Integrated theoretical, computational and experimental programs to understand and develop the physics, chemistry, materials and processing that confidently meet critical naval needs

**High Performance Functional Materials**
- Power Generation & Energy Storage Materials
  - Electrochemical Materials
  - Polymeric and Organic Materials
- Piezoelectric Materials

**High Performance Structural Materials**
- Structural Metallic, Structural Cellular and Composite Materials
- High Temperature Turbine and Ultra-high Temperature Materials
- Welding and Joining
- Optical Ceramics

**Environmental Quality**
- Anti-fouling Release Coatings
- Solid and Liquid Waste Treatment

**Optimization from Design thru System Life**
- Computer Aided Materials Design
- Scarce Element Mitigation Strategies
- Solid Mechanics and Fatigue
- Non-Destructive Evaluation and Prognostics
- Additive Manufacturing
- Integrated Computational Materials Engineering
Mechanical Properties, e.g.

Common Engineering Concepts?

EBSD image

MIL-HBK-5H

Table 5.4.1.9(O). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

<table>
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<tr>
<th>Specification</th>
<th>AMS 4931 and MIL-T-20046, Comp. AB-1</th>
<th>MIL-T-20046, Comp. AB-1</th>
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<tr>
<td>Condition</td>
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<td>Thickness, in.</td>
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Adapted from D. Furrer, April 2013

Distribution Statement A: Approved for public release (DCN 43-2780-17)
Integrated Computational Materials Engineering (ICME)

Integrated Computational Materials Engineering provides the framework for understanding and communicating evolution of microstructure, material properties and behavior, material design capability, component performance, and component degradation.


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Dielectric Materials for Capacitive Energy Storage

Focus on improving energy storage density through improved dielectric materials for cost effective, large scale systems.

- Multi-scale computation and computer aided discovery based on permittivity and breakdown characteristic optimization
- Theory guided synthesis, characterization and feedback to theory
- Understanding thermal stability
- Minimizing loss

Major Participants
Penn State
CWRU and NRL
General Atomics, PolyK Technologies, Polymer Plus

Progress
- Discovered and developing dielectric films based on terpolymer fluoropolymers, multilayer extrusion, aromatic thioureas and related systems and group IV metal containing dielectrics (Si, Sn, Ge).
- Maturing multilayer extruded films and higher temperature fluoropolymer blend systems for optimized manufacturing
- Nanocomposite approach to reduce leakage current at high temperatures

Capacitors can make up 50% of the volume of power storage and conditioning systems.
Focus on understanding and optimizing the mesoscale and bulk properties of materials with internal structures at the nanoscale.

- Both structural and multifunctional nanomaterials, metals and ceramics
- Multi-scale computation guiding and describing processing and stability of structures at mesoscale and beyond
- Advanced characterization techniques
- New synthesis and assembly routes
- Novel assembly and manufacturing, including repair tools

Major Participants
Rutgers U                    Purdue U
U Colorado                  MIT
Johns Hopkins U             NRL
UC Berkeley                 NAVSEA
Integran Technologies

Progress
- Formulated a Frenkel pair model to explain anomalous lattice expansion observed during electric-field-assisted sintering of oxide ceramics.
- Maturing Electroplasticity as a metal forming technique.
- Exploring shipboard in situ repair of Cu-Ni piping in heat exchangers, fire suppression mains, etc
AM of Structural Non-oxide Ceramics by Photothermochemically-assisted Reaction Bonding

**Objective**
- Develop photothermo-chemically-assisted reaction bonding techniques for additive manufacturing (AM) of non-oxide ceramics.

**Approach**
- A binder-free, dense ceramic formed from precursor materials.
- Binary phases will be converted to the same non-oxide ceramic.
- Process optimization will be accomplished using neural networks.

**State of the art:**

(Z. C. Eckel et al., *Science* 2016)

(Distribution Statement A: Approved for public release (DCN 43-2780-17))
Focus on understanding and obviating the damage mechanisms active in the severe temperature and chemical environment in which Naval turbine engines operate to optimize performance (thrust:weight ratio) and confidently minimizing maintenance requirements.

- Create and develop materials for ship and aero turbine engine operating temperatures up 1500oC.
- Characterizing the thermodynamics and kinetics of materials interactions affected by temperature, environment, materials chemistry, and stress
- Integrated theoretical and experimental approach to computational models for design of materials, materials processing, and life prediction
- Establish tools to understand and quantify highly coupled degradation mechanisms as a function of numerous variables (e.g. temperature, temperature gradients, stress, contaminants, interdiffusion, interfacial mobility, thermal stability, oxide growth rates, corrosivity)

**Progress**

- Characterization and understanding of coating strength and grain structure influence on fatigue life under conditions where hold times are present
- Strong bond coats and interdiffusion zones increase life, particularly for thin sections
- Improved understanding of CMAS interactions with TBCs/EBCs leading to materials solutions for enhanced coating durability and improved life prediction models, discovery of CMAG in ship engines

Inherently multidisciplinary, multi-component for confident turbine efficiency in a hostile environment.
Objective / Goal
Lower Total Ownership Costs (TOC) by developing advanced materials package capable of minimum 3X engine life over current gas turbine (GT) materials set

Recent Accomplishments
• Universities beginning coating development, burner rigs at UVA and UC Irvine are running coating/alloy tests evaluating corrosion resistance in RR baseline and new advanced coating systems
• RR and GE evaluating disks, alloy and coating

Technical Approach
• Leverage ONR gas turbine materials development program
• Shipboard GT Marinization Package for Higher Temperature, Higher Pressure Operations
  – Marinized High Temperature Rotor Alloys
  – Oxidation/Hot Corrosion Resistant Blade/Vane Coatings
  – Marinize Single Crystal Alloys

Key Milestones / Projected Transition
• Integrated upgrade materials package (marinized rotor, marinized single crystal alloys, oxidation/hot corrosion-resistant coatings)
• NAVSEA specification to backfit upgrade package during depot MTBR and for future USN/USMC new construction engines

Project TOTAL SAVINGS = $65M to $76M/year
Focus on establishing the scientific basis for processing confidence, enabling the rapid qualification and certification of AM components, and expanding the design space for AM fabrication including tailored geometries, microstructure and properties.

- Multi-scale predictive models for AM materials and processes, enabling engineering applications
- Materials optimized explicitly for AM for Naval applications
- Harnessing the highly coupled and complex design, structure, process, and performance relationships for AM fabricated parts through computational modeling and materials characterization
- Establish verification and validation for robust computational models to enable an accelerated qualification framework for AM parts

Microstructural complexity must be understood and controlled.

**Progress**

- Large scale AM for molds and tooling applications; including development of a full scale optionally manned technology demonstration
- Flight critical AM part demonstration
- Understanding impact of residual stress
Focus on establishing the scientific basis for the discovery of new materials, improving existing materials, and rapid insertion (ICME)

- High Throughput Screening
  - Automation & new algorithm
  - Off-lattice scaling
- Informatics
- Multiscale Simulation

Progress

- Rensselaer Materials Informatics Tools now being used by Lockheed-Martin for discovery/design of polymer composites
- AFLOW Automated Flow for Materials Discovery
- RAPPID (phase diagrams): in progress; beta tests 2017
- “Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways” published, 2016
- PROFESS 3.0 (Princeton Orbital-Free Electronic Structure Software) released, 2016

Major Participants

- Princeton, Stanford, Chicago, Brown, Duke, BYU, RPI, Maryland

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Focus on developing and extending the knowledge base for the design of metal alloys, alloy processing and joining approaches for accelerated engineering application in high-performance, affordable systems.

- Structure→processing ↔ properties ↔ performance relationships for materials
- Characterization and quantification of microstructure features and their statistical correlations
- Advanced tools for characterization, physical and computational
- Development of model-based design and optimization approaches for materials and systems
- Verification and validation of data and models to ensure robust design
- Uncertainty quantification

**Progress**
- Advanced high-strength steel for CVN flight-deck applications
- Demonstration of Ti-alloy valve cores via advanced powder processing
- Shipyard demonstration of friction-stir joining of steel plate

Creep Damage during simulated fire exposure in Al 5083: SEM and X-ray Tomography

Capturing the heterogeneity of alloys for improved component design and asset management.

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ICME for Design & Prediction

Salient Microstructural Feature Size & Distribution

Processing Models and Microstructure Evolution Models

Alloy and Process Design Tool Feedback

Manufacturing Optimization

Damage Models for Prognosis

Multi-Mechanism Failure Prediction

Damage Initiation Probability

Physical Models for Damage Nucleation

Ti 4 processing effects

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Asset Management in Digital Age

Cyber-Physical Environment will enable state-awareness for optimal design, manufacture, maintenance and capability assessment of materials, components, systems and platforms.

Platform State Awareness

Material State Awareness

Prognostics

Approach:
Start with the 60% solution, aim high, and iterate frequently.
Prognostics: Integrated Hybrid Structural Management System (IHSMS)

Capabilities

- Gross Weight (GW) and Center of Gravity (CG) measurements
- Load/load-history tracking for dynamic components and airframe hot spots
- Damage detection and monitoring
- Damage growth and criticality prediction
- Micro-climate environmental monitoring
- Expanded fleet/asset management

Developed and demonstrated a single integrated structural health fleet management system for the CH-53K platform, combining sensors and algorithms to track and assess (cycle-by-cycle) loads, damage, environment, usage and health of the rotor and fuselage.

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Fiber Optic Sensors

Enabling multiple simultaneous measurands (Temp, Strain, Vibration, Impacts, Acoustic Emissions)

<table>
<thead>
<tr>
<th>Measurand</th>
<th>TOW</th>
<th>Temp</th>
<th>Flutter</th>
<th>Strain</th>
<th>Accel.</th>
<th>Vibrat.</th>
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<td>10 – 100</td>
<td>100 – 1k</td>
<td>1k – 10k</td>
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FOBG Strain Sensors have cross sensitivity with Temperature

<table>
<thead>
<tr>
<th>$\varepsilon$ (micro-strain)</th>
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<td>100</td>
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</table>

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Multi-Performer Programs

MURIs:

• *Materials for Smart Multifunctional Superstructures* [(MS)²], FY18-22
• *Advanced Optical Materials that Create Force from Light*, FY18-22
• *In situ Microstructural and Defect Evolution below the Micron Scale in as-Deposited Metal Alloys*, FY18-22
• *Predicting and Validating Pathways for Chemical Synthesis*, FY18-22
• *Phase Change Materials for Photonics*, FY17-21
• *Dynamic Events at Ultra High Temperature and Pressure*, FY17-21
• *Physics, Chemistry and Mechanics of Polymer Dielectric Breakdown*, FY17-21
• *The Science of Entropy Stabilized Ultra-High Temperature Materials*, FY16-20
• *Metalloid Cluster Networks*, FY15-19
• *Computational and Experimental Methods towards Understanding the Chemistry and Physics of Materials >2000°C*, FY15-19
• *Exploring the Atomic and Electronic Structure of Materials to Predict Functional Material Properties*, FY14-18
• *Understanding Energy Harvesting Mechanisms in Polymer-Based Photovoltaics*, FY14-18
• *Replacing Strategic Elements in DoD Materials*, FY13-17
• *A New Way to Dissipate Shock Wave Energy from Detonations*, FY12-17
• *Biological Stability of Future Naval Fuels and Implications for the Biocorrosion of Metallic Surfaces*, FY11-17
• *Atomic-scale Interphases: Exploring New Material States*, FY11-17

BRC:

*A Scientific Basis for Enhanced Manufacturability with Electrical Currents*, FY17-20