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

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Our project addresses 5 key elements towards realization of TEGs for vehicles

1. **Materials** (Romny Scientific, Priya)
   - Our materials efforts focus on rapid and scalable fabrication techniques with abundant, low-cost materials
   - Isostatic pressing of Mg Silicide materials
   - ZnO with Al by solid-state reaction
2. **Thermal management** (Ekkad, Huxtable)
   - Models and experiments to characterize heat sinks and system-level designs to predict/demonstrate performance
3. **Heat exchangers** (Ekkad, Huxtable)
   - Experiments and models of efficient heat sinks using, e.g., pin fins and and jet impingement
4. **Interfaces & Durability** (Huxtable, Romny Scientific)
   - Measurements of adhesion electrical transport and species mixing and diffusion through interfaces
   - Effects of thermal history adhesion, properties, & transport
5. **Metrology** (all)
   - Nano-macro TE and structural characterization of materials (SEM, EDX, XRD, Seebeck, electrical & thermal conductivity, etc.

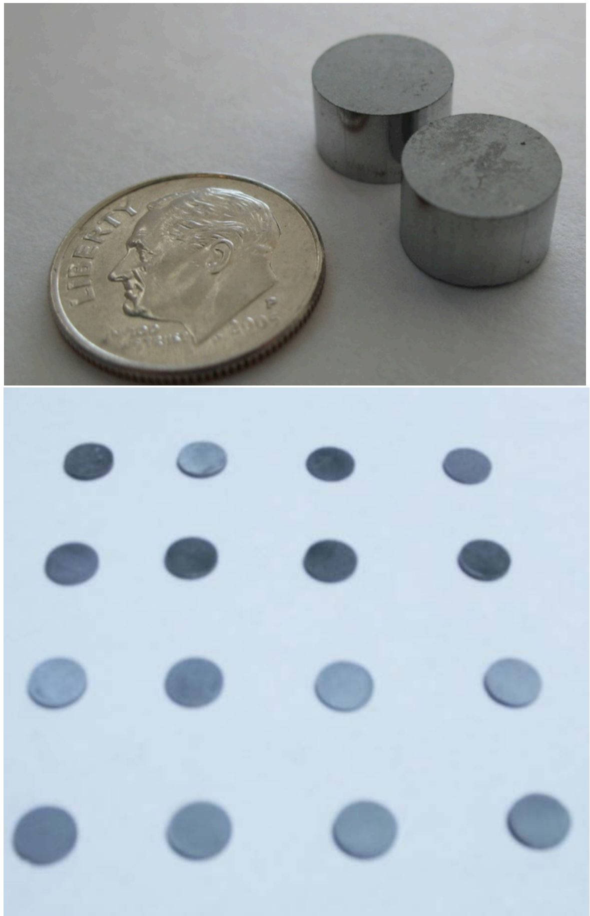
Romny Scientific has created high quality Mg-Silicide N-type elements with isostatic pressing

Our approach towards “high performance” TE materials focuses on metrics beyond high ZT. For automotive applications, ZT/(Material Production Cost) is also a critical metric.

Silicides are promising TE materials as they provide low mass, are environmentally benign, inexpensive, and offer high ZT.

We use a hot pressing fabrication approach that 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. Initial measurements indicate large tolerance for impurities.



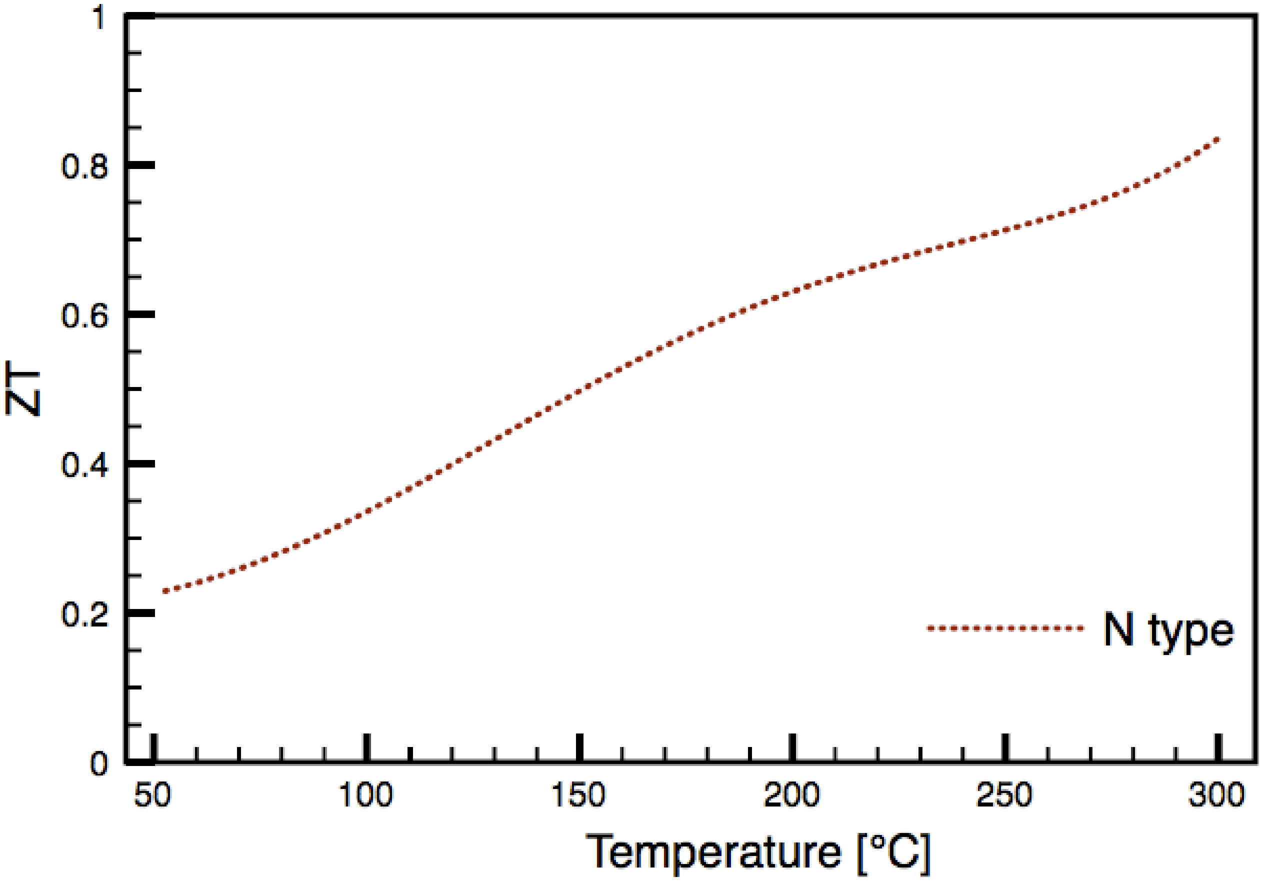
Mg-Silicide ingots (top) and pucks (bottom) hot-pressed by Romny

Romny Scientific has created high quality Mg-Silicide N-type elements with isostatic pressing

N-type $Mg_2Si_xSn_y$ produced by Romny give ZT of ~ 0.83 at 300 °C

Materials hot-pressed by Romny

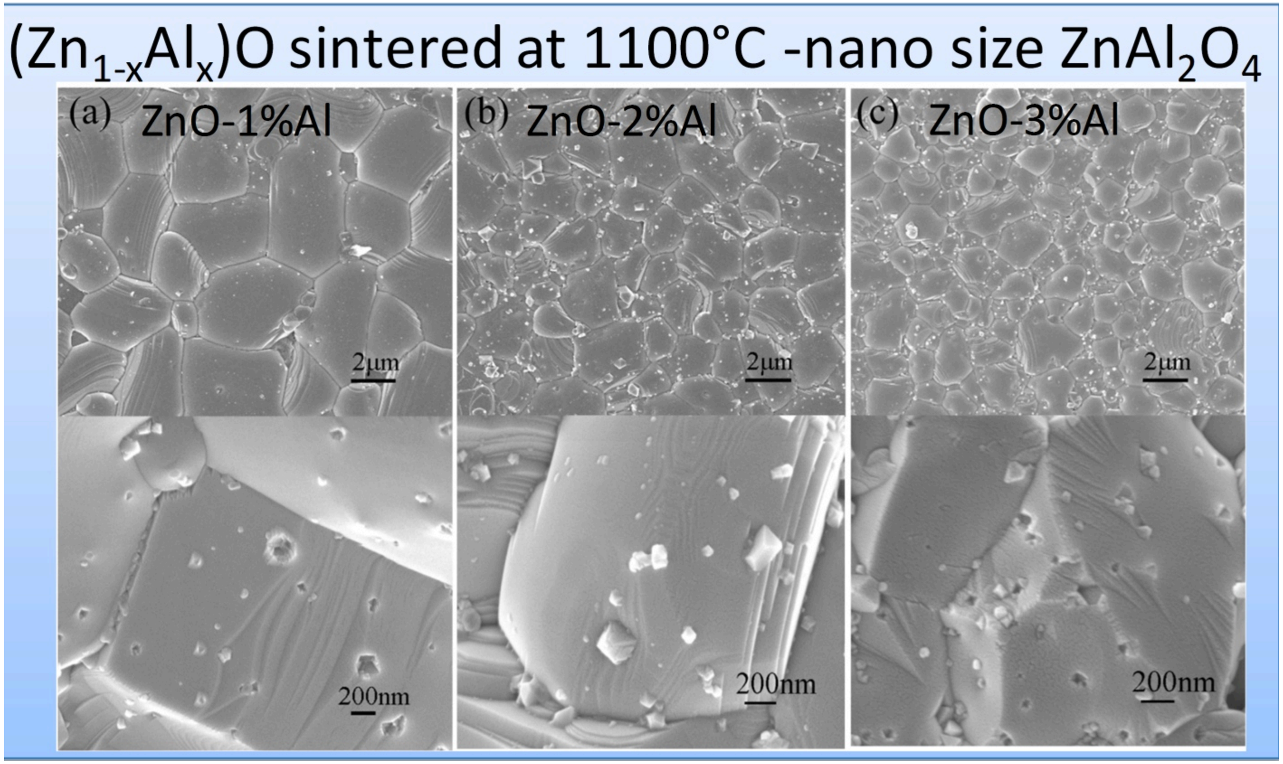
Measurement systems benchmarked with ORNL provided BiTe and other NIST traceable materials



Romny's N-type $Mg_2Si_xSn_y$ shows promising ZT of up to 0.83 at 300 °C (with potential room for improvement with further refinement in manufacturing processes)

We created ZnO with nanoscale $ZnAl_2O_4$ precipitates

ZnO is a promising material for high temperature TE applications. However, lattice thermal conductivity must be reduced significantly.



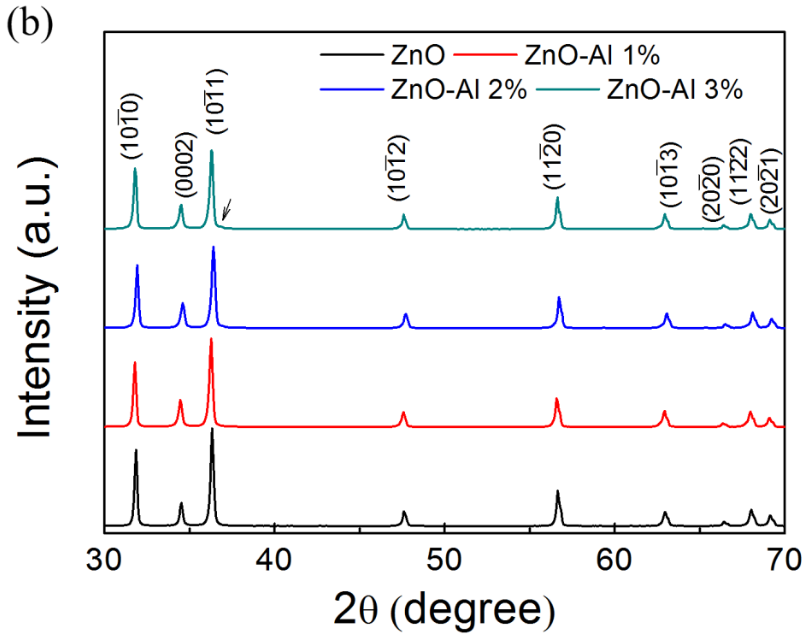
$(Zn_{1-x}Al_x)O$ sintered at 1100°C -nano size $ZnAl_2O_4$

Strategy:

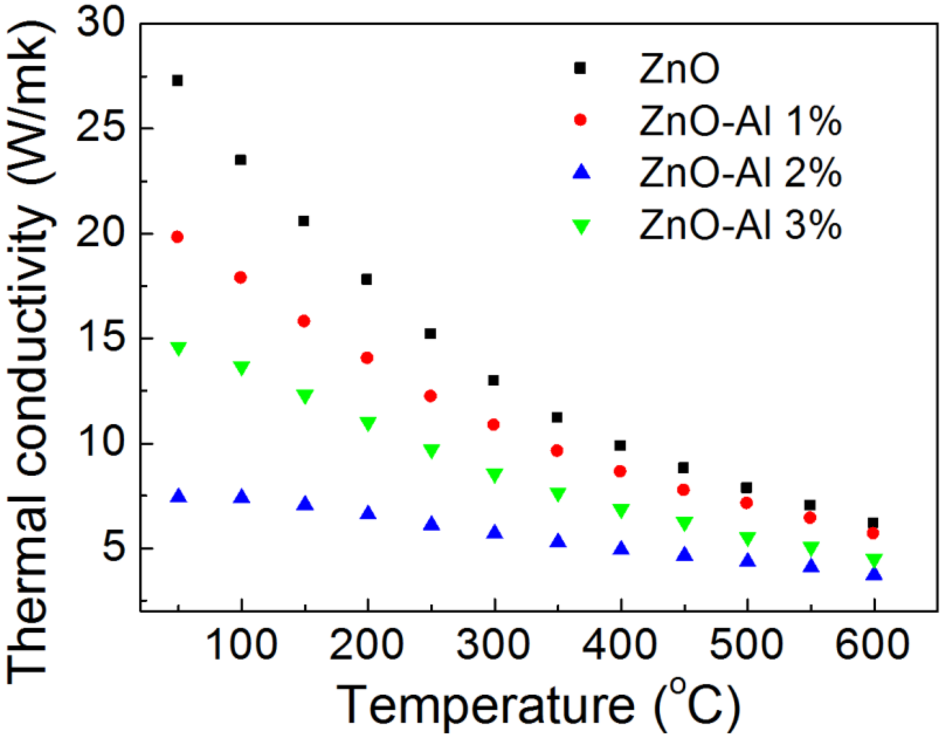
We aim to capture the advantages seen in other nanostructured materials by developing nanostructured bulk materials that can be fabricated with scalable techniques.

Here we use solid-state reaction techniques to create ZnO materials with nanoscale precipitates of $ZnAl_2O_4$.

The nanoscale $ZnAl_2O_4$ precipitates create a large reduction in thermal conductivity

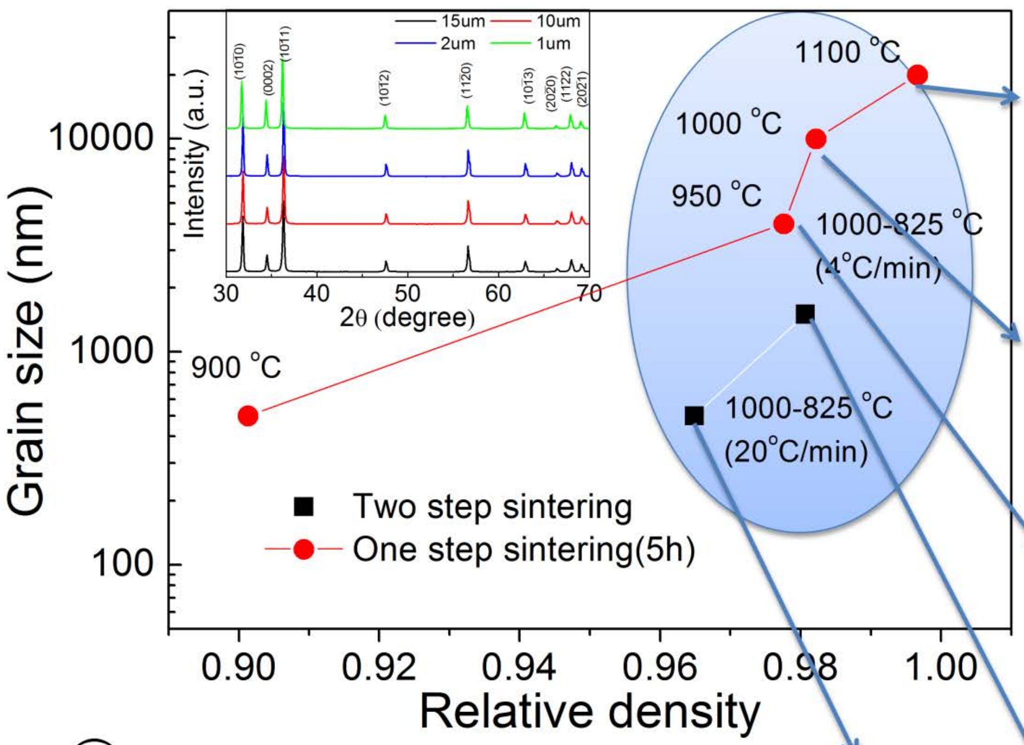


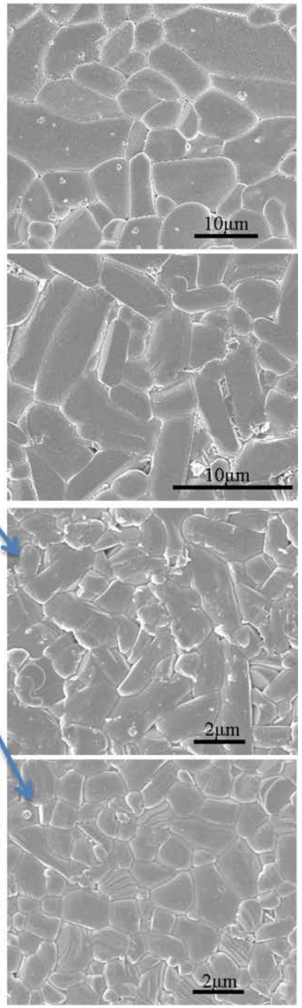
The ZnO samples with nanoscale precipitates primarily contain ZnO with hexagonal wurtzite structure as the primary phase. The secondary phase is $ZnAl_2O_4$.

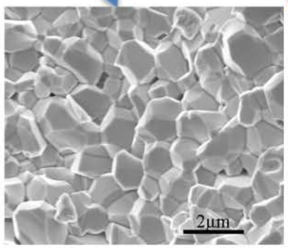


The nanoscale precipitates and, to a lesser degree, the grain boundaries create a significant reduction in thermal conductivity

Variations in grain size have a weak, but noticeable, effect on thermal conductivity

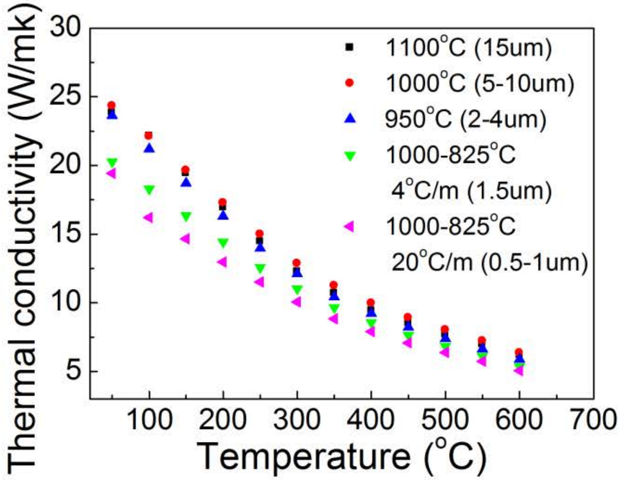






Grain size is controlled through sintering.

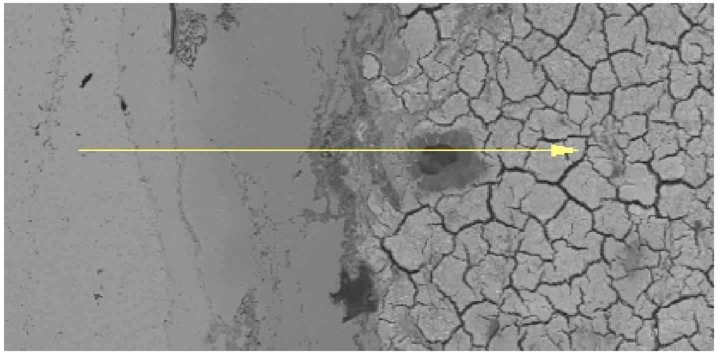
Grain size has a small effect on thermal conductivity.

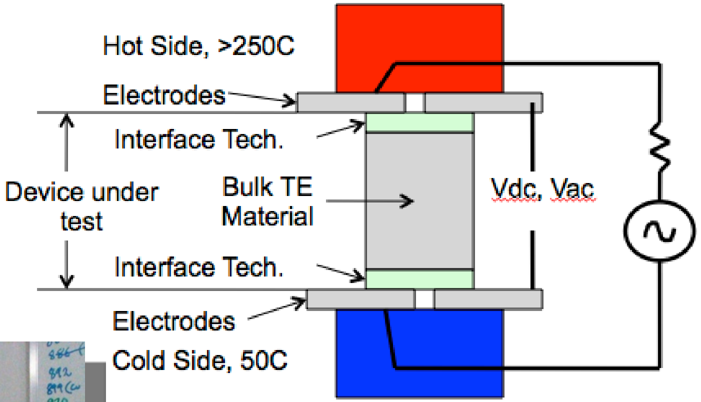


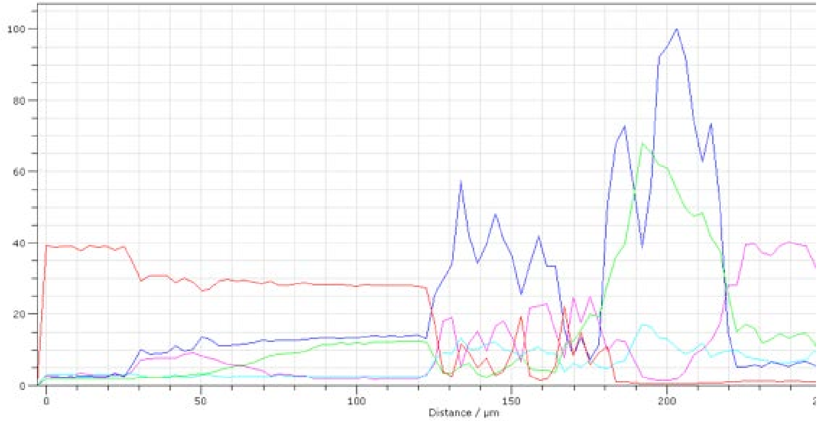
Our samples have suffered from poor control of electrical conductivity.

We examine interface quality and stability through a variety of techniques

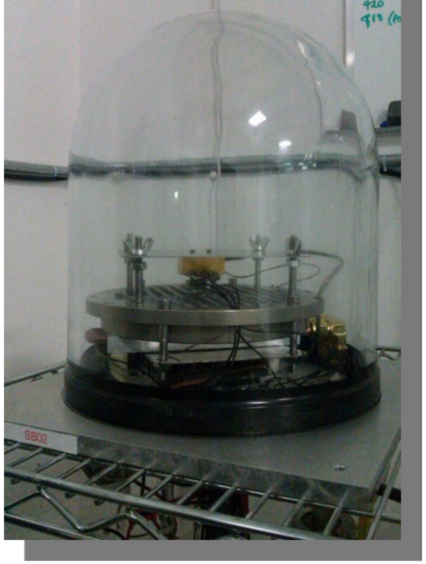
We examine the properties, reliability, and stability of interfaces through a combination of electron microscopy, energy dispersive x-ray spectroscopy, electrical resistance and Seebeck measurements.







SEM (top) and EDX (bottom) give insight into species diffusion at interfaces and interface quality



Stability Testing of Interfaces

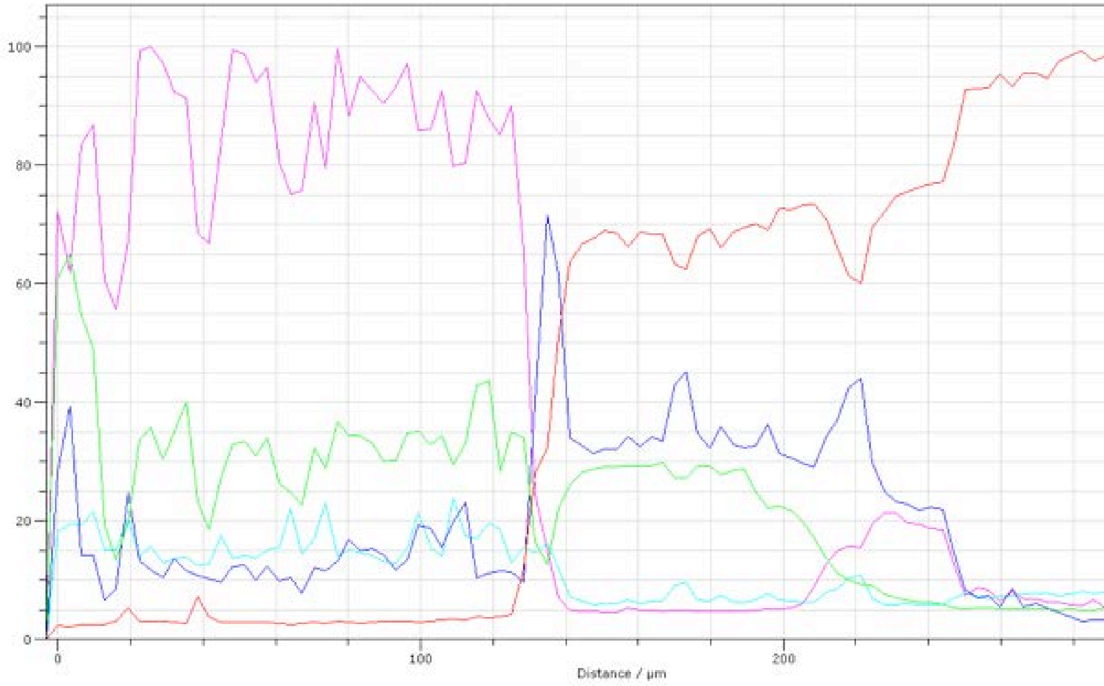
We monitor the stability of the bulk resistance, interface resistance, and Seebeck voltage over time (as shown by Romny this morning)

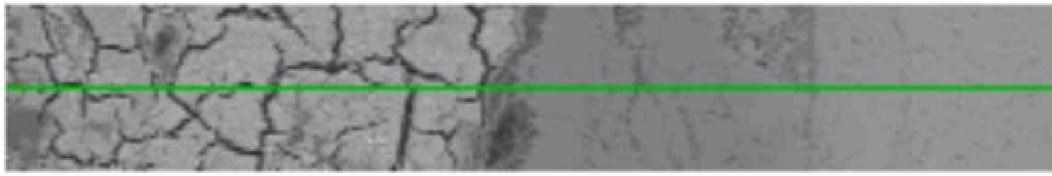
Cu and Fe make good interfaces with our Mg Silicides, while Ni was poor

SEM and EDX give insight into interface mixing, diffusion, and correlation of bulk and interface properties with structure.

Further measurements show the effects of high temperature aging on diffusion.

Several materials including Ni, Cu, and Fe were examined with Silicides



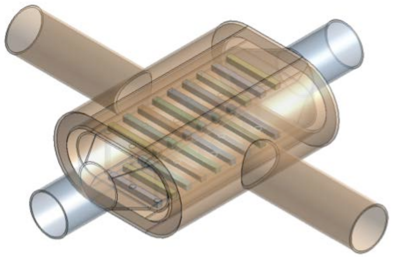


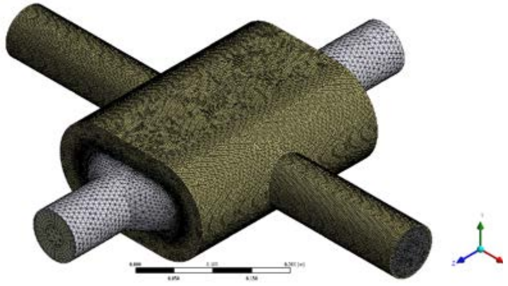
Ni gave poor performance as a contact material (despite being an excellent contact barrier in BiTe and PbTe material systems)

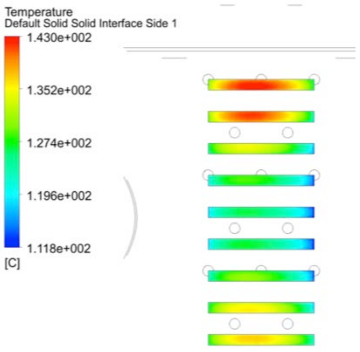
Cu and Fe show good initial results. Further work required for long-term aging and thermal cycling.

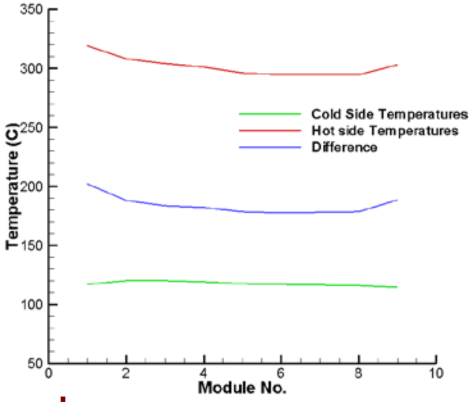
Prototype heat exchangers are designed, modeled, fabricated, and tested at VT

To improve heat sinks and thermal management in TE devices for vehicle applications we use a combination of modeling and experiments.

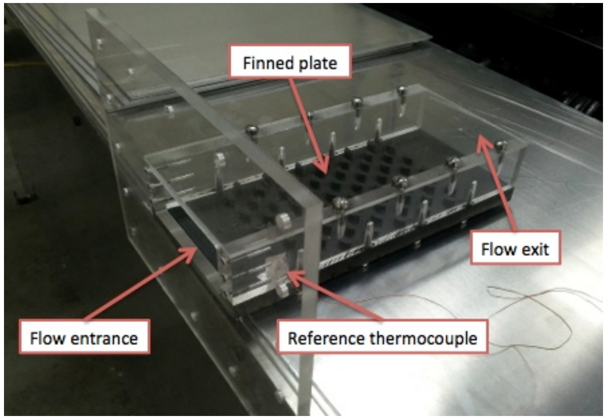


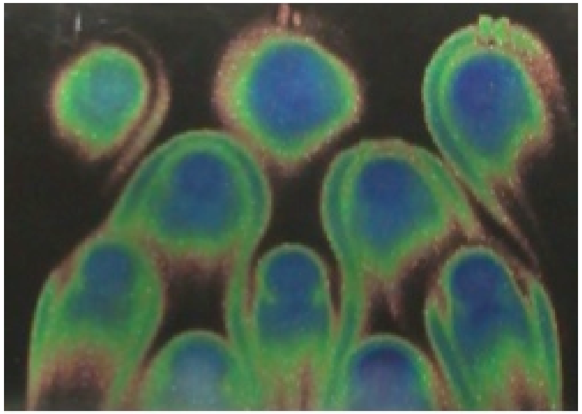






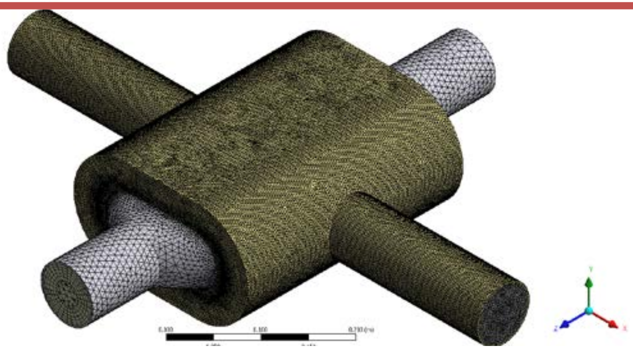
Component and system level models are used to examine various heat exchangers as well as system layout



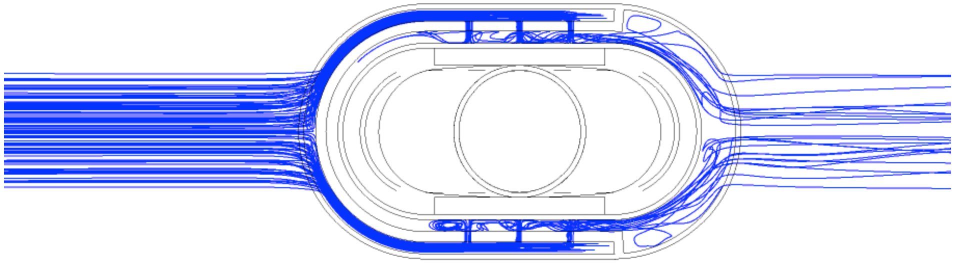


Prototype heat exchangers are fabricated with 3-D printing and tested with transient liquid crystal techniques

Impinging jets provide excellent heat transfer with limited pressure drop



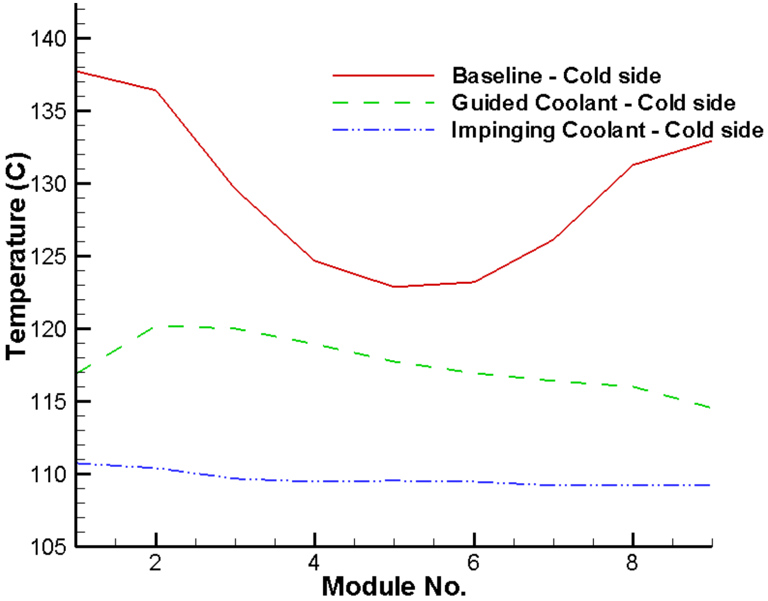
Cross-flow type of heat exchanger designs modeled with CFD. Here, hot exhaust gases flow through the internal pipe (light color), while coolant flows through the outer shell.



On the cold side, we examined baseline, guided flow, and impingement cases (streamlines for an impingement case shown at right).

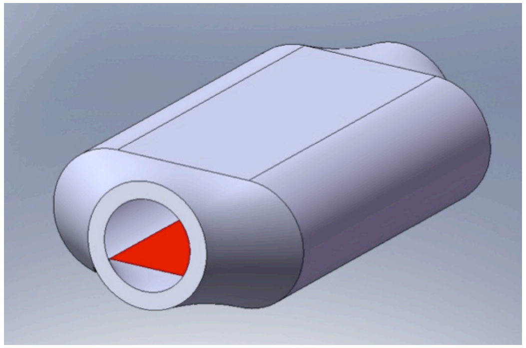
Impinging jets provided the most uniform temperature distribution and best cooling.

Impinging jets were superior to all guided flow cases, and provided excellent heat transfer with limited pressure drop penalty.

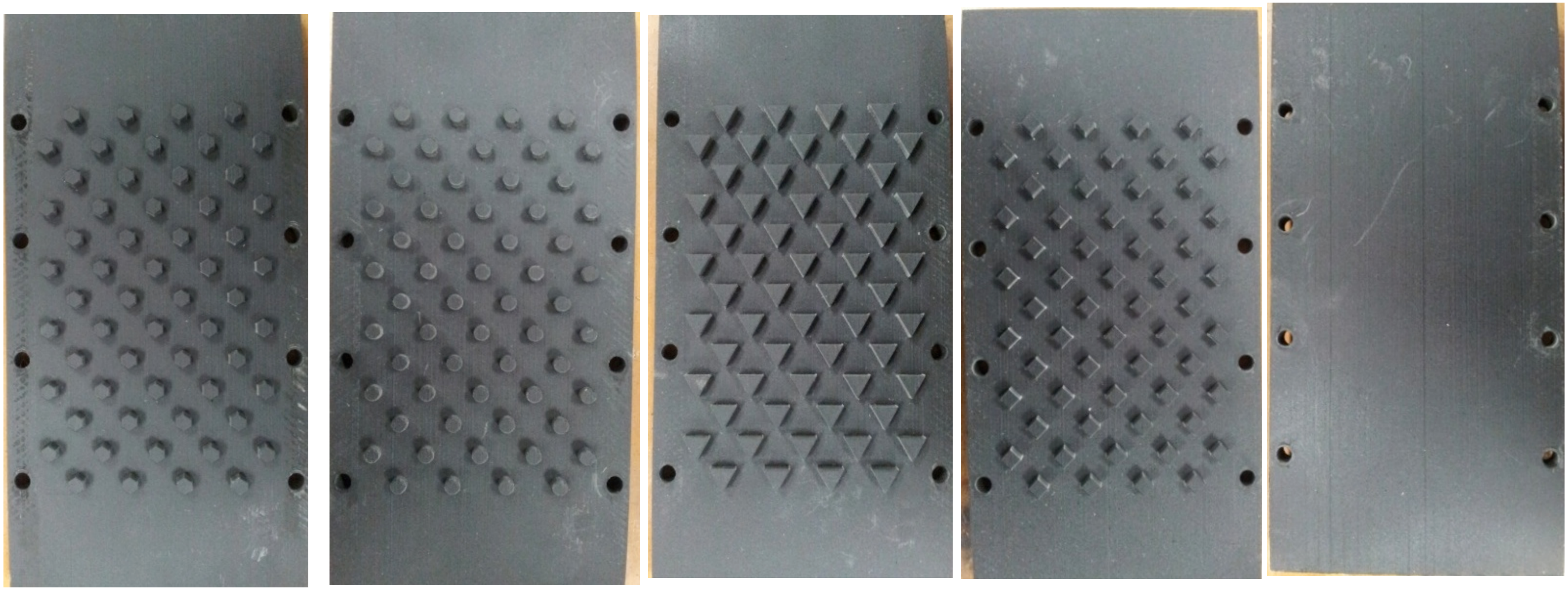


Pin fins were examined for air-side heat exchangers

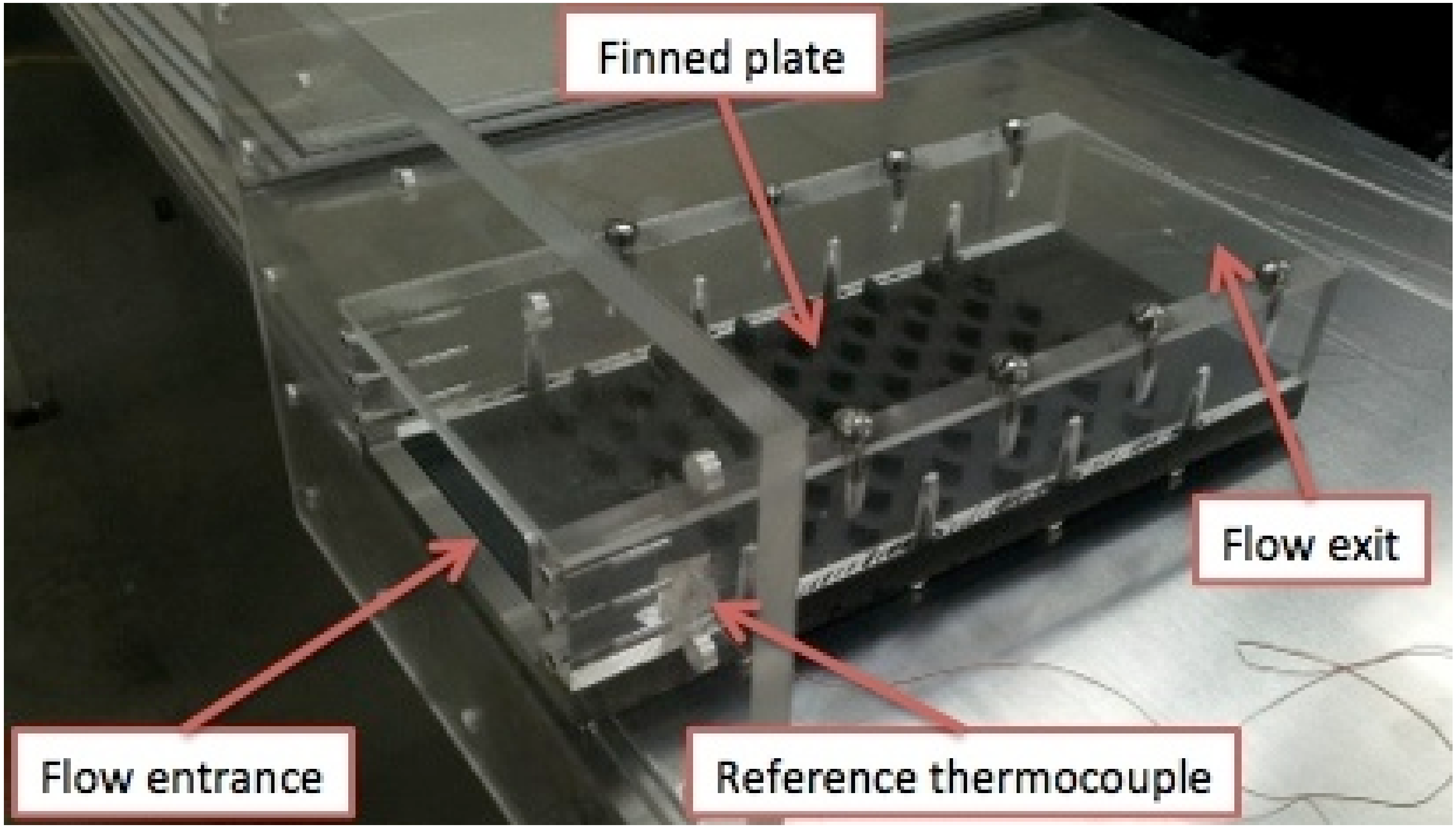
Pin-fins of various geometries were modeled and tested experimentally to enhance heat transfer from exhaust gases (placed inside exhaust system shown in schematic at right)



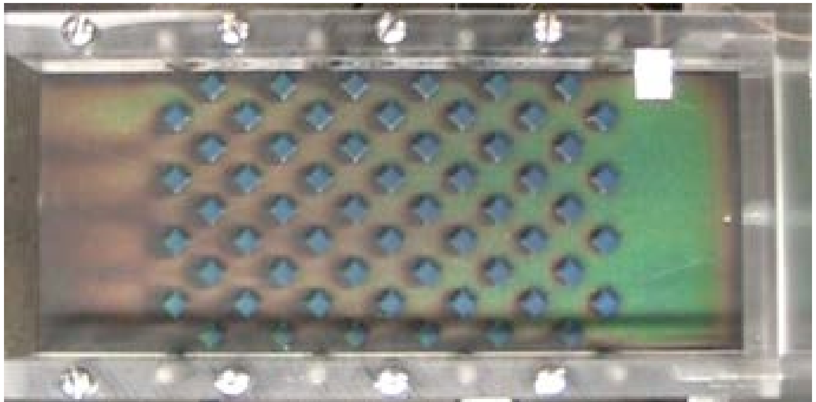
Diamond, triangle, hexagonal, and circular shaped pin-fins are shown below. These prototypes were fabricated at Virginia Tech with 3-D printing.



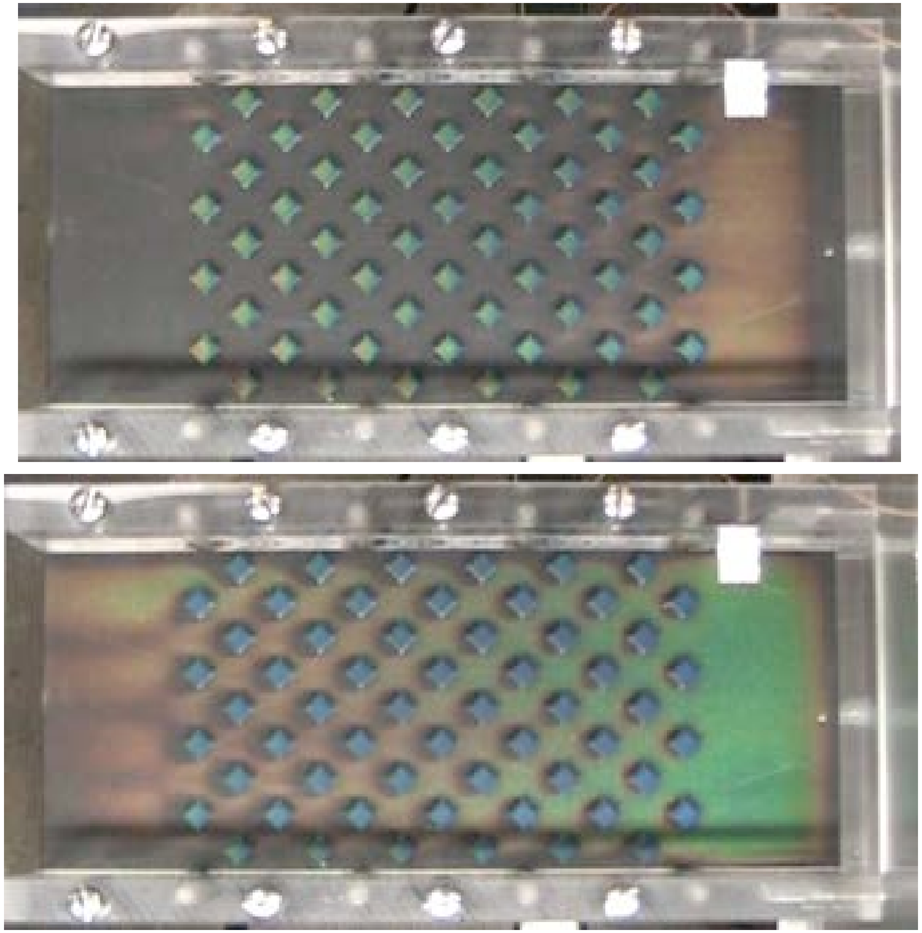
Pin fins are examined with a transient liquid crystal technique

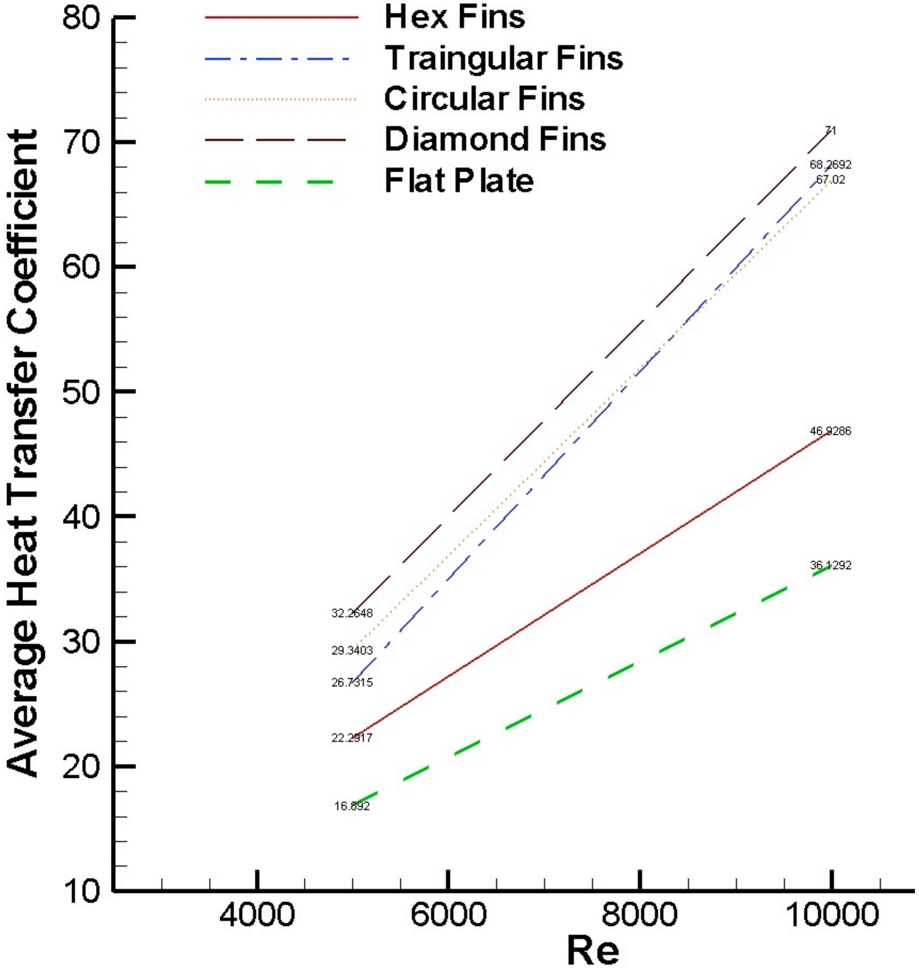


Prototypes are coated with liquid crystals. The liquid crystal spray coating changes color with temperature. Color is calibrated with thermocouple measurements, and heat transfer coefficients are extracted.



Simple pin fins increased heat transfer by a factor of two





Simple pin-fins with length <15% of the channel height increased heat transfer rates by a factor of two. Results are highly dependent on pin-fin geometry.

In summary, we are examining materials, thermal management, heat sinks, and interfaces

- Successfully produced high-quality N-type $Mg_2Si_xSn_y$ with ZT of up to 0.8 at 300 °C (Romny Scientific)
- These Mg Silicide materials are a factor of ~20 better than PbTe in terms of ZT/$ (Romny Scientific)
- Demonstrated that the creation of nano-inclusions through spontaneous precipitation is a simple and promising way to reduce thermal conductivity in ZnO (and related) TE materials.
- Initial measurements show stable interfaces and bulk elements for Mg Silicide with various interface materials (Cu and Fe were good interface materials, while Ni was poor)
- Impinging jets provided excellent heat transfer with limited pressure drop penalty for cold-side heat exchangers (10-20 °C lower temperatures for geometries tested with guided flow)
- Simple pin-fins with length <15% of the channel height can increase heat transfer rates by a factor of two on the exhaust-side heat exchanger.

Future/ongoing work includes materials development,

Materials development

- Further refinement of N-type Mg silicide materials
- Development of a P-type compliment material (efforts underway with P-type Mg_2Si_X)
- Further development of ZnO materials to include stronger reduction of thermal conductivity with spontaneous precipitation of nanoparticles while maintaining electrical conductivity.
- Perform full structural characterization (elastic modulus, hardness, thermal expansion, etc.) on the refined TE materials.

Thermal management & Heat exchangers

- Finish system-level experimental testbed for verification of CFD models.
- Compare system-level models and experiments, and use refined models to evaluate system sensitivity parameters in order to direct system design.
- Explore additional heat transfer enhancement features (e.g. dimples) and further evaluate pin spacing and pin heights for hot-side heat exchanger
- Development of a system optimization tool to determine best configuration and geometry of TEG modules in the system based on available input data.

Interfaces

- Long term testing of contact technologies to show electrical stability, limited diffusion, and mechanical stability through thermal cycling.

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- Dr. Andrew Miner
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Additional Collaborators

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