2008 DOE OVT Annual Merit Review

Combustion & Fuels
Waste Heat Recovery & Utilization Project
Project Technical Lead - Thermoelectric Analysis & Materials

27 February 2008

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This Presentation Does Not Contain Any Proprietary of Confidential Information

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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 ≥ 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 < ~$1/W
- Component & System Durability & Reliability Not Demonstrated

Technical Approach

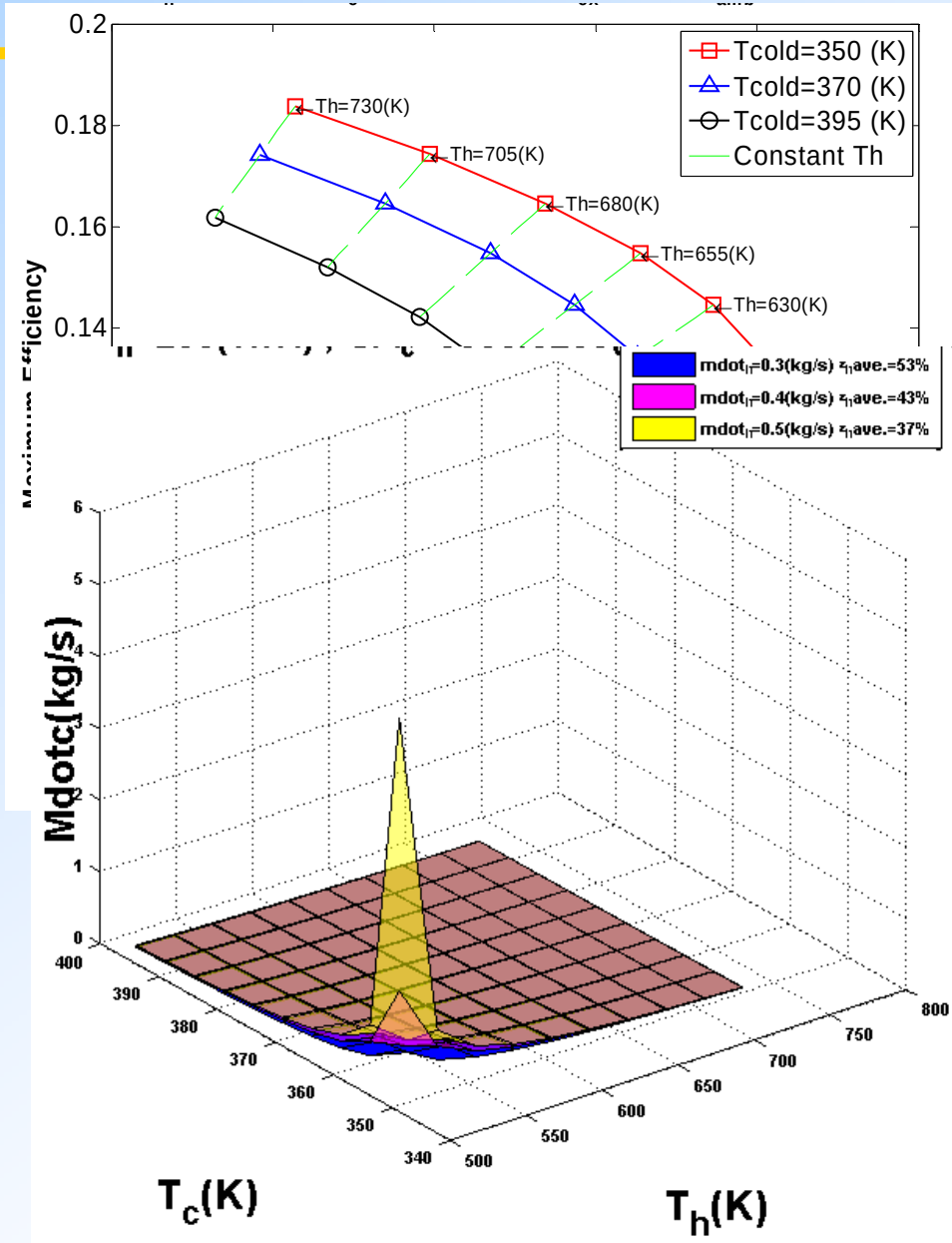
- Advanced TE System-Level Analysis Integrated With Advanced TE Materials & Testing R&D
  - Monitor, Review & Incorporate Advanced TE Materials R&D Results Across Multiple Government/Industry Projects
    - National / International Projects
    - DOE
    - DOD - DARPA & ONR
    - Industrial Research & 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

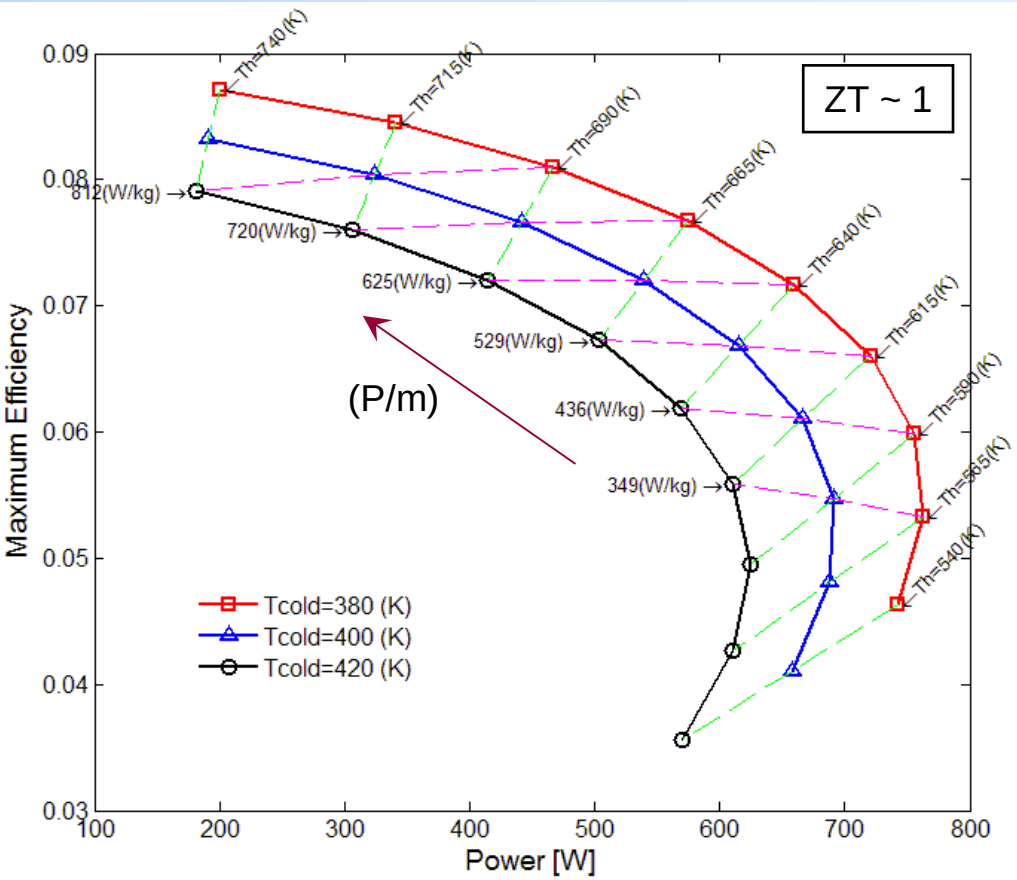
Typical System Efficiency – Power Maps

- 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

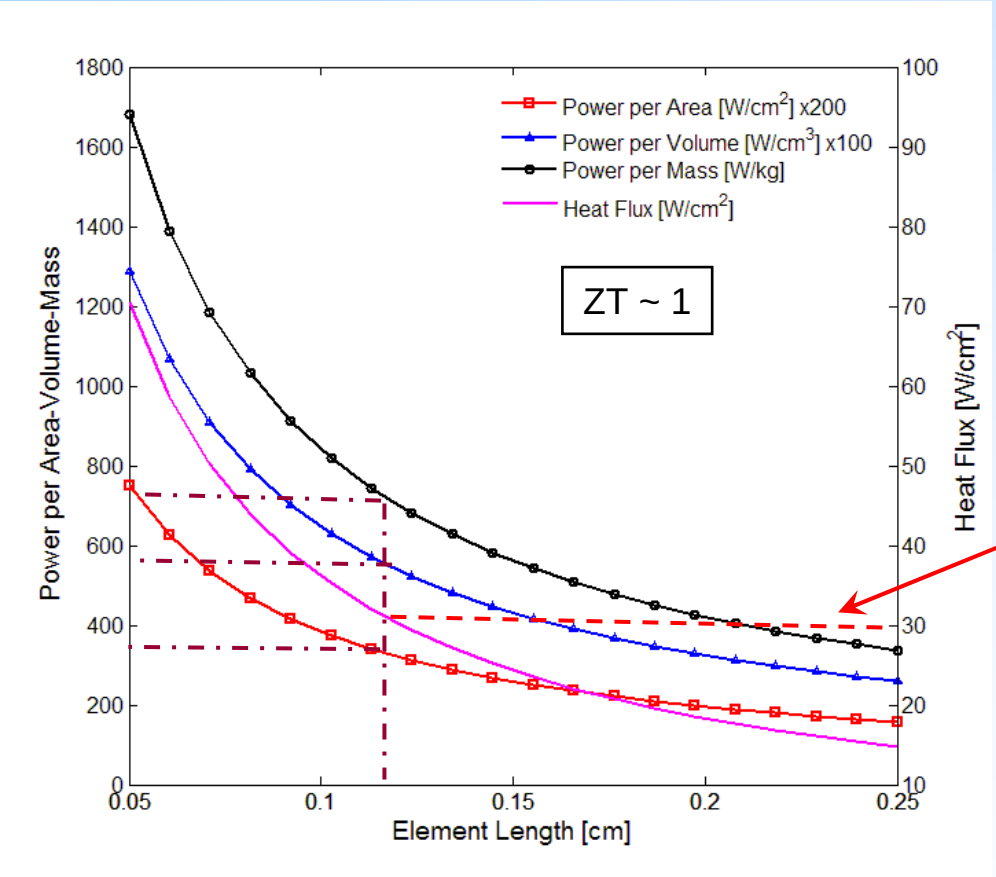
- (P/m), (P/A), & (P/V) Analyses Coupled with η - P Maps
  - Illustrates Critical Relationships
  - Illustrates Critical Tradeoffs
- (P/m), (P/A), (P/V) All Follow Similar Lines on η - P Maps
- η - P - (P/m) or η - (P/m) Clearly Shown on One Map
- Prime Example of Depth of System Understanding @ PNNL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



(P/m)=Specific Power Density [W/kg];
(P/A)=Power Flux [W/cm^2];
(P/V)=Volumetric Power Density [W/cm^3]

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

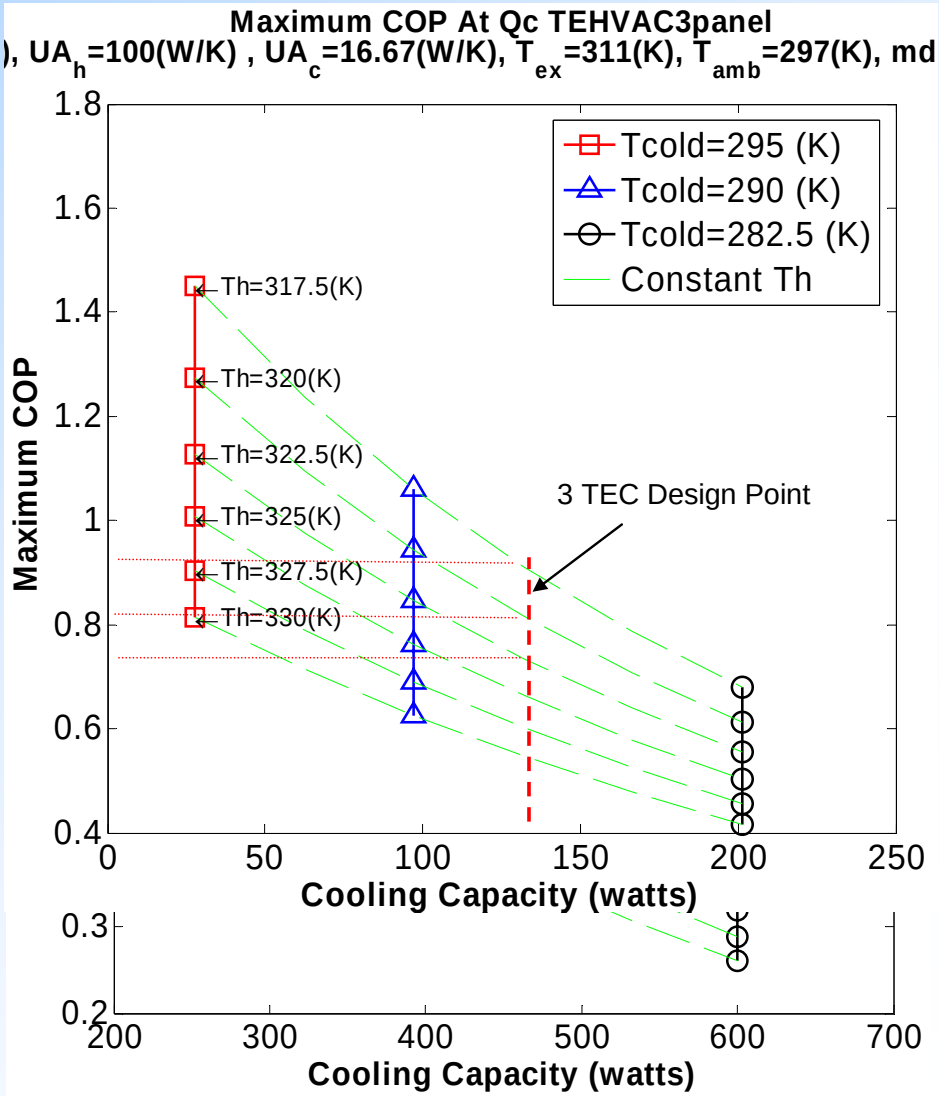


Example Hot-Side Heat Exchanger Heat Flux

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

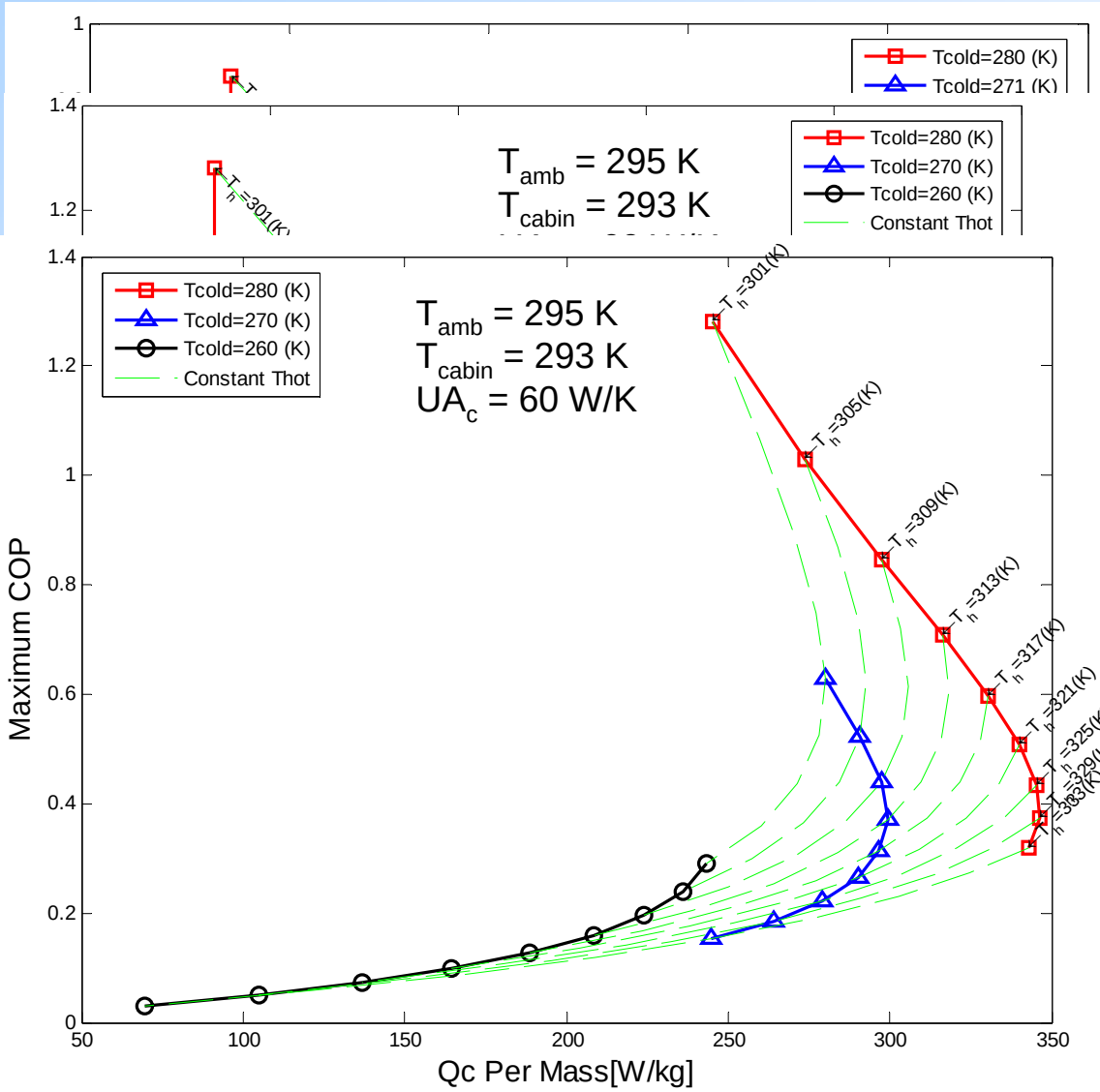
ZT ~ 1 TE Materials



TE Cooling Systems – Automotive HVAC

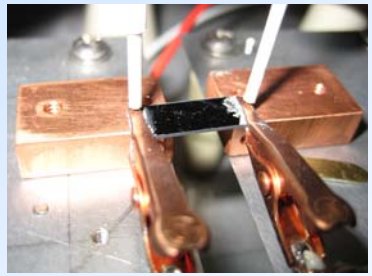
Bi_2Te_3 Materials

- Evaluate TE Cooling System Characteristics & Parametric Relationships
- (P/A), (P/m), & (P/V) Analyses Coupled with COP - Q_c Maps
  - Critical Relationships / Trends
  - Critical Tradeoffs
- Establish Project Goals & Targets
- Establish Fact vs. Fiction

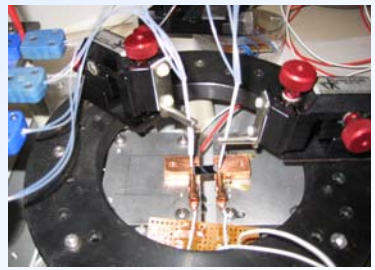


Si/SiGe Thin-Film Material Validation

- 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 ΔT_{max} Tests @ TE Couple Level
  - External Validation of Thermal Efficiency / ΔT_{max} Tests ASAP

ONAMI
OREGON NANOSCIENCE AND MICROTECHNOLOGIES INSTITUTE

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.

Mission –

- Grow micro & nano R&D supporting high tech industry
- Increase and accelerate commerciallization 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

+ HP, FEI, ESI, …
OHSU, PNNL, UO, OSU, PSU

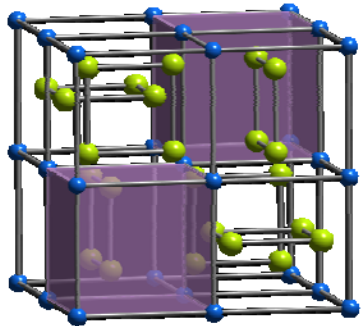
Multiple Rattlers in Skutterudites: $R_xR_y'Co_4Sb_{12}$

- **PNNL & ONAMI Collaboration on Advanced "Multiple - Rattler" Skutterudites & Advanced Oxides**

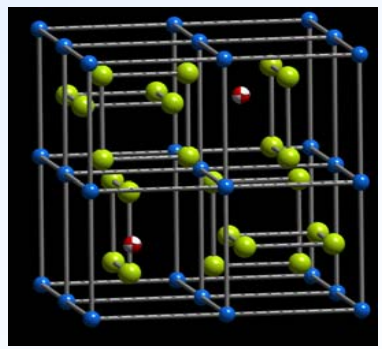
Multiple Rattlers:

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



Co_4Sb_{12}



$R_xCo_4Sb_{12}$

- $In_xCo_4Sb_{12}$ 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
  - Hendricks, T.J. and Karri, N.K., "Design Impacts of Stochastically-Varying Input Parameters on Advanced Thermoelectric Conversion Systems", TE Theories and Phenomena Session, Paper #O-M-1
- ASME Energy Sustainability 2007 Conference, Long Beach, CA, June 2007
  - Hendricks, T.J. and Karri, N.K., "Probabilistic Design & Analysis for Robust Design of Advanced Thermoelectric Conversion Systems", Nano- & Micro-Scale Devices/Energy Systems Session, Paper #ES2007-36085
- *Journal of Energy Resources Technology, ASME, New York, 2007*
  - Hendricks, T.J., "Thermal System Interactions in Optimizing Advanced Thermoelectric Energy Recovery Systems", Vol. 129, No. 3
- AIAA International Energy Conversion Engineering Conference, St. Louis, MO, June 2007
  - Karri, N.K. and Hendricks, T.J., "Probabilistic Modeling Approach to Thermoelectric Systems Design Optimization", Paper #81312
- 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 & Probabilisitic 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
  - Continue Government / Industry Collaborations in TE Materials, Devices & Systems, and Testing

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