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This Presentation Does Not Contain Any Proprietary of Confidential Information
Agenda

- Goals and Objectives
- SMMR I Review Comments & Responses
- Technical Barriers
- Technical Approach
- Accomplishments
- Publications/Presentations
- Collaborations/Interactions
- Plans for Next Fiscal Year
- Summary
OVT Goals & Project Objectives

Relevant OVT Goals:
- Develop Advanced Technologies to Dramatically Reduce Fuel Consumption & Emissions in All Petroleum-Fueled, Personal Vehicles Through Improved Energy Efficiency
- Develop Technology to Improve Commercial (Mid- & Heavy-Duty) Vehicle Fuel Economy Through Improved Energy Efficiency (Double Fuel Economy in Mid- & Long-Term)

Project Objective:
- Develop Waste Energy Recovery Systems Capable of Increasing Vehicle Fuel Economy by up to 10%
- Provide Technical Leadership to OVT Waste Energy Recovery & Utilization Project (John Fairbanks – Project/Technology Manager)
- Project Focusing on Advanced TE Materials & Systems & New Initiative Development

Project Initiated in FY 2007
- $100K Authorized to PNNL in October 2008
- $200K Authorized to PNNL in May 2007
  - High ZT Materials Validation With NASA-JPL & ORNL
  - PNNL / University Collaboration in Advanced TE Materials & Systems
SMMR I Reviewers’ Comments

- Generally Quite Positive Comments From SMMR I
  - High Relevance
  - Providing High-Quality Technical Support to the DOE-OVT & Project Subcontractors

- 2007 SMMR I Reviewers Indicated Need for:
  - Adding Project Cost Effectiveness Analysis
  - Adding Focus on Transient System Analysis & More Parametric Optimization
  - Ability/Mechanism to Interact More Closely With Industry Given Industry IP Concerns

- Response to 2007 SMMR I Reviewer Comments
  - Items 1 & 2 Would be Great Additions to the Project if Only We Had the Funding to Support – Discussions Underway with OVT
  - There is a Mechanism Available to Us to Work More Closely With Industry, But It is Partially a Funding Issue ($ to Engage) & Effort to Overcome IP Inertia
    - Interaction With the BSST Team in the Last Year (Analysis Details, Advanced TE Materials)
    - Interaction With GM/GE Team in the Last Year (HVAC Systems, Probabilistic Design)
    - Constant Level of Effort to Identify Ways/Methods to Provide Technical & Programmatic Support to Industry
Technical Barriers

- Low Component & System Performance
  - Advanced TE Materials Need to Exhibit Higher ZT’s Over the Anticipated Temperature Ranges
    - $ZT \geq 1.5$ @ $400 - 873$ K Really Needed to Achieve Project Goals and Make Industry Business Cases
  - Advanced TE Materials MUST be Replicated and Validated at Multiple Laboratories / Locations
  - Advanced TE Materials MUST be Demonstrated and Validated in Advanced TE Devices & Systems

- High Component & System Costs
  - Advanced TE Systems Costs Must Be $< \sim$1/W

- Component & System Durability & Reliability Not Demonstrated
Technical Approach

- Advanced TE System-Level Analysis Integrated With Advanced TE Materials & Testing R&D
  - Monitor, Review & Incorporate Advanced TE Materials R&D Results Across Multiple Government/Industry Projects
    - National / International Projects
    - DOE
    - DOD - DARPA & ONR
    - Industrial Research & Development
  - Evaluate Advanced TE Materials Against Project Goals
  - Provide Verifying Design Optimization & Performance Analyses
  - Evaluate Advanced TE Devices/Systems Against Project Goals
    - TE Device Integration with Heat Exchangers
    - Vehicle Drive Cycle Effects on TE System Integration
    - Vehicle System Integration

- Light-Duty / Heavy-Duty Vehicles
- Industry/Government Agency Collaborations & Interactions
Accomplishments & Contributions

- PNNL Served as Project Technical Lead
  - Attend & Support Project Reviews With Technical Leadership & Guidance
  - Provided Technical Comments & Guidance to OVT Project Manager, NETL Program Managers, and Subcontractors
    - Advanced TE Materials
    - Advanced TE System Analysis
    - Advanced TE Testing Systems
  - Coordinated With ORNL Thermoelectrics Program
  - Coordinated With Outside Government Agency Programs
- Provide Scientific & Analytic Foundation in Accomplishing Project Goals & Evaluating Project Technical Progress
- Independent, Normalized Evaluation of Project Results to Gauge Project Progress
- Technical Accomplishments & Contributions Illustrated In Following Slides
  - Provided Technical Knowledge & Leadership Exemplified Below to OVT Project Manager & NETL Program Managers
Typical System Efficiency – Power Maps

- Integrated TE System Analysis
  - TE Device
  - Heat Exchangers

- System η-P Map
  - Identifies System Tradeoffs
  - Identifies Power Output Potential
  - Performed for Various TE Material Combinations
  - Quickly Shows System Impact of Increasing Materials ZT

- System Cold-Side Cooling Needs
  - Identifies Challenging Cooling Conditions
  - Also Performed for Various TE Material Combinations

- Project-Specific Analyses
  - GM / GE System
  - MSU System
  - BSST / BMW System
TE Device Specific Power Density, Power Flux & Volumetric Power Density

- (P/m), (P/A), & (P/V) Analyses Coupled with $\eta$ - P Maps
  - Illustrates Critical Relationships
  - Illustrates Critical Tradeoffs
- (P/m), (P/A), (P/V) All Follow Similar Lines on $\eta$ - P Maps
- $\eta$ - P - (P/m) or $\eta$ - (P/m) Clearly Shown on One Map
- Prime Example of Depth of System Understanding @ PNNL
  - Analysis Performed for Any Advanced TE Material of Interest
  - Quickly Shows System Impact of Increasing Materials ZT

Analysis Performed for Any Advanced TE Material of Interest

(P/m)=Specific Power Density [W/kg];
(P/A)=Power Flux [W/cm²];
(P/V)=Volumetric Power Density [W/cm³]
Thermoelectric / Thermal Systems Interactions

- Available Hot-Side Heat Exchanger Flux Dictates Much About the System Potential Power, Mass, & Volume
- Dependent on TE Materials – Couples TE Materials & System Design

Example Hot-Side Heat Exchanger Heat Flux
TE Cooling Systems – Automotive HVAC

Automotive HVAC is Critical
- Solid State System to Eliminate Greenhouse Gas Impacts
- Key Enabling Technology for Hybrid Vehicles

Analysis Performed to Support Automotive HVAC Initiative Development
- Quantify Performance Expectations vs. Materials
- Integrate TE Materials with System Expectations
- Quantify Key Impact Phenomena
- Evaluate Design Configuration Differences
- Establish Project Goals
- Establish Project Targets

Overarching System-Level Analysis to Separate Fact vs. Fiction

ZT ~ 1 TE Materials

Maximum COP At Qc TEHVAC3panel, \( U_{A_h} = 100 \text{ (W/K)} , U_{A_c} = 16.67 \text{ (W/K)} \), \( T_{ex} = 311 \text{ (K)} \), \( T_{amb} = 297 \text{ (K)} \), md

- \( T_{cold} = 295 \text{ (K)} \)
- \( T_{cold} = 290 \text{ (K)} \)
- \( T_{cold} = 282.5 \text{ (K)} \)

3 TEC Design Point

Cooling Capacity (watts)

Maximum COP

Temperature (K)

ZT - 1.0 TE Materials
Evaluate TE Cooling System Characteristics & Parametric Relationships

- Critical Relationships / Trends
- Critical Tradeoffs

Establish Project Goals & Targets

Establish Fact vs. Fiction

Optimal COP for $T_{amb} = 295$ K and $T_{cabin} = 293$ K

$UA_c = 60$ W/K
PNNL is leading an effort to validate (or not) latest thin-film Si/SiGe materials.

- NASA-Jet Propulsion Laboratory
- Oak Ridge National Laboratory
- NIST

Early results with JPL (September 2007):
- Contractor supplied 100 Si/SiGe layers (10 nm thick) on 400 um Si substrate
- High Seebeck coefficient & low electrical resistivity measured
- However, thick Si substrate significantly clouded the results
  - Thick Si substrate in the measurement circuit – not acceptable

PNNL recommended a 4-step test validation process:
- Perform testing on Si/SiGe multi-layers on SIMOX samples – electrically eliminate Si
  - JPL
  - ORNL
- Develop multi-layer electrical model of test sample configuration
  - Guide / provide critical interpretations of test results
  - Draw conclusions on important test circuit parameters & their impact on test results
- Perform thermal efficiency &/or $\Delta T_{\text{max}}$ tests @ TE couple level
- External validation of thermal efficiency / $\Delta T_{\text{max}}$ tests ASAP
**Mission**
- Grow micro & nano R&D supporting high tech industry
- Increase and accelerate commercialization of micro & nano technology
- Develop micro & nano technology leaders

**Research thrusts**
- "Green" nanomaterials and nanomanufacturing
- Microtechnology-based energy and chemical systems
- Nanolaminates, materials/processes for nanoelectronics
- Nanoscale metrology

**Facility Network**
- CAMCOR - UO Materials Characterization and Nanofabrication
- MBI – OSU/PNNL Micro Chemical and Energy Devices & Micro/Nano Fabrication
- CEMN - PSU beam metrology & nanofabrication

Oregon’s first “Signature Research Center”
Expanding Oregon’s role as micro & nano R&D nexus with largest micro-nano R&D community in U.S.
Multiple Rattlers in Skutterudites: $R_xR_y'Co_4Sb_{12}$

- PNNL & ONAMI Collaboration on Advanced “Multiple - Rattler” Skutterudites & Advanced Oxides

**Multiple Rattlers:**

| $R^{2+}$: Ba, Sr, Ca, Ag, Pd, |
| $R^{3+}$: La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, In, Sc |

- $In_xCo_4Sb_{12}$ Shows High ZT ~1 at 573 K
- $In_xCe_yCo_4Sb_{12}$ Increases the ZT >1.3 at 573K
- Synthesis of More Rattler Combinations in Progress
- Goal for Advanced Materials
  - ZT ~ 1.6-1.8 @ 600-700 K
  - Similar Materials Confirmed By ORNL and Purdue Univ. Measurements
- Later Focus On Mixed Valent Transition Metal Oxides

**High Performance TE Materials Expected**

- Bulk-Type Materials for Easier Device Manufacture & Integration
- Results Expected At the End of FY 2008
- Expect to Transition Results to Projects As Appropriate & Quickly As Possible
DOE / ONAMI Project (Continued)

Objectives

- Optimize the Synthetic Conditions & Properties of Newly Discovered Thermoelectric Compositions
- Optimize Compositions
- Test & Characterize TE Material Properties (ONAMI & PNNL)
  - Seebeck Coefficient
  - Electrical Resistivity
  - Thermal Conductivity
- PNNL to Characterize System-Level Benefits of Material Compositions in Waste Energy Recovery Applications

- Project Duration: Through FY 2008
- Sponsor: John Fairbanks, Technology Manager, OVT
- FY 2007 Funding: $100K
Publications / Presentations

- **26th International Conference on Thermoelectrics, Jeju, South Korea, June 2007**

- **ASME Energy Sustainability 2007 Conference, Long Beach, CA, June 2007**


- **AIAA International Energy Conversion Engineering Conference, St. Louis, MO, June 2007**

- **Micro Nano Breakthrough Conference, Invited Plenary Session Speaker, Portland, OR, September 2007**
  - Title: Advanced Energy Recovery & Conversion Systems Employing Micro Technology
Collaborations & Interactions

- GM / GE
  - Automotive HVAC Systems & Probabilistic Design
- Michigan State University & Tellurex, Inc.
  - LAST-m TE Material Properties
- BSST, Visteon, BMW
- ORNL
  - Advanced Si/SiGe Thin-Film TE Material Testing & Validation
- NASA-JPL
  - Advanced Si/SiGe Thin-Film TE Material Testing & Validation
- NIST
- ONAMI
  - Joint Project in Advanced TE Materials Development
- ONR DTEC Program Review – August 2007
- Japanese NEDO Delegation – November 2007
- 26th International Conference on Thermoelectrics
  - Japanese METI NEDO TE Project – Japanese Program Managers
  - United Kingdom R&D – UK Program Managers
FY 2008 Plans

► FY 2008 AOP Will Govern Our Activities in FY 08
► Several Technical Ideas Identified for FY 2008 AOP
  ● Provide Project Technical Leadership, Scientific, & Analysis Support
    ■ Advanced TE Materials
    ■ Advanced TE Devices & Systems
    ■ Advanced Testing Systems
  ● Develop Advanced System Concepts
  ● Advanced Analytic Techniques & Methodologies
  ● Develop PNNL / Industry / University Joint Projects on Advanced TE Materials & Systems
Summary

PNNL Provides Support to WHR&U In Several Areas

- Independent WHR&U Project Technical Evaluation & Leadership
- In-Depth Thermoelectric Analysis
  - Advanced TE Power Systems
  - Advanced TE Material Effects
- Advanced Test System Support
- New Project Initiative Development
  - “Initiative” Analytic Justifications
  - New Project Ideas / Concepts to Achieve / Accelerate Goals
- Critical International Collaborations & Interactions
  - Constant State-of-the-Art and State-of-Research Barometer
  - How to Leverage National / International R&D Progress & Successes
- Industrial / Theoretical Experience
  - TE Materials
  - TE Systems
Advanced Thermoelectric System Design

- System-Level, Coupled Design Analysis
  - Hot Side Heat Exchanger
  - TE Device
  - Cold Side Heat Exchanger
- Single & Segmented TE Material Legs
- Temperature-Dependent TE Materials
- Accounts for Hot/Cold Thermal Resistances
- Accounts for Electrical Contact Resistances
- Accounts for HX / TE Device Thermal Losses
- Optimum Heat Exchanger / TE Design
  - Parameters Determined Simultaneously
- Maximum Efficiency & Maximum Power Density Designs Are Possible
- Off-Nominal & Variable Condition Performance Analysis