Nanostructured High Temperature Bulk Thermoelectric Energy Conversion for Efficient Waste Heat Recovery

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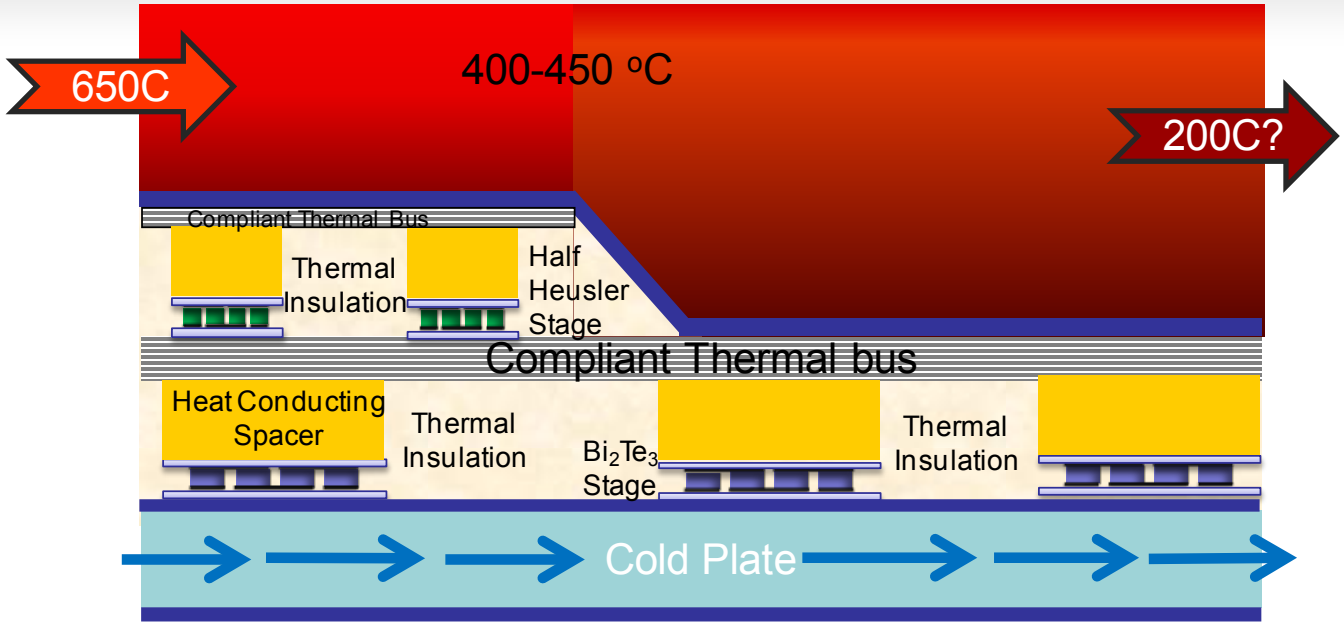
NETL: Carl Maronde

2012 DOE 3rd Thermoelectrics Applications Worshop
March 22, 2012

Outline

- Program Overview
  - Overall Program Goals
  - Team Introduction
- Phase 1 Experimental Details
  - Materials Research
  - Device Fabrication and Testing
  - Heat Exchanger Model and Design
  - Vehicle Model and Baseline Performance Testing

Program Overview



- Proposed two-stage TEG system with half-heusler as the first stage, and Bi_2Te_3 as the low temperature stage. Thermal buses and high thermal conductivity spacers, together with thermal insulation are used to concentrate heat to low-profile generators, significantly reducing the amount of materials used for the TEGs.
- 5% fuel efficiency improvement with TE generator integrated and tested in vehicle platform under US06 drive cycle

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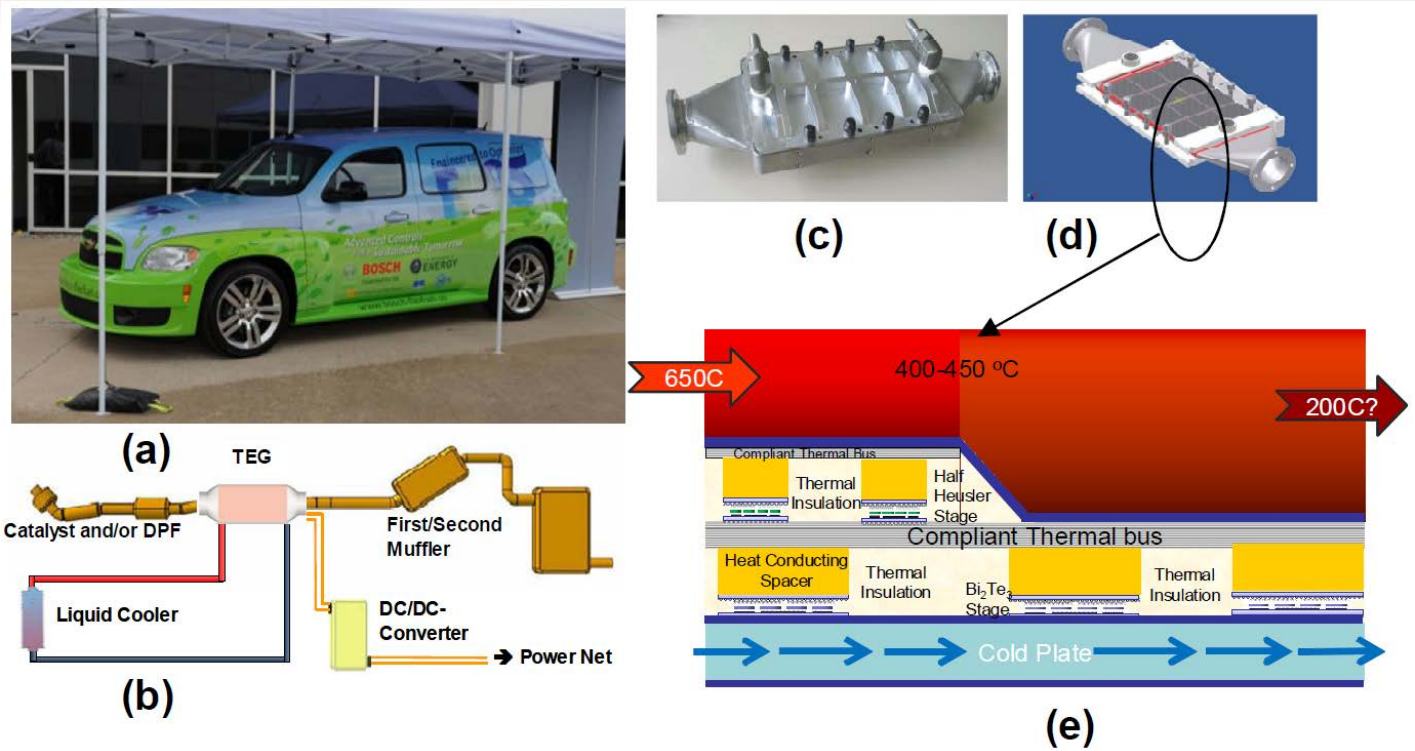
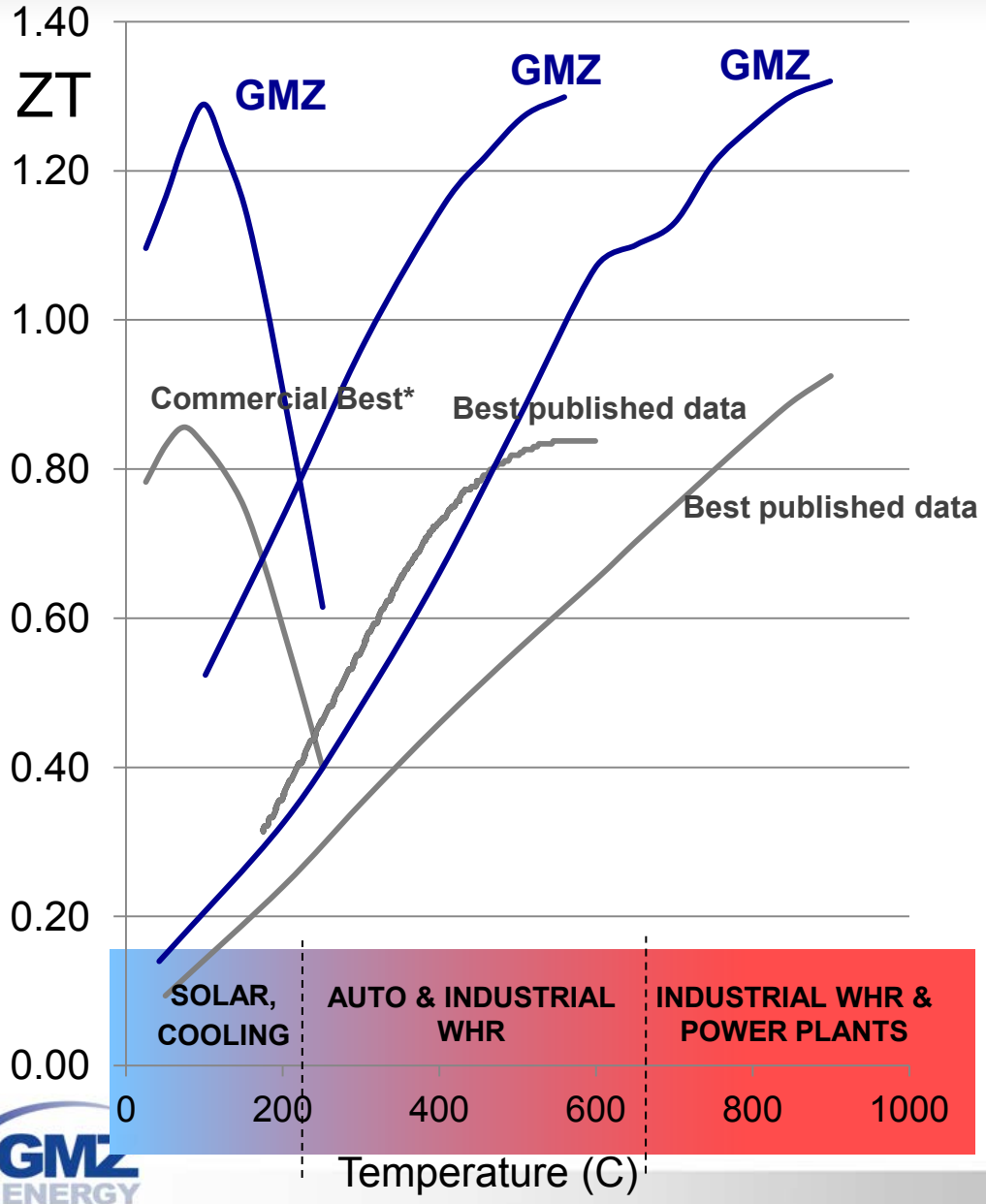
Proposed Program Overview

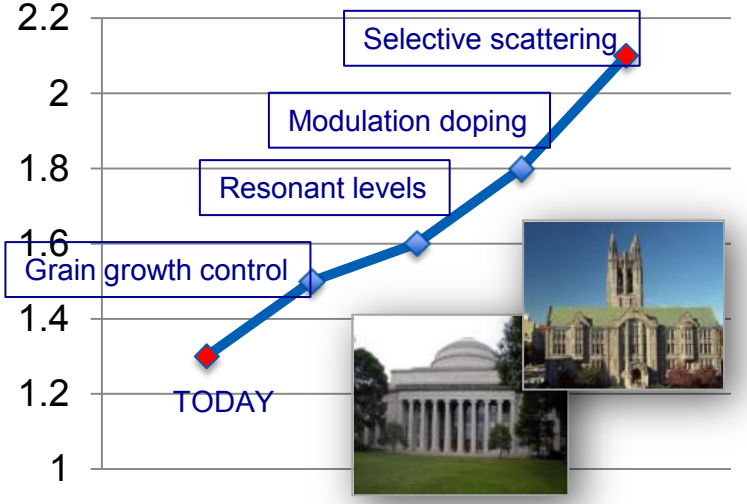


- Proposed cascade TEG system and prototype (a) Chevrolet HHR vehicle, (b) exhaust system, (c) a prototype built at Bosch, (d) and (e) illustration of the two-stage cascade design. Half-heusler serves as the first stage, and Bi_2Te_3 as the low temperature stage. Thermal buses and high thermal conductivity spacers, together with thermal insulation are used to concentrate heat to low-profile generators, significantly reducing the amount of materials used for the TEGs.

GMZ TE LEADERSHIP: Across all Markets



ZT Roadmap: Achieving 2.0



Powerful Technology

- Independent of material family
- Covers all applications & markets
- Sustaining performance advantage

*it is possible to acquire specialty non-commercial material with ZT~1 for 5x cost.

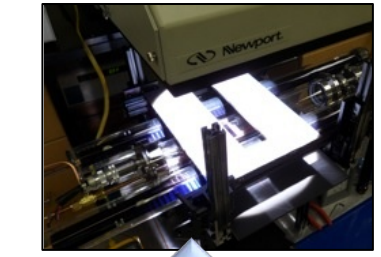
Materials Manufacturing Through System Development

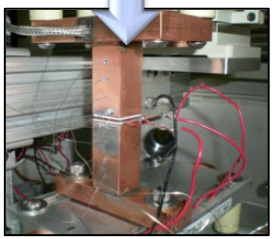
Power Generation

System Level Development

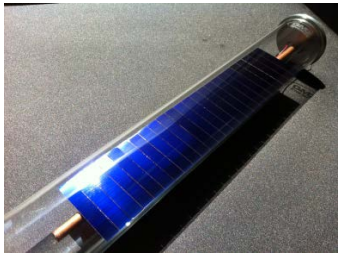
Materials Production

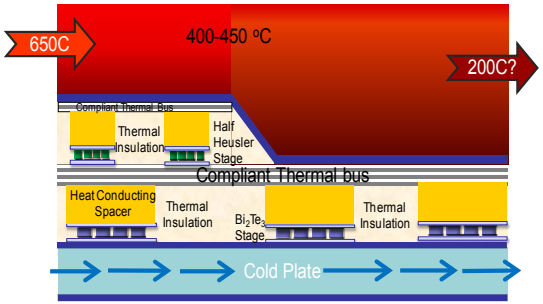
TE leg Production





COP/ΔT test





- Electrical, Thermal Characterization (ρ,α,κ)

- XRD – compositional verification
- SEM – particle size
- TEM – grain size

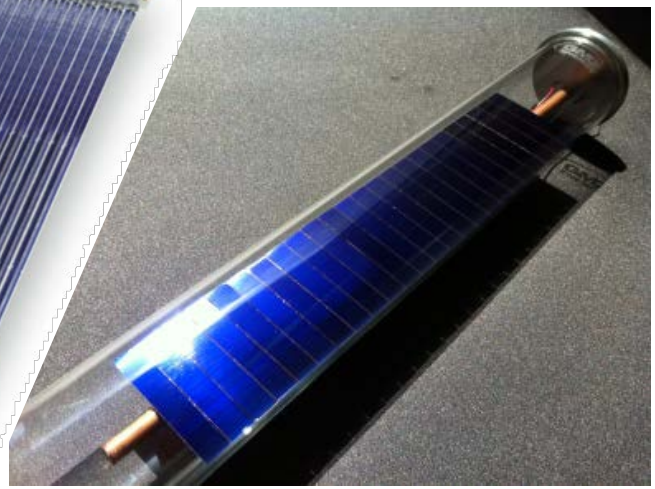
- Contact Resistance
- Device Resistance
- Performance Testing
- System Engineering

Hybrid Electric & HW Solar Thermal System

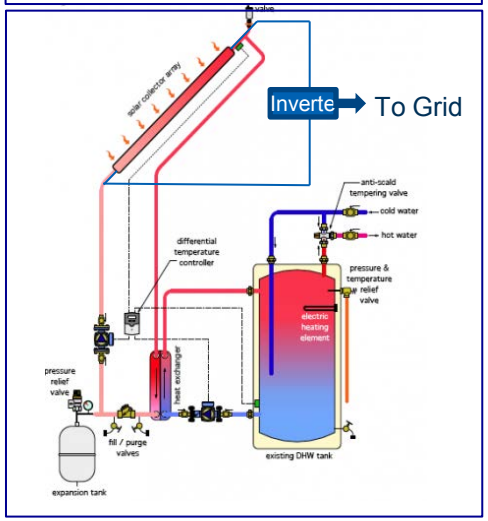
World's First Integrated Electricity & Solar Thermal HW Module

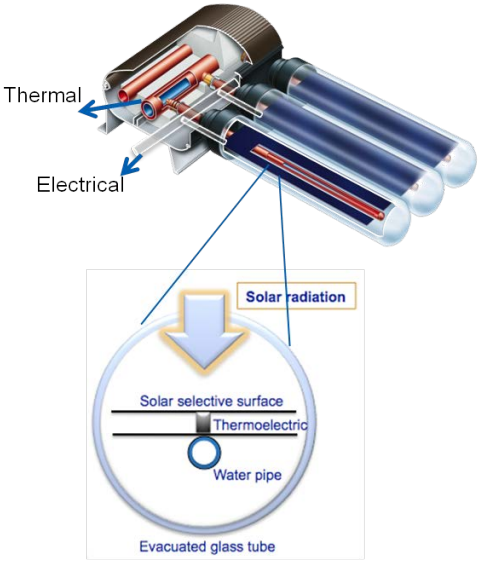
Hot Water

Electricity



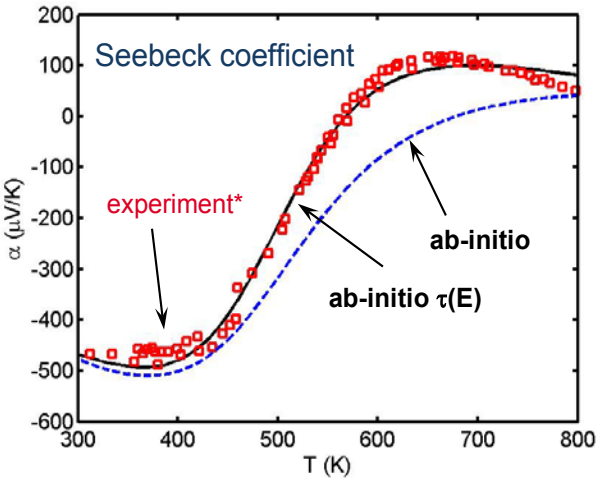
Baseline Solar Thermal

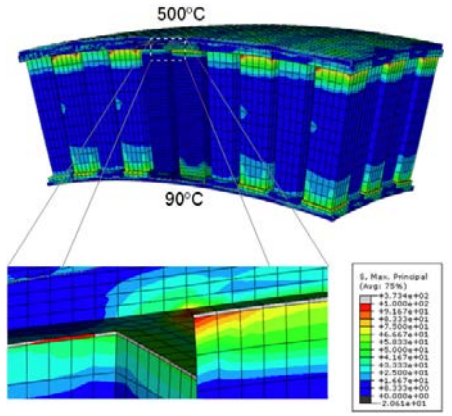


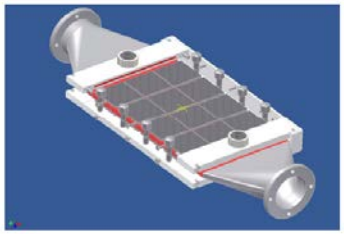


Bosch – wide ranging contribution to VTP

- Bosch will interact with tasks from their perspective as a Tier One OEM supplier as well as through a basic materials and device development perspective.
  - Corporate Research (CR) through Research and Technology Center (RTC)
    - Atomistic modeling of materials and device contact layers and joints
    - Conjugate heat flow CFD simulations and heat exchanger design will be performed using ANSYS FLUENT, and system level simulation using ANSYS and COMSOL for coupled thermo-mechanical/electronic FEM modeling of modules under a variety of operating conditions.
  - Gasoline System Engineering (GS) will work closely with ORNL on integrating the thermoelectric component into a full vehicle for testing and modeling
  - Automotive Electronics (AE) will support the electrical integration of the thermoelectric generator system into the vehicle for testing.

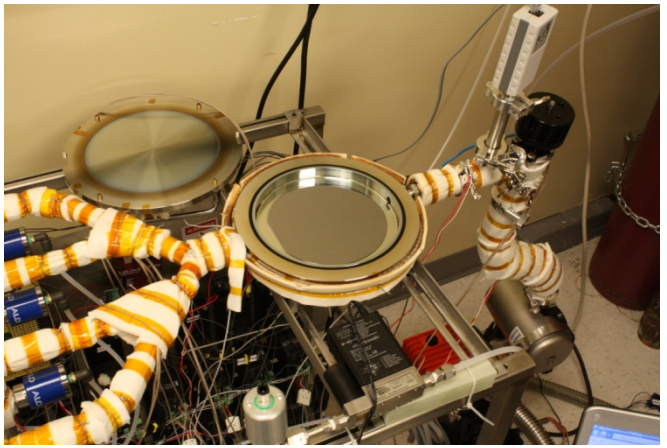


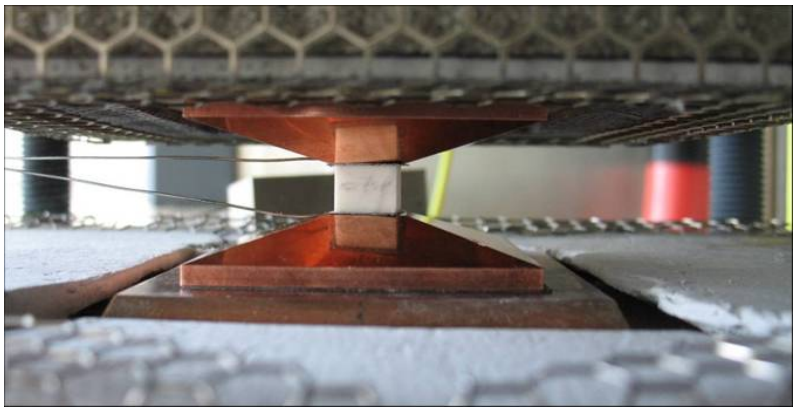




Bosch CR/RTC Background: Thermoelectric Generation

- Bosch RTC has developed a unique chemical vapor deposition setup that allows precise control of coating composition and morphology of protective layers for materials.
- Full-scale TE precise module efficiency test bench
- Reliability test bench under vibration and elevated temperature
  - Hot side temp. up to 700° C
  - Shaker frequency: 10-4000Hz
  - Shaker acceleration up to 8g.





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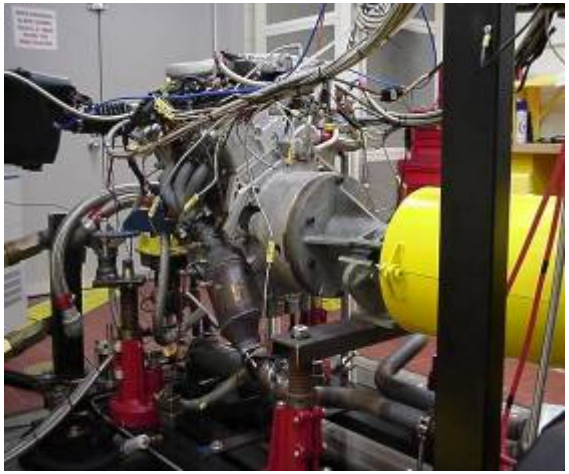
Bosch GS Background

- A dedicated Engine Dynamometer Operations team at Bosch is responsible for operating and maintaining nine engine dynamometer test cells. From durability to full engine mapping with emissions capabilities this team meets all needs:
  - Data Acquisition System: MTS-DSP ADAPT
  - Automated Test Schedule Capability
  - Fuel Measurement Capabilities (0-200 lb/hr)
  - Oil, Coolant and Fuel Temperature Control
  - Emission Bench: Horiba Mexa-7500D
  - Fuel Measurement System: Pierburg PII401



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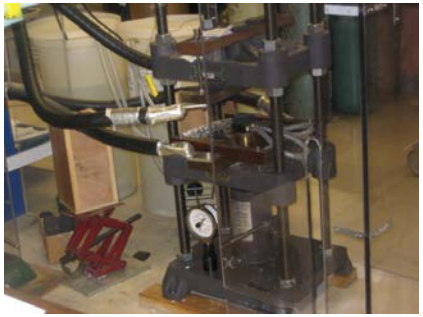
Boston College

- BC contributing founding work in nanostructured materials and fundamental understanding of thermoelectric thermal systems.
  - Continue to develop the materials to increase ZT and understand compositional changes and the effect on the temperature range of ZT.
  - Fundamental studies on thermo-mechanical properties of joints.
  - Materials cost reduction via reduction/elimination of Hf from half-heusler compositions while maintaining performance



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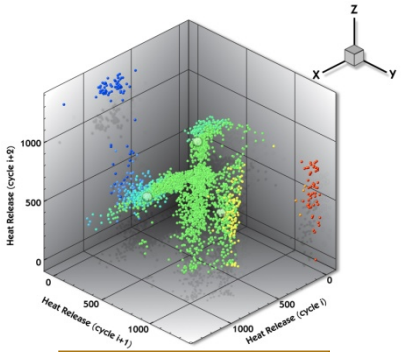
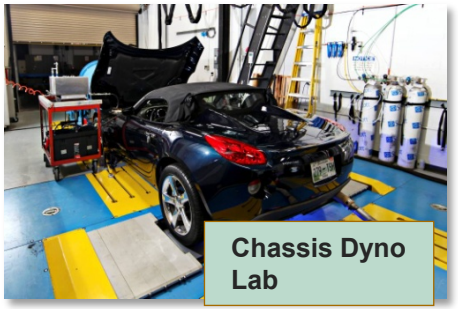
ORNL: Fuels, Engines, and Emissions Research

…. a comprehensive laboratory for advanced transportation technologies

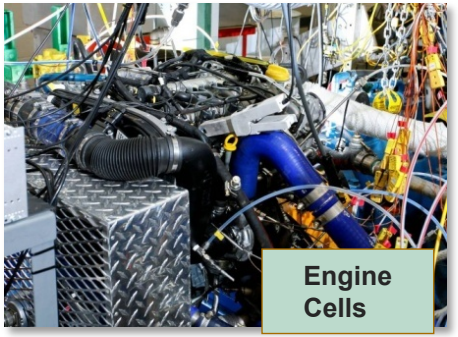
- A DOE National User Facility
- Research and development to achieve key DOE milestones in transportation efficiency and emissions.
- **Work with DOE and industry to resolve barriers to deployment of efficient vehicles and alternative fuels.**
  - Efficient and effective emissions controls.
  - Advanced combustion processes and fuel effects.
  - Thermodynamic fundamentals and energy management.
  - Enabling technologies including materials, diagnostics, etc.



Models and Controls

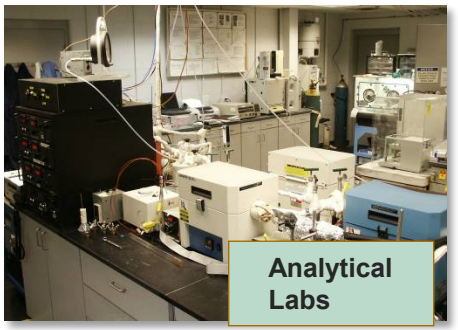


Chassis Dyno Lab



Engine Cells

- **Vehicle systems integration for understanding potential and issues under real world conditions.**
- Third party DOE lab to verify and oversee testing of the thermoelectric exhaust waste heat recovery system and take part in steady-state dynamometer testing at their facility with a prototype system fitted to an engine supplied by Bosch.
- Give input and oversee the vehicle model developed by the team and the vehicle-integrated dynamic drive cycle dynamometer testing at Bosch.



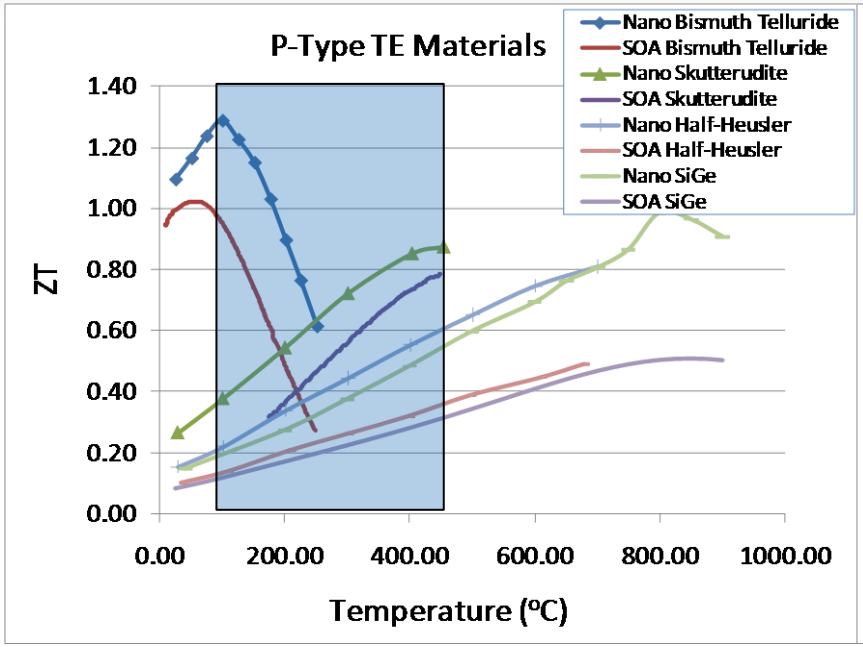
Analytical Labs

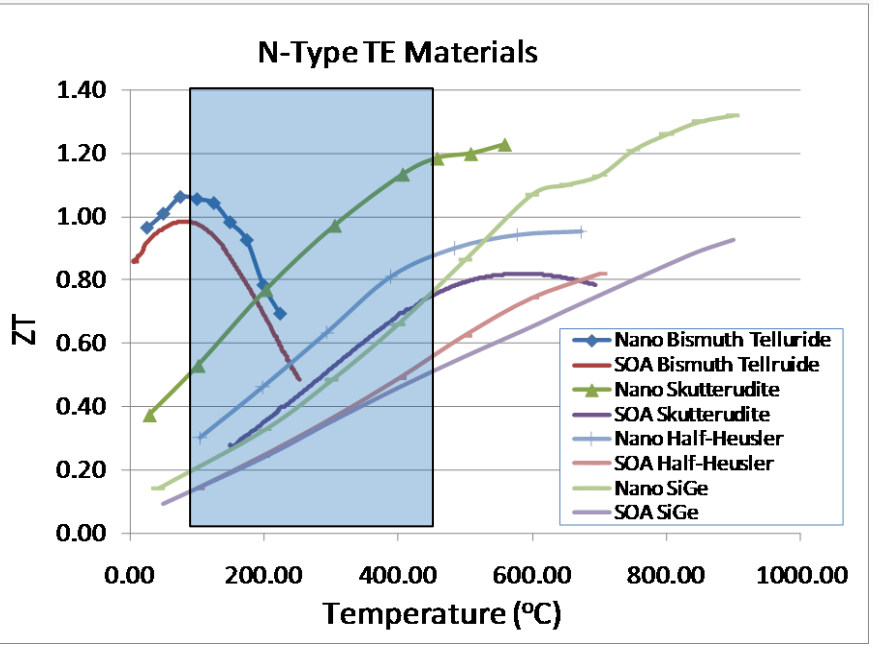
GMZ ENERGY

OAK RIDGE National Laboratory

Phase 1 Experimental Details

Materials Selection Rational

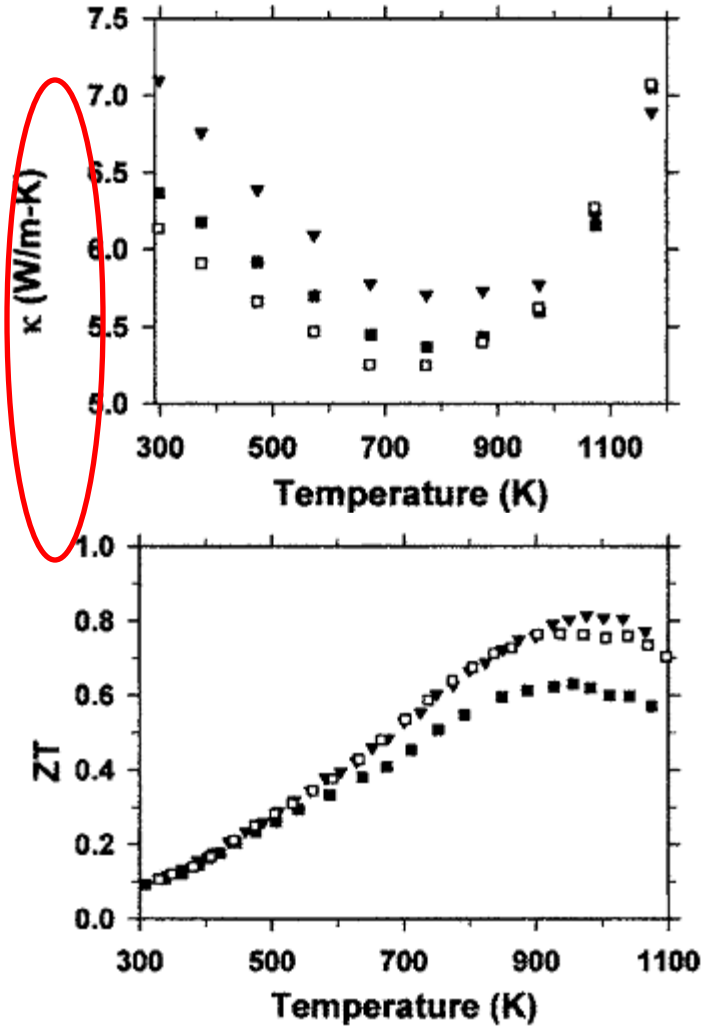




- Nanostructured materials show increased ZT across many families and temperature ranges
- For best combination of temperature stability/reliability and performance, Bi_2Te_3 and Half-Heuslers were chosen for this work

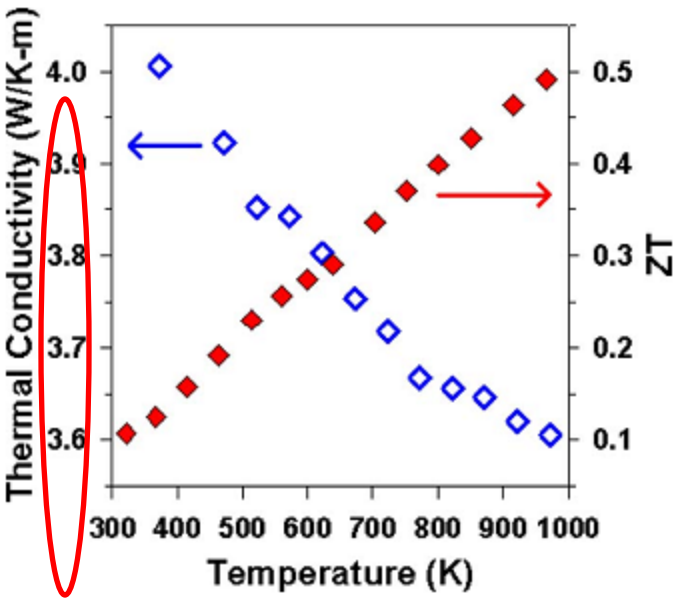
Status of Half-Heuslers

N type, $Hf_{0.75}Zr_{0.25}NiSn_{0.975}Sb_{0.025}$



Culp et al., *Appl. Phys. Lett.* **88**, 042106 (2006)

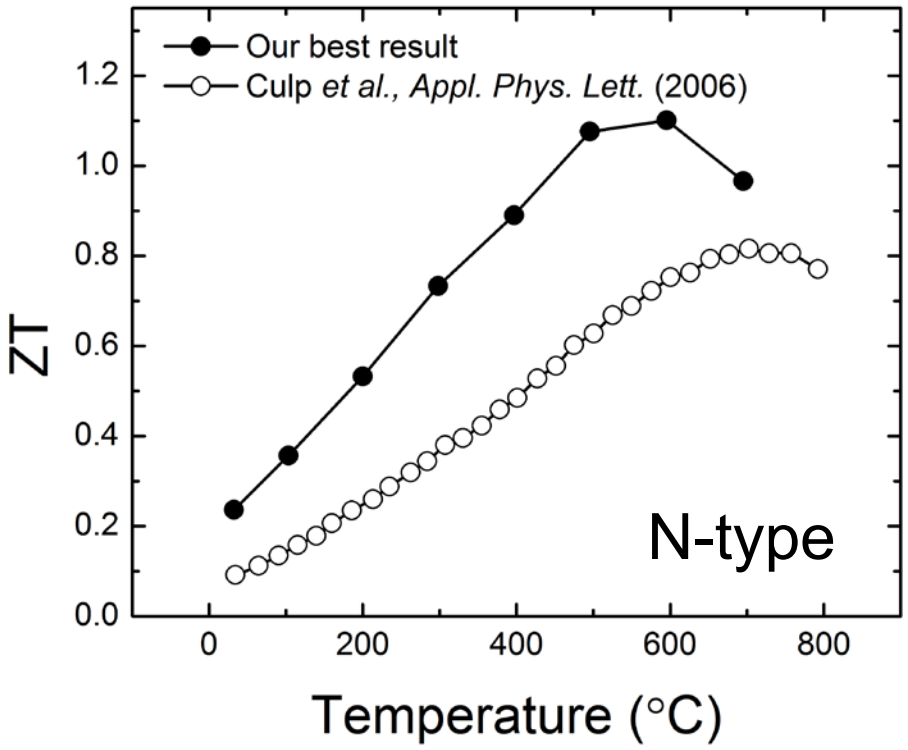
P type, $Zr_{0.5}Hf_{0.5}CoSb_{0.8}Sn_{0.2}$

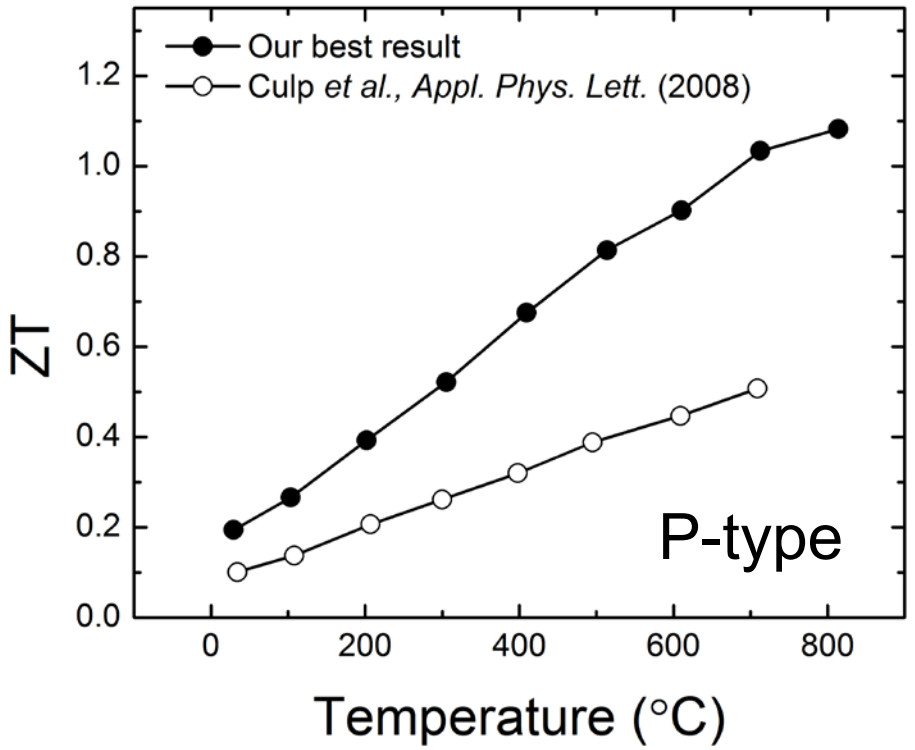


Culp et al., *Appl. Phys. Lett.* **93**, 022105 (2008)

- Thermal conductivity too high!
- Nanocomposite approach: reduce thermal conductivity

Summary


Our best result
Culp et al., Appl. Phys. Lett. (2006)
ZT
Temperature (°C)
N-type
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
200
400
600
800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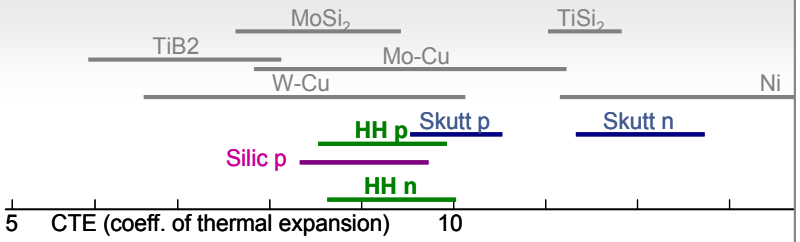
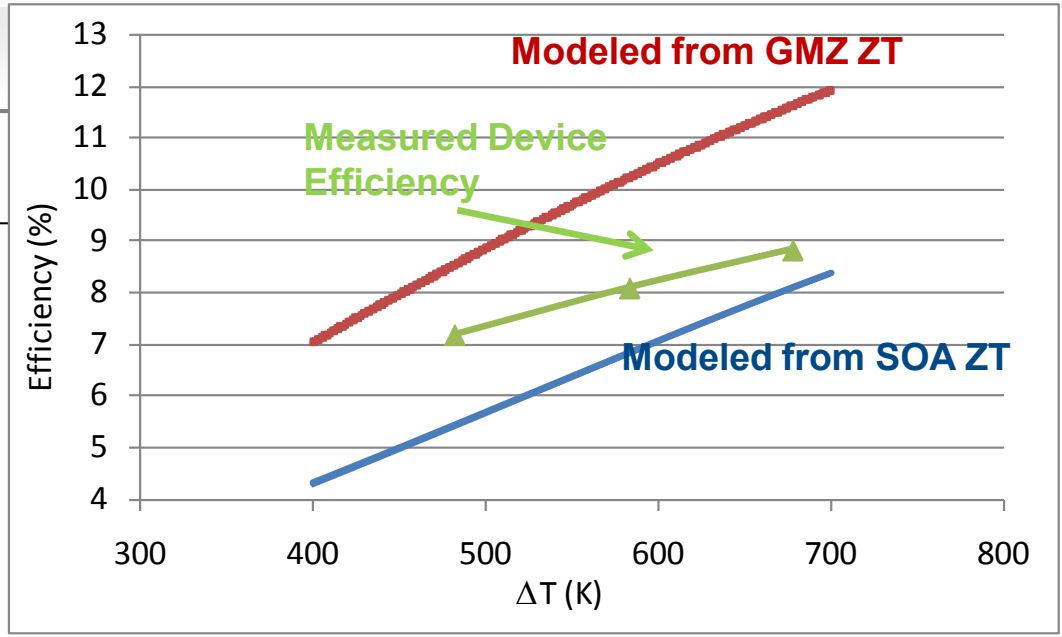
GMZ Devices and Testing – Previous Work



- Coefficient of thermal expansion (CTE) data shows HH materials well matched for lower thermal stress.
- Similar situation for Bi_2Te_3 materials

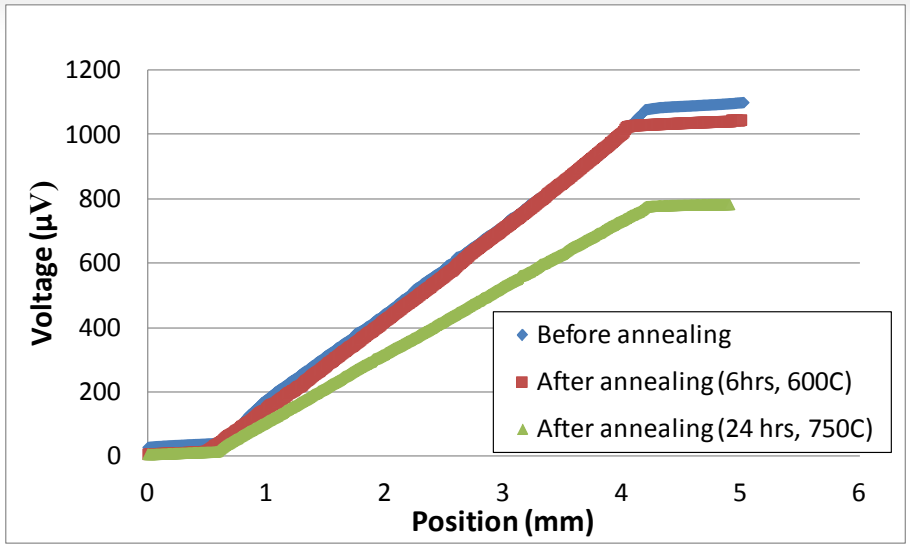


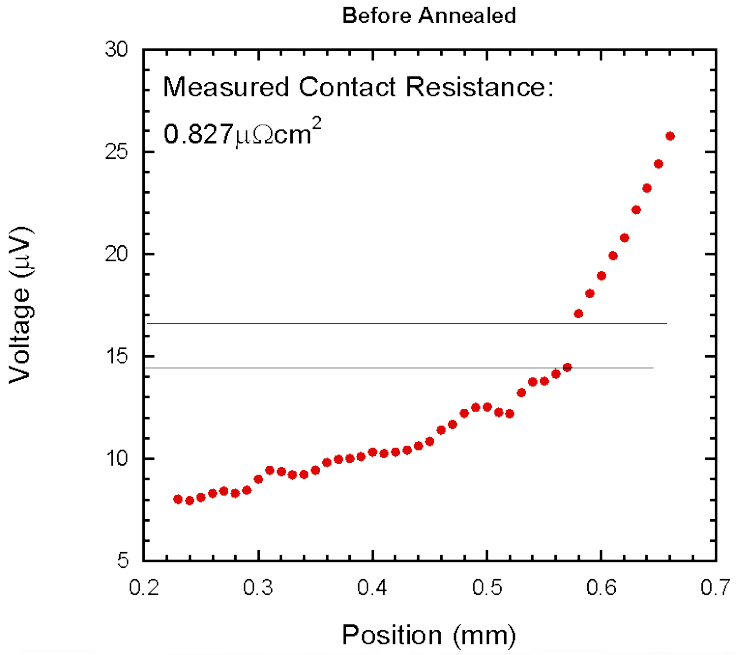
Measured efficiency of Half-Heusler device fabricated and tested at GMZ

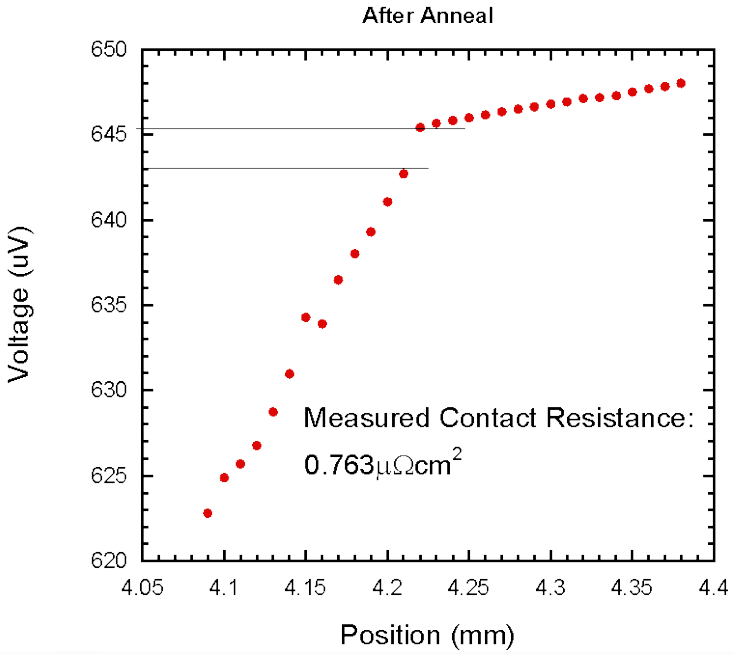
- GMZ will build on its experience in Bi_2Te_3-based and initial high-temperature half-heusler devices, which have shown superior power generation efficiency
- ***Measured efficiency for GMZ devices is better than the ideal modeled efficiency for SOA materials***.
- There is room for improvement with further materials and device development.

Half-Heusler Contact Studies at GMZ

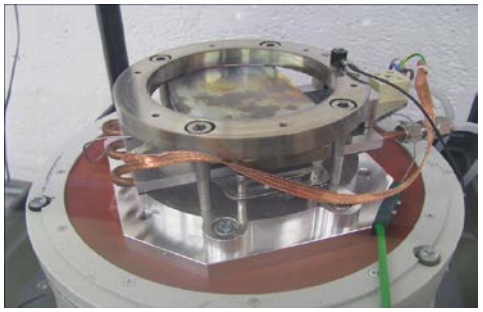
- In order to make good devices, good contact layers are needed
- GMZ has successfully applied thick (diffusion barrier) contacts with low contact resistivity – precursor to high-performance devices and modules

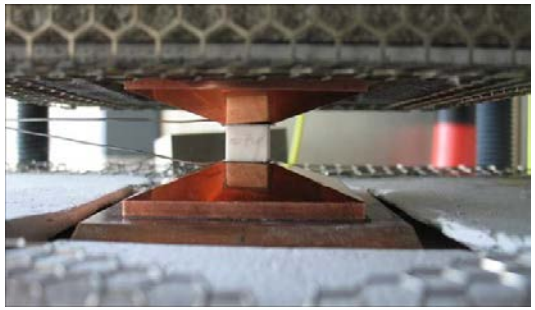


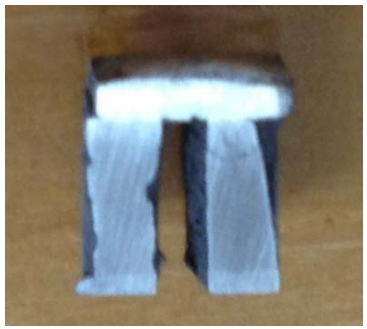


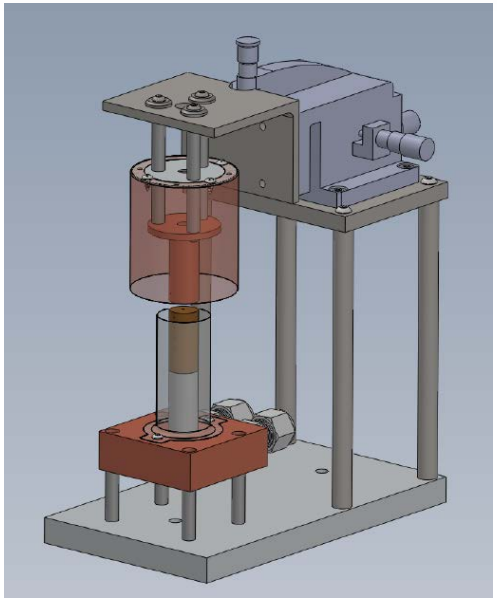


Device Testing and Reliability



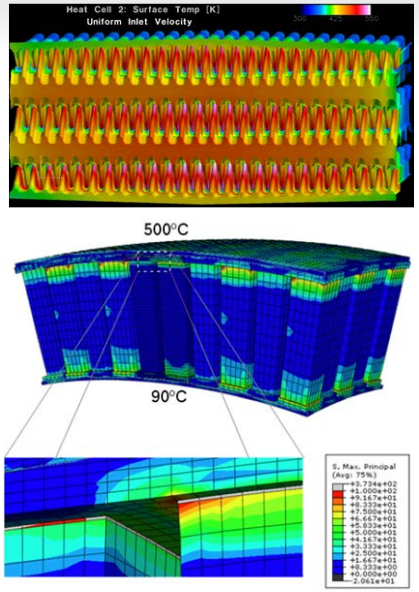


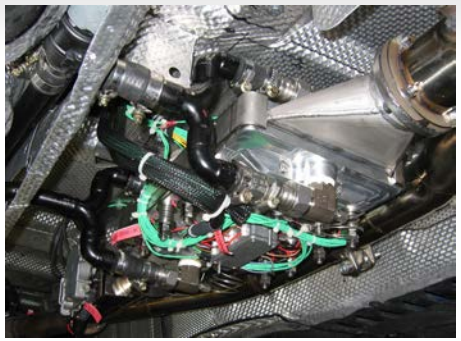


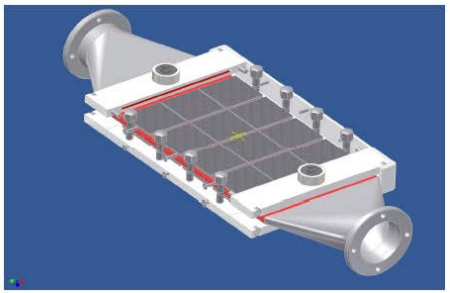


- Precise module efficiency testing equipment at Bosch and GMZ will be used to measure thermoelectric device performance and long term stability (thermal cycles).
- Thermal-mechanical strength and failure modes will be tested in conjunction with BC and potentially an outside consultant

Heat Exchanger Design – System Integration







- GMZ and Bosch will work together to take advantage of past experience, modeling tools and hands-on experimentation to find a robust, reliable and cost effective system design – including TE devices, heat exchangers and system level integration

- Bosh has direct experience with TE device integration and testing
- GMZ and Bosch will bring an integrated modeling concept from individual legs, to modules, interfaces and systems
- Sub-system testing will be accelerated to find empirical confirmation of designs – module and sub-system testing in phase 1.

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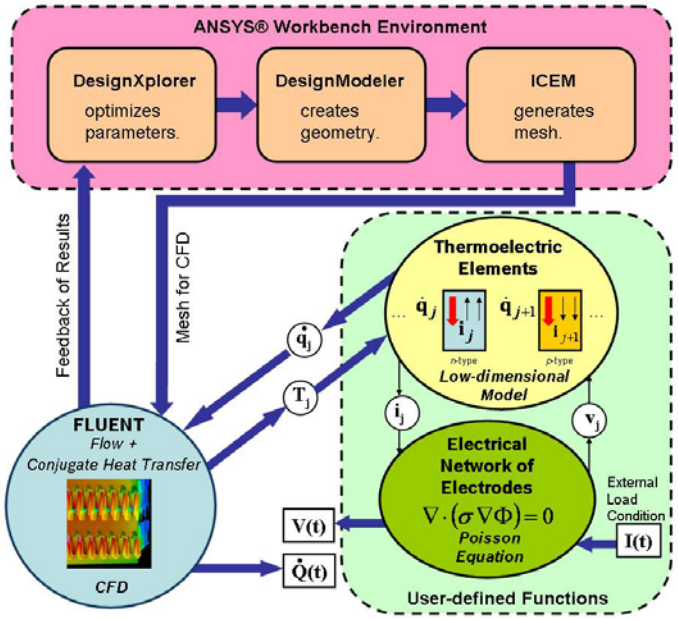
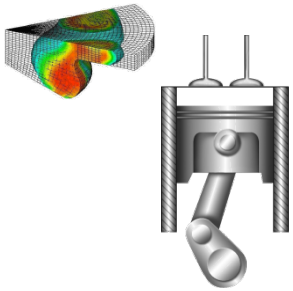
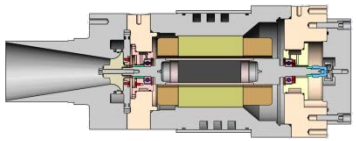
Vehicle/System Model and Electrical Integration

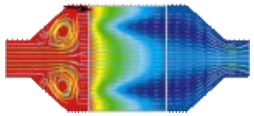
- Using GT-Drive and GT- Power as main tools
- US06 and FTP75 drive cycle and both for gasoline and E85
- Semi-automated environment to optimize the geometry of a thermoelectric generator, seamlessly integrating flow physics and solid-state physics
- Predicted electrical output (voltage, current) to size DC/DC converter (buck vs boost or combination) and Maximum Power Point Control (MPP) control





Thermal Energy Recovery





Aftertreatment

Combustion / Engine → Engine System → Vehicle System

Conclusions

- The team is positioned well to execute on all objectives
- Program gaining momentum and will have device data in next quarter – efficiency, thermal cycles and mechanical properties
- Module and system architectures to be defined by the end of phase 1 – Jan 2013.