An integrated approach towards efficient, scalable, and low cost thermoelectric waste heat recovery devices for vehicles

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NSF/DOE Thermoelectrics Partnership: An integrated approach towards efficient, scalable, and low cost thermoelectric waste heat recovery devices for vehicles

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Overview

Timeline
• Start date: 10/1/10
• End date: 9/30/13
• Percent complete: 14%

Budget
• Total project funding
  – DOE share: $750k
  – NSF share: $750k
• FY10 funding - $0
• FY11 funding - $500k

Barriers
• Barriers addressed
  – A. Cost of TE systems
  – B. Scale-up to a practical thermoelectric device
  – C. Thermoelectric device/system packaging

Partners
• Romny Scientific
  • Thermoelectric materials development
• Project lead – Virginia Tech
Objectives

Practical thermoelectric systems for waste heat recovery in vehicles require advances in materials, thermal management, durability, and metrology.

1. Thermoelectric materials (Romny, Priya)
   - Microstructure design of high-performance oxide thermoelectric materials
   - Isostatic pressing of appropriately scaled silicide materials

2. Thermal management (Ekkad, Huxtable)
   - System level models and experiments to characterize system and predict performance
   - Experiments and models of efficient heat sinks using, e.g., minichannels and swirl jet impingement

3. Interfaces & Durability (Inman, Huxtable)
   - Measurements of adhesion, electrical and thermal transport through interfaces and methods for improvement
   - Effects of vibration, thermal cycling on adhesion & transport

4. Metrology (all)
   - Complete nano-macro TE and structural characterization (HRTEM, TDTR, XPS, Auger, XRD, laser flash, etc.)
Objectives, continued

These objectives are relevant to the Vehicle Technologies program as described below.

1. Thermoelectric materials (Romny, Priya)
   • Our thermoelectric materials are low-cost, abundantly available, scalable, and environmentally friendly, thus ensuring that our devices could be widely deployed in practical applications

2. Thermal management (Ekkad, Huxtable)
   • Heat exchangers are developed that are low-cost, efficient, and appropriately scaled for the specific application

3. Interfaces & Durability (Inman, Huxtable)
   • Parasitic losses through interfaces are examined and minimized
   • System models address durability and lifetime of devices

4. Metrology (all)
   • Evaluation of full structure-property relationships allow for optimization of thermoelectric materials
## Milestones for upcoming year

<table>
<thead>
<tr>
<th>Month/Year</th>
<th>Milestones</th>
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<tbody>
<tr>
<td>August 2011</td>
<td>Complete high temperature thermal conductivity, Seebeck, thermal expansion</td>
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<tr>
<td></td>
<td>and electrical conductivity measurement systems</td>
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<td>October 2011</td>
<td>Complete initial thermoelectric measurements on first round of silicide</td>
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<td></td>
<td>samples from Romny and textured oxides from Priya’s group at VT</td>
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<tr>
<td>November 2011</td>
<td>Complete first dynamic and thermo-fluid system level models</td>
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<tr>
<td>January 2012</td>
<td>Fabricate first round of TE samples using 3-D aerosol printing</td>
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<tr>
<td>May 2012</td>
<td>Prototype system structure and geometry defined</td>
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Layered cobalt oxides, such as Na$_x$CoO$_2$ and Ca$_3$Co$_4$O$_9$, have natural superlattice structure.

**Strategy:**
- We aim to capture the advantages seen in exotic nanostructured materials by developing nanostructured bulk materials that can be fabricated with scalable techniques.
- Design the novel microstructures to control $\sigma$ and $\kappa$ (Textured CaCo$_x$O$_y$ ceramics).
Approach for TE materials development, p. 2

- Textured thermoelectric bulk ceramics
  - Composition: CaCo\(_x\)O\(_y\) Ceramics
  - Template: \(\beta\)-Co(OH)$_2$
  - Target: >90% textured ceramics

For piezoelectric ceramics, we have achieved a 2~5 time increase in \(d_{33}\) by texturing. By artificially texturing materials we aim to allow for rapid, low-cost, and scalable growth of “superlattice-like” efficient TE materials.
Approach for TE materials development, p. 3

- Fabrication 3D-TEG device at micron scales
  - Deposition of Complex patterns
  - Design textured microstructures to control material properties
  - Grow graded structures
  - Direct growth on various substrates

We have made complex structures using 3D aerosol printing
Approach for dynamic system analysis

We start with simple models before going to full finite elements in order to understand the basic phenomena. Models are verified through road tests of instrumented vehicles.

\[ \tau \nabla^2 w(x, y, t) = \rho w_{tt}(x, y, t), \quad x, y \in \Omega \]

\[ \sum (\rho A(x) \frac{\partial^2 w(x, t)}{\partial t^2} + \frac{\partial}{\partial x^2} \left[ EI(x) \frac{\partial^2 w(x, t)}{\partial x^2} \right]) = f(x, t) \]
Approach for thermal management

Finite element models are used to model the thermo-fluid characteristics of a vehicle exhaust system.

Thermoreflectance measurements give insight into interface thermal resistances.

Novel cooling approaches such as swirl jet impingement are evaluated.

Heat exchangers are designed and fabricated in-house at Virginia Tech.
Progress – synthesis of reactive template

Effect of CoCl₂ Concentration on phase and purity of Co(OH)₂ template

**Pure β-Co(OH)₂**

**Pure α-Co(OH)₂**

High aspect ratio (>50) and highly pure β-Co(OH)₂

We have successfully fabricated templates, and have improved our growth process.
Initial work has demonstrated the feasibility of synthesizing matrix powders. We will continue to optimize reaction conditions to improve the purity of Ca₄Co₃O₉ matrix powders.
Progress – synthesis of silicide TE elements

Silicide based thermoelectric ingots that have recently been fabricated using hot pressing by Romny are shown on the right.

Silicide materials provide low mass, are environmentally friendly, low cost, and offer high performance.

This hot pressing fabrication approach can be scaled up to high volume production and can produce TE elements of various sizes and shapes.

Optimizations in particle size, particle size distribution, densification times and temperatures enable performance per cost to be maximized.
Progress – preliminary instrumentation on vehicle

Preliminary temperature and vibrational measurements were performed on a Jeep.

Demonstration done in order to develop and refine real-time data collection on vehicle. These data will be crucial in refining our dynamic models.

Dynamic response of finned heat exchangers examined with a shaker in benchtop experiments.

Note: Cold side heat exchanger to air shown in photo was used only for initial demonstration purposes. Current thermoelectric generator systems use liquid coolant for cold side heat exchanger.
Progress – preliminary analysis of heat exchangers

We use CFD tools to predict thermo-fluid performance of heat exchangers, and lab experiments to verify models. Prototypes have been fabricated and benchmark experiments show favorable results in comparison with commercial models.

Comparison of preliminary heat exchanger designs with commercial model is shown on the right.

CFD model for swirl impingement flow heat exchanger

Example of mini-ribbed heat exchanger design (A) and prototypes (B & C) made through metallic molds. Prototypes are ~ 20 x 60 x 5 mm.
With our thermoreflectance system we can simultaneously extract thermal conductivity and interface thermal conductance. These measurements are critical for evaluating and understanding thermal transport in nanostructured materials.

We can also map thermal conductivity with ~3 μm resolution. This can be useful for measuring local conductivity on cross-sections of graded materials, and thermal interface materials.
Progress – High temperature Seebeck and electrical conductivity measurement system under construction

A high temperature (500 °C) vacuum oven system is under construction.

Robust system will allow for measurements on samples of a variety of shapes and sizes (unlike commercial systems)

Expected to be operational by summer 2011

Measurement system is modeled after system designed and built by Zhou and Uher (Rev. Sci. Instrum. 76, 023901, 2005)
Collaborations

- Our research team at Virginia Tech includes
  - Scott Huxtable: PI, thermal management & system design
  - Shashank Priya: co-PI, materials development
  - Srinath Ekkad: co-PI, heat sinks & thermal management
  - Dan Inman: co-PI, dynamic modeling & durability
- Industry collaborator
  - Romny Scientific (Dr. Andrew Miner, founder & CEO)
  - Romny is providing high quality silicide TE materials as well as critical industry knowledge
- Additional collaborations
  - Doug Nelson (Virginia Tech). Doug is an expert in electric vehicles and is providing general vehicle assistance
  - The Virginia Tech Transportation Institute. VTTI conducts applied research to develop new techniques and technologies to study transportation challenges from various perspectives: vehicle, driver, infrastructure, and environment.
Future work for next year

- Materials development
  - Fabrication of textured $\text{CaCo}_x\text{O}_y$ ceramic TE elements
  - Formation of initial TE elements with 3D aerosol deposition
  - Fabricate prototype TE generator with current silicide materials

- Metrology
  - Complete high temperature Seebeck and electrical conductivity measurement system & fully characterize initial round of materials (including thermal conductivity & ZT)
  - Complete structural characterization (XPS, EDS, etc.) of initial round of materials to develop structure-property relationships

- Thermal management
  - Finish thermo-fluid system model & benchmark with experimental testbed results

- Dynamic system
  - Modeling the combined TEG/heat exchanger/exhaust system dynamic response using substructure techniques
Summary

• We are developing an integrated approach towards the use of thermoelectric devices for waste heat recovery in vehicles that will result in significant improvements in fuel economy and reduction in emissions.

• Our TE materials (e.g. silicides and layered oxides), are abundant, low cost, and non-toxic. Our fabrication techniques are scalable and can produce elements of various shapes and sizes.

• We are developing low cost heat exchangers that are optimized for low pressure drop in exhaust and coolant flows and can be mass produced.

• Our approach includes extensive system level optimization such that TE elements are scaled and carefully matched with appropriately sized heat sinks.

• Quantitative measurements of thermal and electrical contact resistance of interfaces between TE materials, diffusion barriers, brazes, heat spreaders, and heat sinks are used to reduce parasitic losses.

• Complete dynamic analyses including shock, vibration, and thermal stresses are examined in conjunction with experimental measurements on road tested vehicles, in order to address lifetime and durability concerns.