “Stop and Go” process

As previously mentioned, the fabrication of the “smart parts” is comprised with the interruption of the EBM process in order to insert the piezoceramic sensor and wiring system. To achieve this goal, the “stop and go” process has been developed, and consists of six steps. A schematic diagram of process sequence is shown in Fig. 1 to demonstrate the fabrication of a simple design of “smart parts”.

Step 1: EBM fabrication of bottom part (box shaped with cavity) using Ti-6Al-4V along with “insert” part.

Step 2: Stop the process and assemble the piezoceramic sensor and wiring into the cavity of bottom part, followed by “insert” part.

Step 3: Fabricate mask plate using CNC machining.

Step 4: Set up the entire part with the use of the mask plate.

Step 5: Continue building top part.

Step 6: Clean up the finished “smart parts” and perform sensor testing.
Fig. 1. Process sequence in the fabrication of “smart parts” using EBM technology

The “insert” part would be designed oversize to make tight fitting with the cavity, and the mask plate would be built undersized compared to the bottom part. This will help maintain fitting during thermal expansion and avoid the misalignment of the bottom part during fabrication of “smart parts”. Additionally, an intended hole will be made for sensor wiring. The registration issue would be compensated by calculating the thermal expansion of materials and offsetting accordingly in the CAD design.

Conclusion

The work presented here demonstrates a conceptual design for fabricating “smart parts”. The ultimate goal of this work is to fabricate real life energy system components using the EBM, which will enable the possibility to get in-situ information in real time. This work will enable the possibility of multi-step EBM fabrication, which can be a guideline for future production of embedded electronics, focusing different applications.

References


Analysis of ferroelectric ceramic fabricated by binder jetting technology

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keywords: binder jetting technology, ceramics

Abstract

ExOne’s system binder jetting technology was used to fabricate 3D structures of two different ceramics for applications that include dielectric capacitors, sensors, and integrated circuits. This project presents results obtained for BaTiO$_3$ fabricated by the M-Lab system[1] and the continuation of the work which consists on the fabrication of alumina (Al$_2$O$_3$) samples. An organic binding agent was utilized during the printing process and later burned out at ~600°C prior to sintering. Multiple building parameters and sintering profiles were analyzed and compared in an attempt to obtain dense parts.

Introduction

Barium titanate (BaTiO$_3$ or BTO) has been a ceramic of interest for several applications, due to the fact that it possesses good ferroelectric, piezoelectric and dielectric properties. Some applications include semiconductors with positive temperature coefficient of resistivity (PTCR) [2] dynamic access memories (DRAM), and IR sensors [3] Alumina (Al$_2$O$_3$) has been subject to study due to its good thermal and electrical insulation properties. Common applications include bearings and pressure-resistant windows [4]. Some other uses include wireless temperature sensors, which are highly sensitive on the porosity of the part since the changes in dielectric properties depend highly on the water uptake of the pores[5].

This project involves the fabrication of BTO and alumina samples using binder-jetting technology with the purpose of developing a wireless temperature sensor. Samples were built using different building parameters and sintering profiles, this in order to develop parts with a density close to theoretical density. The density of the samples was measured using ASTM B962-13 standard. Further studies included scanning electron microscopy of both the powder and the fabricated samples.

Methodology

ExOne M-Lab system is a binder jetting technology that uses an organic agent to bind layers of ceramic powder. The thickness of the layer is a parameter that can be adjusted to meet fabrication requirements dependent on powder
Another parameter that can be modified is the binder saturation. The binder used for this project is ethylene-glycol-monomethyl-ether. The binder is cured at 195°C after building, and then burned out during the sintering process. The system has two chambers which move in the X-direction, the build and the feed (Fig 1). The feed provides the powder and the build is the chamber where the powder layer is spread from the feed by a roller. The binder is later deposited by a printhead that moves in the Y-direction.

Simple geometries were fabricated using the M-Lab system. For BTO, an initial thickness of 15µm was used. These samples were too brittle to test, so the thickness was doubled to 30µm, regardless of initial powder size (spherical ~1µm in diameter powder). Experiments with three different binder saturations were performed: 60%, 75% and 120%. After fabrication, the binder was cured at 195°C with a hold of two hours. After curing, the samples were cleaned and then sintered. The recommended sintering temperature is around 0.8T_m, so based on this, three different sintering temperatures were used. The holding time for all three profiles was 4 hours, and the temperatures used were 1260°C, 1330°C and 1400°C. A hold at 600°C was used to burn out the binder. After sintering, density values were obtained based on Archimedes’ principle. This standard requires samples to be weighed in air, then impregnated with oil at 7kPa for 30 minutes. The next step consists of measuring the weight in air and suspended in water. A small drop of soap was added to the water in order to reduce the surface tension. This gives off two measurements, referred to as sintered density (out of the furnace) and impregnated density (after oil impregnation). The next step of the analysis of the samples was performed by using a TM-1000 Tabletop SEM with an accelerating voltage of 15kV. No sample preparation was required.

For alumina, the layer thickness used was 60µm, this based in the powder particle size (angular powder size was ~66µm). Based on the results obtained from the BTO parameters, the binder saturation used for the alumina samples was 60%. The same process for curing was performed on the alumina samples. For the sintering process however, the profiles had to be modified since T_m=2040°C. The sintering temperature for the three profiles was 1600°C, and the holding times were 8, 15 and 30 hours. Further experiments included density measurements using the standard described previously and scanning electron microscopy.

### Results

Different binder saturations and sintering profiles were used and the obtained density was compared to select the best build parameters. Table 1 shows that the highest value obtained from BTO was from sample built using 60% binder saturation sintered at 1260°C for 4 hours. The low values obtained can be attributed to the fact that the samples were

<table>
<thead>
<tr>
<th>Material</th>
<th>Sintering Profile</th>
<th>Sintered Density (g/cm³)</th>
<th>Impregnated Density (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BTO</td>
<td>1260°C for 4 hrs</td>
<td>1.30</td>
<td>1.58</td>
</tr>
<tr>
<td>BTO</td>
<td>1330°C for 4 hrs</td>
<td>1.22</td>
<td>1.39</td>
</tr>
<tr>
<td>BTO</td>
<td>1400°C for 4 hrs</td>
<td>1.21</td>
<td>1.37</td>
</tr>
<tr>
<td>Alumina</td>
<td>1600°C for 8 hrs</td>
<td>1.41</td>
<td>1.85</td>
</tr>
<tr>
<td>Alumina</td>
<td>1600°C for 15 hrs</td>
<td>1.41</td>
<td>1.88</td>
</tr>
<tr>
<td>Alumina</td>
<td>1600°C for 30 hrs</td>
<td>1.41</td>
<td>1.84</td>
</tr>
</tbody>
</table>

Table 1. Density measurements obtained
exposed to pressureless sintering. Since the samples fabricated using 60% saturation used less binder than those fabricated using a higher saturation, less empty spaces were left behind. Figure 2 shows an SEM image of a BTO sample that was sintered at 1260°C. These samples showed less open spaces between grains than samples sintered at higher temperatures, thus yielding a higher density.

![Fig 2. BTO sintered at 1260°C for 4 hours.](image)

For the alumina samples, the binder saturation used was 60%, since it resulted in a higher density for BTO samples. Samples were then sintered using profiles mentioned before and the density results obtained are discussed in Table 1. Figure 3 shows alumina after sintering at 1600°C for 30 hours. A possible sintering Stage I is observed, meaning that for fully sintered parts a longer holding time or higher temperature are required. A higher density value is obtained from samples sintered for 15 hours, this can be attributed to the fact that samples are developing a film between powder particles when sintered at this profile, nonetheless, further investigation is required.

![Fig 3. Alumina sintered at 1600°C for 30 hours.](image)

### Conclusion
It can be observed that a higher density is achieved with Alumina samples (50%) but BTO samples (26%) possess better dielectric properties. Based on this assumption, further work consists of fabricating alumina samples and infiltrating with different concentrations of BTO. The goal is to combine both properties observed in these ceramics while obtaining dense-functional parts.

### References

Literature Review of Mechanical Testing of Ti-6Al-4V Fabricated by Electron Beam Melting

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Keywords: Electron-beam melting (EBM), Titanium-6Al-4V, Fatigue

ABSTRACT

Electron beam melting (EBM) of Ti-6Al-4V powder is used to create complex, three dimensional components layer by layer using CAD. With the ability to create layer by layer components, the possibility to fabricate complex “smart parts” is increased. “Smart parts” are energy systems components containing embedded sensors. The “smart parts” will be fabricated with the use of necessary methodology of EBM multi-step process, and stop-and-go techniques necessary for the embedment of sensors into Ti-6Al-4V parts. This paper focuses on the literature review of mechanical testing (tensile and fatigue) of Ti-6Al-4V fabricated by EBM. In addition, found results will be implemented for the aforementioned fabrication of sensor embedment and its mechanical testing.

Introduction

“Smart parts” are referred to energy systems with embedded piezoceramic sensors to provide high temperature and pressure feedback from exhaust tubes, gas turbine fuel/air premixers, and many more. By doing so, parts will fabricated at a lower cost with a more efficient process, reducing the energy cost of production. Using electron-beam melting (EBM) for the creation of these components, a method to stop the process, in the middle of the built, and allow the insertion of a sensor to create “smart parts” will be attempted. Once the “smart parts” have been created, mechanical testing will be performed to characterize its properties. This paper provides a literature review of mechanical testing performed previously on Ti-6Al-4V fabricated by EBM. Found results will be implemented for the testing of the “smart parts” previously mentioned, and by using the W. M. Keck center facilities located at the University of Texas at El Paso, fabrication of “smart parts” by EBM will be attempted.

Methodology

EBM is a well-developed technology for 3D fabrication, where metals parts are created layer by layer. Powder metal is melted using an electron beam at roughly 30mA in a vacuum chamber of
The desired design is created as a .stl file and further layered by the arcam builder software. EBM has the ability to work with a range of metal powders. According to Arcam, the standard materials that are used for EBM include: Ti-6Al-4V, Ti-6Al-4V ELI, Titanium grade 2, and cobalt-chrome ASTM F75. EBM can be described as a three-step process: 1) the powder is spread on even distributed layers using the raking system, for Ti-6Al-4V the layer created is 70µm thick [3]; 2) the electron beam then strikes the powder with a low intensity to sinter it; 3) the powder is then melted with the full power of the electron beam to achieve a fully dense layer. The build table is then lowered one layer thickness and the three steps repeat for every layer until the 3D part is completed. Several are the advantages to using EBM for the fabrication of metal parts [3], the most important being the ability to fabricate non-conventional geometric parts (such as mesh and foam structures) that can be used for high strength to weight ratio applications.

**Experimental Procedure**

Mechanical properties of the EBM fabricated Ti-6Al-4V is a concern for the “smart parts” that will be created for this project. Tensile and fatigue testing will be performed on samples with and without piezoceramic sensors.

Murr, *et al.*, reported tensile testing results for wrought and annealed Ti-6Al-4V and compared them to that of EBM fabricated Ti-6Al-4V. The ultimate tensile stress (UTS) of EBM fabricated Ti-6Al-4V ranges from 1.1 to 1.4 MPa, while annealed Ti-6Al-4V reported a UTS value of 0.95MPa, and for wrought a UTS value of 1.29 MPa was obtained. Percent Elongation was also reported and values obtained are as follow: 25% elongation for EBM fabricated Ti-6Al-4V, 14% elongation for annealed specimens and 15% for wrought [1].

Microstructure is also an important feature that needs to be addressed for this project. The microstructure of the EBM fabricated Ti-6Al-4V, wrought, and annealed Ti-6Al-4V processes were all examined. Murr, *et al.*, analyzed the microstructures of all three specimens. First microstructure examined was the top portion of the EBM sample, showing a α and β Widmanstätten structure. Then the bottom portion of the EBM sample microstructure was analyzed, where a finer lamellar microstructure is present. The average acicular α-plate thickness of the top and the bottom portions of the EBM sample were measured and compared, the top α-plate thickness value were 3.2 µm, while the corresponding average acicular α-plate thickness was 1.6 µm in the bottom section (Figure 1). The microstructure of wrought Ti-6Al-4V has an acicular α-plate microstructure, and for annealed Ti-6Al-4V there is a equiaxed α/β microstructure [1].

![Optical metallographic images comparing acicular α-plates in the top (~1 cm) section of EBM-2 samples (a) and the bottom section (~1 cm) (b). Magnification is the same as shown in (a) [1].](attachment:image.png)
Fatigue Testing
Fatigue life is another characteristic of the components that will be evaluated for “smart parts”. Rafi, et al., performed fatigue testing on Ti-6Al-4V for two different additive manufacturing processes. The two processes that were compared were EBM and selective laser melting (SLM). Both samples were tested using ASTM standards E466. The tests were performed at a stress ratio of 0.1, frequency of 50Hz, and stopped after $10^7$ cycles; if the sample did not fail. Figure 2 graphs the results of the tests that were conducted. Fig. 2a) plots the results of SLM and b) represents the results obtained for the EBM process. The information that is plotted on graph b) indicates that EBM Ti-6Al-4V has a fatigue limit of 340MPa, while annealed Ti-6Al-4V has a fatigue limit of 510MPa [2].

![Fig. 2: S-N curve showing fatigue behavior of Ti64 samples (a) SLM and (b) EBM [2].](image)

Conclusion
Future investigation would need to be conducted in order to achieve successful “smart parts”. Once the “smart parts” have been created, the mechanical properties, including tensile, hardness, and fatigue life will be tested and compared to data obtained from literature.

References
4 Conclusion

Surface diffusion of adatoms plays an important role in modeling selective-area growth. MD is able to solve the position of atoms as a function of time. This method allows us to solve the diffusivity of Cd and Te by tracking of time the displacement of the atoms at various substrate temperatures.

Acknowledgement

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References


Calculating Diffusion Coefficient of Cd and Te on CdS and SiO2 by Molecular Dynamics Simulations

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1 Introduction

Cadmium telluride (CdTe) is a p-type semiconductor used for low-cost CdTe/CdS solar cells to convert sunlight into electrical energy. While semiconductor theory predicts that these devices have a theoretical value of 29\% of efficiency, the maximum recorded efficiency for this technology only 19.6\% [1]. One cause for the lower efficiency is the high density of crystal defects in the CdTe film which is mainly attributed to the large lattice mismatch (10\%) between CdTe and CdS. Nanoscale selective-area growth is one method that is being studied to reduce the defect density. In this method, CdTe is deposited on a SiO\textsubscript{2}/CdS/SnO/glass substrate in which the SiO\textsubscript{2} is nanopatterned with an array of holes. This allows the CdTe to selective deposit on the CdS but not the SiO\textsubscript{2} [2]. This is presumably due to the larger surface diffusion length (diffusivity) of Cd (and Te) adatoms on SiO\textsubscript{2} compared to on CdS. This hypothesis is being studied by solving the continuity equation, using appropriate boundary conditions for a patterned surface, and applying distinct Cd and Te diffusivities. However, the diffusivities of Cd and Te are not well known. Molecular dynamics (MD) can be used to visualize the motion of individual atoms during simulated growth and therefore calculate the diffusion length of Cd and Te on SiO\textsubscript{2} and CdS at various temperatures. In this paper, a method to obtain the diffusivity of the Cd and Te adatoms on both CdS and SiO\textsubscript{2} substrates at different environments by molecular dynamics simulations is presented.

2 Method

The diffusion length is expressed as

\[ L = \sqrt{D\tau} \] (1)

where D is the diffusivity in m\textsuperscript{2}/s and \( \tau \) is the residence time in seconds. Molecular dynamics essentially determines the motion of atoms in the vapor, surface and solid during simulated growth by solving Newton’s equation of motion for each atom. An interatomic potential is used to determine the repulsive and attractive forces between atoms as a function of distance between atoms, temperature, and time. Due to the large number of atoms and corresponding equations that need to be solved during crystal growth simulation, super computers are used to obtain results within reasonable time frames. In this study, the Large-Scale Atomic/Molecular Massively Parallel Simulator LAMMPS molecular dynamics program [3] was used to perform the deposition simulation. LAMMPS was used to explore the crystal growth behavior of CdTe on two distinct substrates: CdS and SiO\textsubscript{2} on the Virgo computer cluster at UTEP.

The substrate used in this simulation is a CdS wurtzite lattice [0001]. The molecular system consist of 7200 atoms. This computational structure (15.8 x 1.6 x 9.11 nm\textsuperscript{3}) (See Figure 1) with lattice constants a=4.58 Å and c=7.48 Å was used to observe the diffusivity on surface. The
substrate temperature was set to 1200K. It will deposit 800 atoms above the substrate at random positions. The simulation will release the atoms directly to the substrate surface. We computed the mean-squared displacement (MSD) to determine the displacement of the deposited atoms.

![Image](image_url)

*Figure 1. Initial CdS wurtzite structure and atoms of Cd and Te.*

### 3 Results and discussion

Data obtained from the simulations are visualized and analyzed for diffusivity of the CdTe in the surface layer. Separate depositions with 200 atoms was released each 100ps. Figure 2 shows Cd and Te atoms on the CdS surface. Next, we plot the mean-square displacement (MSD) of the atoms of the system as function of time and shown in Figure 3. Diffusivity is determined by the slope of the MSD versus time.

![Images](image_url)

*Figure 2. Diffusivity CdTe on CdS substrate, at time of a) 0ps, b) 104ps, c) 204ps, and d) 400ps.*

![Graph](image_url)

*Figure 3. MSD of CdTe atoms during 400ps simulation. Depositions was set each 100ps.*
4 Conclusion

Surface diffusion of adatoms plays an important role in modeling selective-area growth. MD is able to solve the position of atoms as a function of time. This method allows us to solve the diffusivity of Cd and Te by tracking of time the displacement of the atoms at various substrate temperatures.

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References


