NSF-DOE Thermoelectrics Partnership:

Automotive Thermoelectric Modules with Scalable Thermo- and Electro-Mechanical Interfaces

Prof. Ken Goodson
Department of Mechanical Engineering
Stanford University

Prof. George Nolas
Department of Physics
University of South Florida

Dr. Boris Kozinsky
Energy Modeling, Control, & Computation
R. Bosch LLC

ACE067

Novel Materials Laboratory
University of South Florida

Overview

Timeline

- Start – January 2011
- End – December 2013
- ~40% complete

Budget

- $1.22 Million (DOE+NSF)
- FY12 Funding = $423K
- Leveraging:
  - ONR (FY09-11)
  - Fellowships (3 NSF, Sandia, Stanford DARE)

Barriers (2.3.2)

- Thermoelectric Device/System Packaging
- Component/System Durability
- Scaleup

Partners

- K.E. Goodson, Stanford (lead)
- George Nolas, USF
- Boris Kozinsky, Bosch

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Relevance: Addressing Key Challenges for Thermoelectrics in Combustion Systems

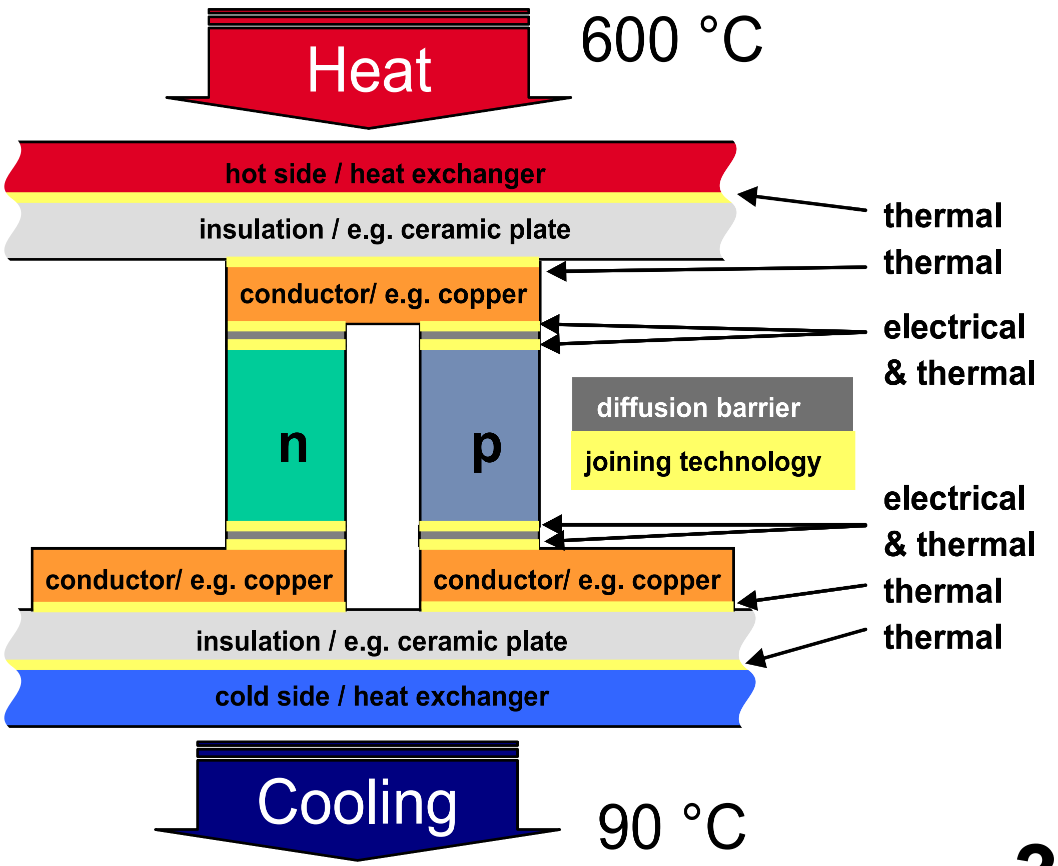
Improvements in the intrinsic ZT of TE materials are proving to be very difficult to translate into efficient, reliable power recovery systems.

Major needs include…

…Low resistance interfaces that are stable under thermal cycling.

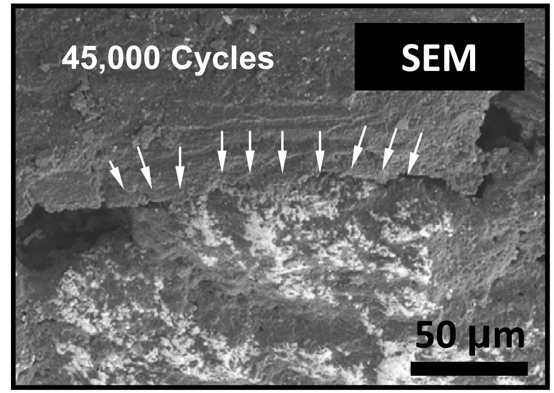
…High-temperature TE materials that are stable and promise low-cost scaleup.

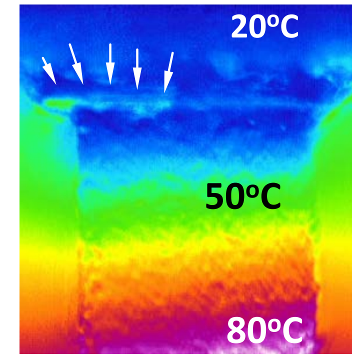
…Characterization methods that include interfaces and correlate better with system performance.



Relevance: Thermoelectric Interface Challenge

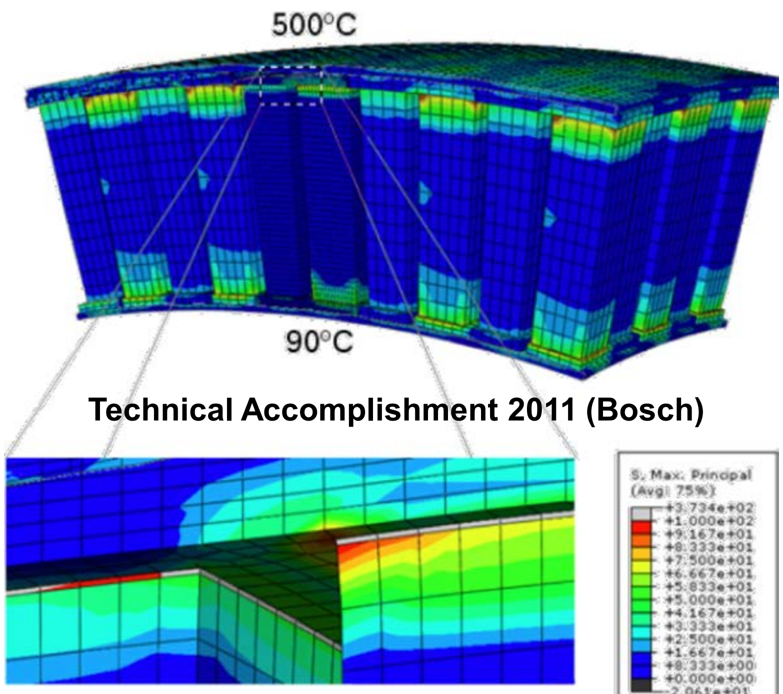
- Combustion TEG systems experience enormous interface stresses due to wide temperature spans.
- Thermal cycling degrades interface due to cracks, delamination, reflow, reducing efficiency.
- Our simulations show importance of thermodynamic stability (chemical reactivity, inter-solubility, etc.) and elastic modulus.

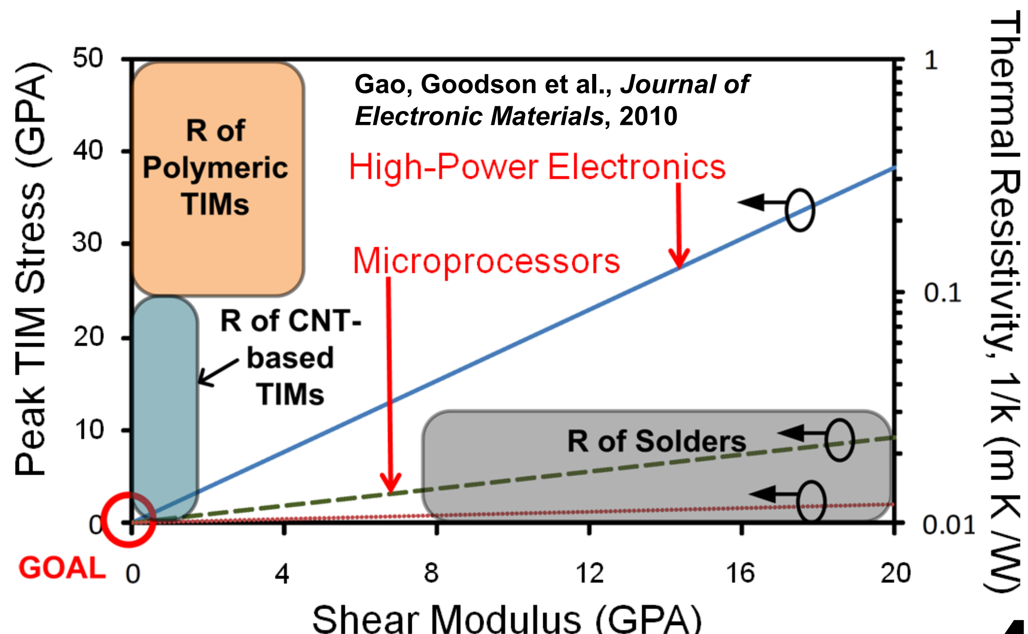




Infrared

From our New Paper: Barako, Park, Marconnet, Asheghi, Goodson, "Infrared Imaging and Reliability Study of Thermoelectric Modules under Thermal Cycling," Proceedings of ITHERM, San Diego, May, 2012.





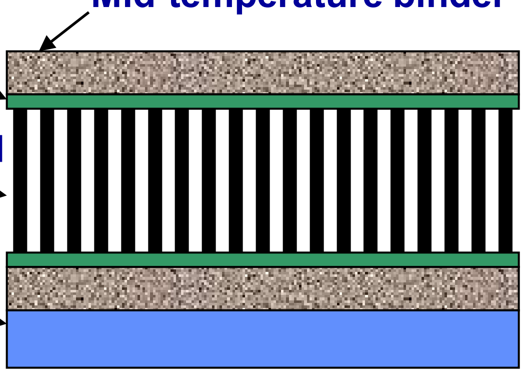
Research Objectives & Approach

OBJECTIVES

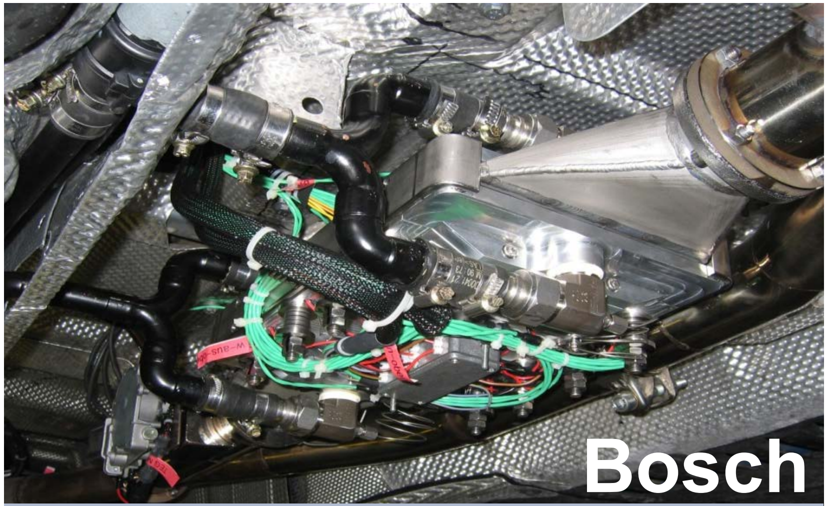
Develop, and assess the impact of, novel interface and material solutions for TEG systems of particular interest for Bosch.

Explore and integrate promising technologies including nanostructured interfaces, filled skutterudites, cold-side microfluidics.

Practical TE characterization including interface effects and thermal cycling.



Panzer, Goodson, et al., Patent Pending (2007)
Hu, Goodson, Fisher, et al., *ASME JHT* (2006)
Won, Kenny, Fisher, et al., *CARBON* (2012)



Prototype TEG in exhaust system

APPROACH

Multiphysics simulations ranging from atomic to system scale.

Advanced materials development including CNT and metal nanowire TIMS, and high temperature thermoelectrics.

Photothermal metrology including Pico/nanosecond, cross-sectional IR. MEMS-based mechanical characterization.

Research Approach

Additional Faculty & Staff beyond PIs
Prof. Mehdi Asheghi, Stanford Mechanical Engineering
Dr. Winnie Wong-Ng, NIST Functional Properties Group
Dr. Yongkwan Dong, USF Department of Physics

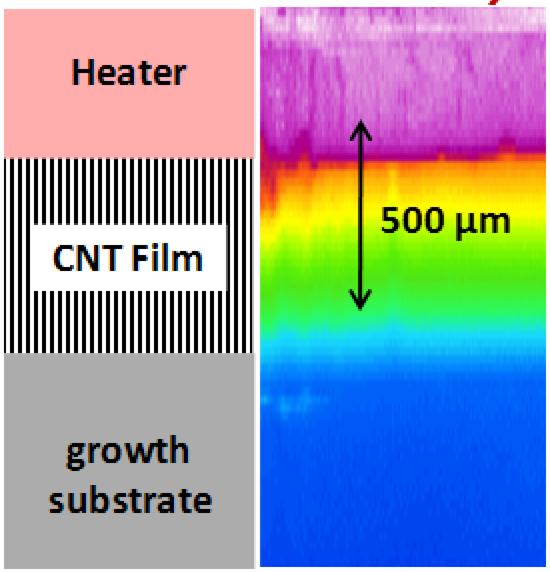
Stanford Students:
Michael Barako, Yuan Gao (NSF Fellow), Lewis Hom (NSF Fellow), Saniya Leblanc (Sandia Fellow), Woosung Park, Amy Marconnet (NSF Fellow), Sri Lingamneni, and Antoine Durieux

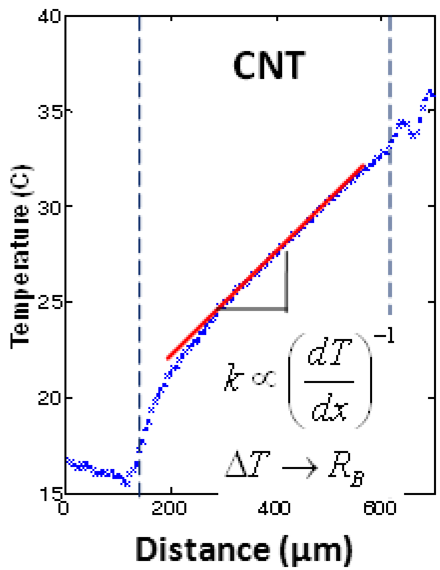
Interfaces **100%**	Nanostructured films & composites, metallic bonding Ab initio simulations and optimization	Stanford Bosch
Metrology **100%**	$(ZT)_{eff}$ including interfaces, thermal cycling High temperature ZT	Stanford USF/NIST
Materials **100%**	Filled skutterudites and half Heusler intermetallics Ab initio simulations for high-T optimization	USF Bosch
Durability **50%**	In-situ thermal cycling tests, properties Interface analysis through SEM, XRD, EDS	Stanford Bosch
Heat sink **50%**	Gas/liquid simulations using ANSYS-Fluent Novel cold HX using microfluidics, vapor venting	Bosch Stanford
System **50%**	System specification, multiphysics code Evaluation of research impacts	Bosch Stanford

Approach: Thermal & Mechanical Properties of CNT Interface Films

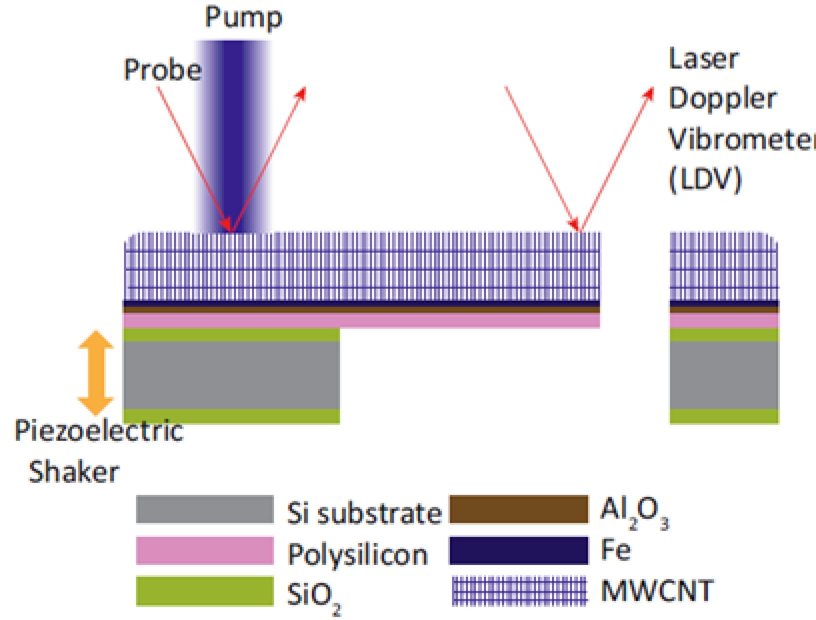
(special thanks to ONR/Mark Spector)

Cross-sectional IR Microscopy with in-situ Thermal Cycling

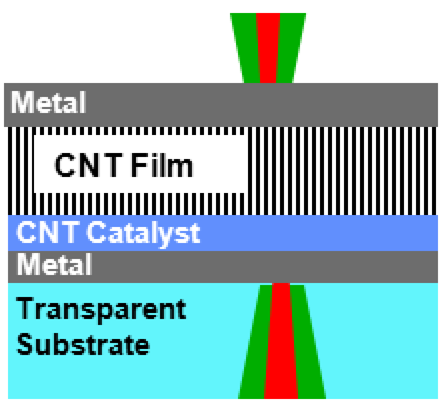




Mechanical Characterization



Pico/Nanosecond Thermoreflectance

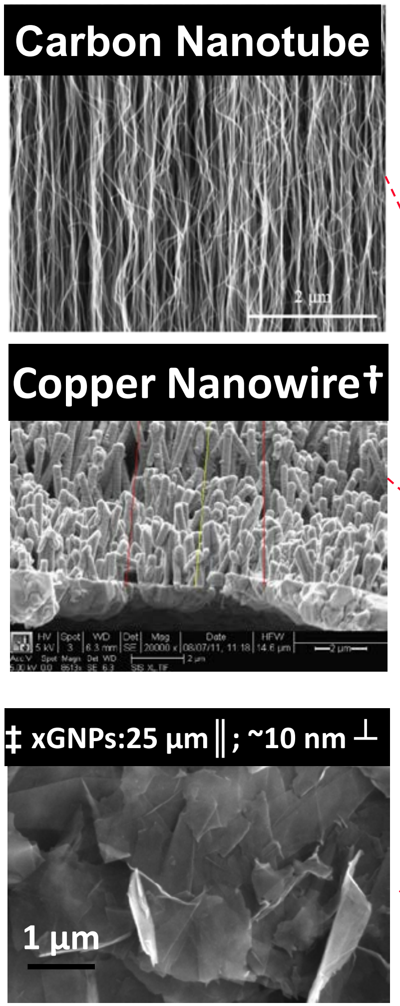


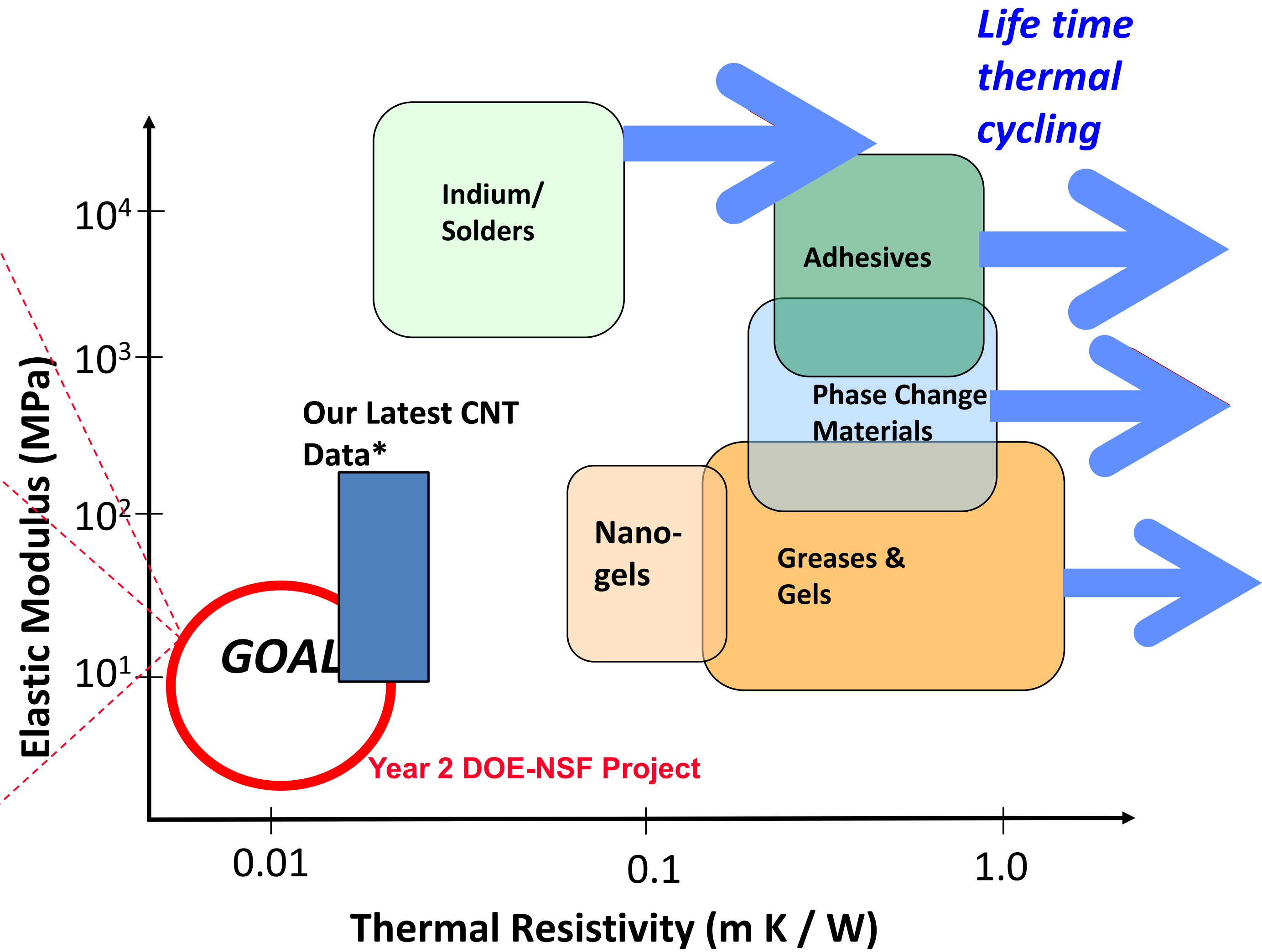
Four Separate Papers at ITHERM, May 2012

Gao, Won, Godson, et al.,	*Carbon*	(2012, in press)
Won, Gao, Panzer, Goodson, et al.	*Carbon*	(2012)
Marconnet, Panzer, Goodson, et al.	*ACS Nano*	(2011)
Gao, Shakouri, Goodson et al.	*J. Electronic Materials*	(2010)
Panzer, Murayama, Goodson et al.	*Nano Letters*	(2010)
Panzer, Goodson	*J. Applied Physics*	(2008)
Panzer, Dai, Goodson et al.	*J. Heat Transfer*	(2008)
Hu, Fisher, Goodson et al.	*J. Heat Transfer*	(2006, 2007)
Pop, Dai, Goodson et al.	*Nano Letters*	(2006)
Pop, Dai, Goodson et al.	*Physical Review Lett.*	(2005)

Approach: Nanostructured Interfaces

Nanostructured Interfaces





******Gao, Goodson, et al., J. Electronic Materials* (2010).
Won, Goodson, et al., Carbon (2012a, 2012b)

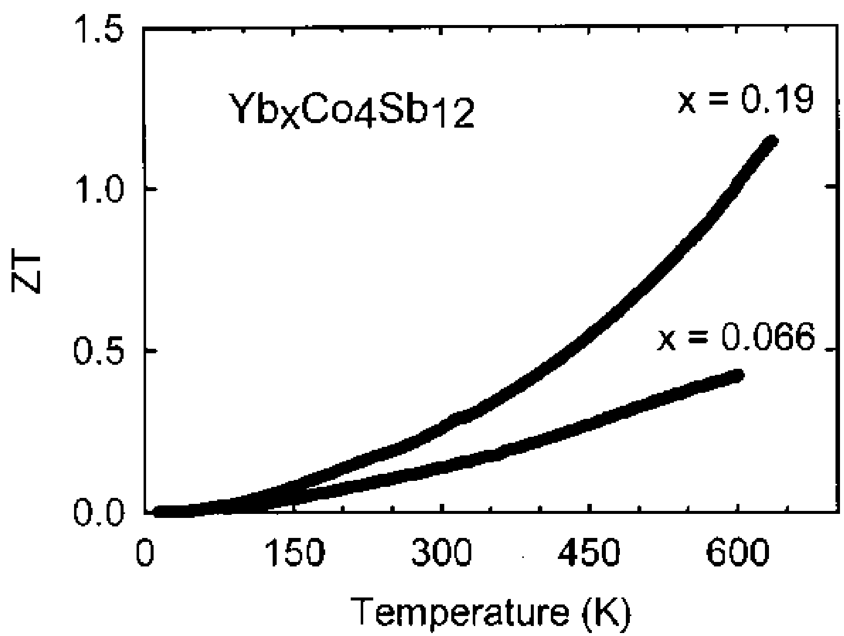
†In collaboration with group of Prof. Fritz Prinz, Stanford
‡www.xgsciences.com

Approach: Bulk TE Materials for Vehicles

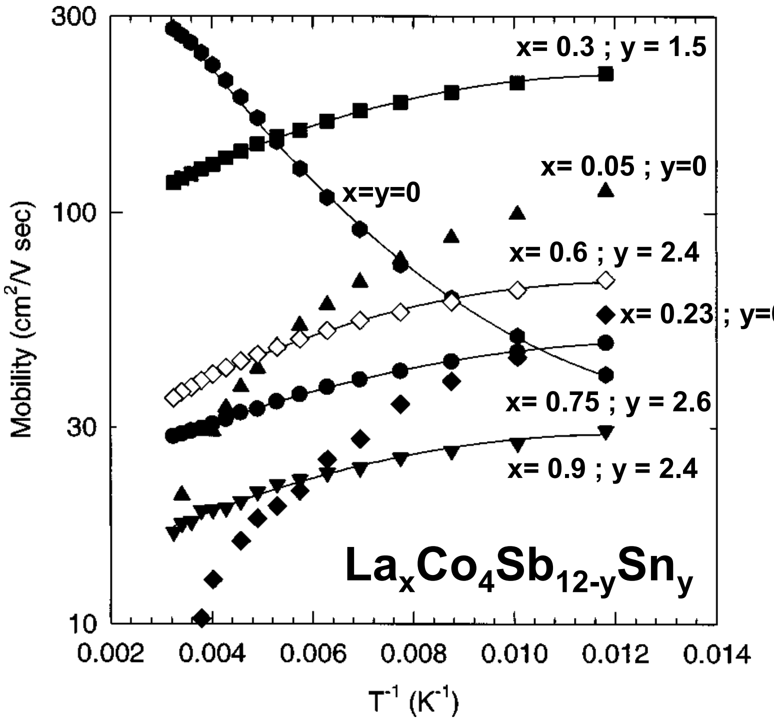
Nolas, Kaeser, Littleton, Tritt, APL 77, 1855 (2000), Nolas, JAP 79, 4002 (1996)
Lamberton, G.S. Nolas, et al APL 80, 598 (2001)

• *Skutterudites with partial filling using heavy, low valence "guest" atoms*

Heavy-ion Filling Yields Lower Thermal Conductivity. Low Valence Filling Facilitates Optimization of Power Factor.



Partial Filling – Optimization of Power Factor & Thermal Conductivity



• *Half-Heusler alloys: small grain-size provides for disordered state*

George S. Nolas
Department of Physics,
University of South Florida

NOVEL MATERIALS LABORATORY
UNIVERSITY OF SOUTH FLORIDA

Approach: Materials Computation

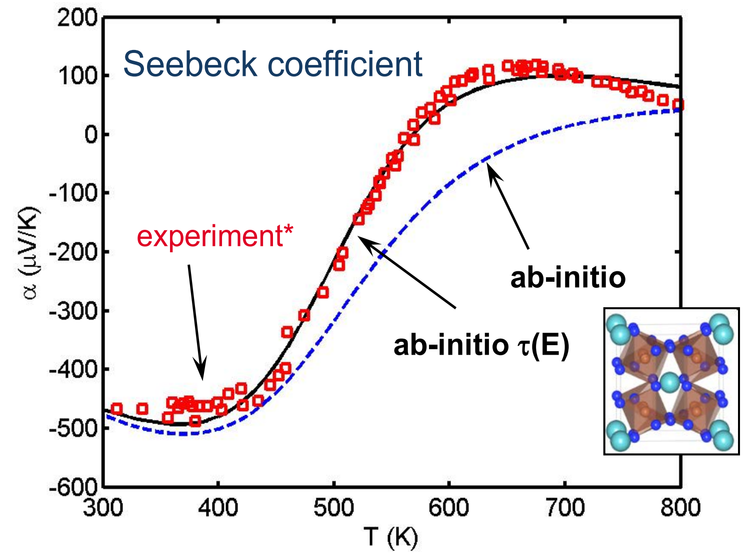
- Predictive computations of TE materials
  - Electronic conductivity
  - Seebeck coefficient
  - Thermal conductivity

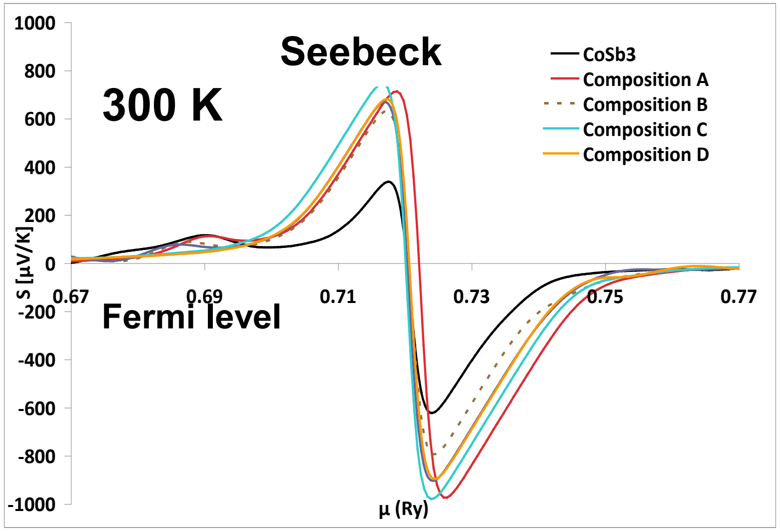
- Understanding of transport mechanisms on atomic level and composition trends from ab-initio

- Composition screening in skutterudites
  - Several new compositions predicted with higher Seebeck than base-line $CoSb_3$

- Trade-offs with conductivity investigated

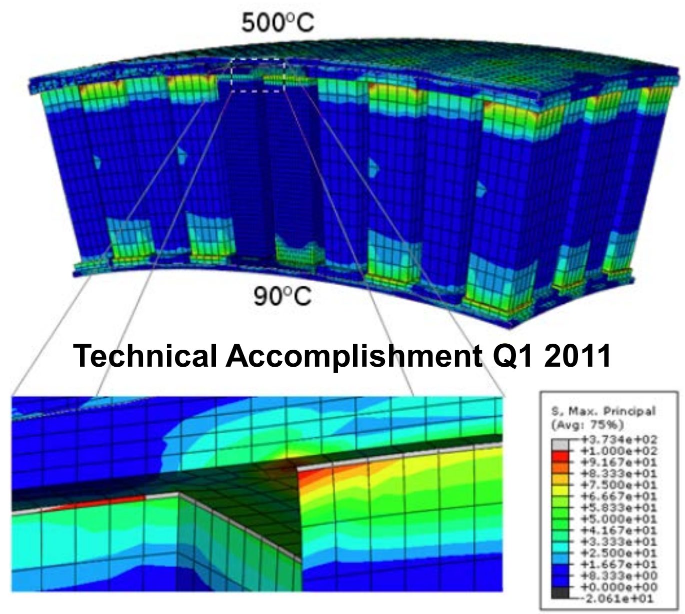
- Collaborative work with Nolas group focuses on Yb and Eu-filled skutterudites

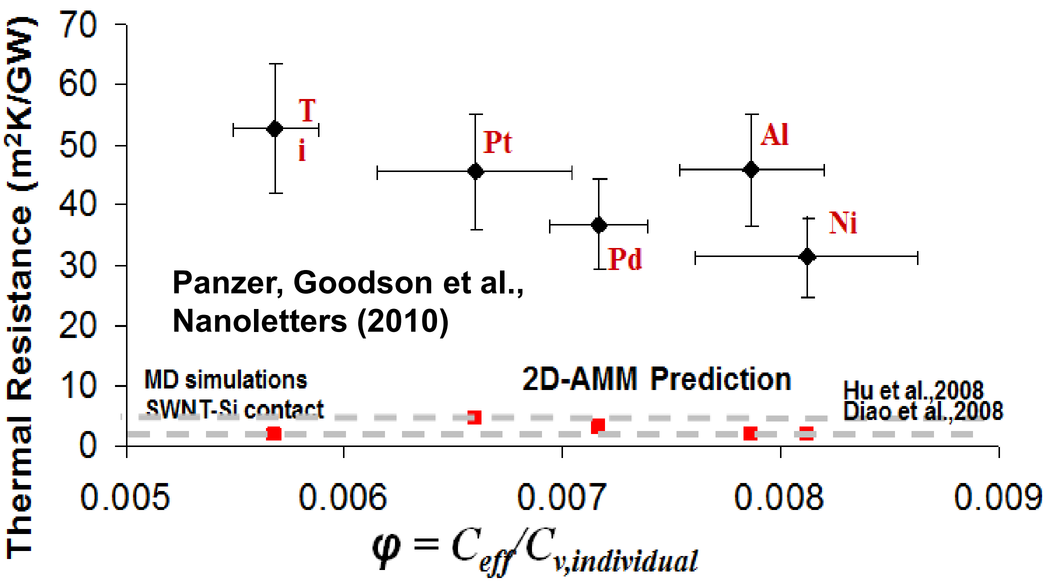


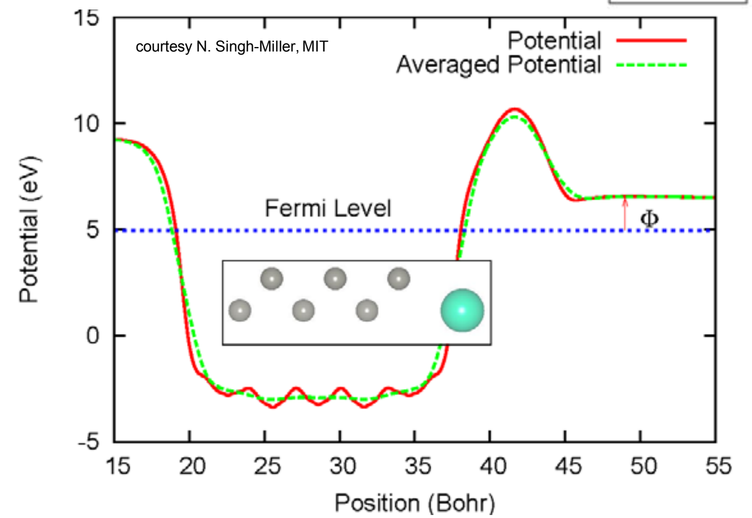


Approach: Interface Optimization

- **Thermal characterization** focuses on interface engagement, nanotube wetting, and stability
- **Mechanical modeling** of interfaces allows screening of compositions to improve thermo-mechanical stability
  - Chemical reactivity at interfaces considering phase stability
  - Ab-initio computations and measurements of modulus, CTE
  - Q1/2011: Analysis of mechanical stresses at interfaces – in-plane stress limitations using computed and measured CTE
  - Q1/2011: Cross-section of leg found to be related to the critical stress, strong implications for materials strength for cost reduction
- **Electronic transport across contacts**
- Work function and barrier calculations set up and calibrated
- Key numerical screening criteria identified: Fermi level and band offsets, Schottky barrier heights







Computed electrostatic potential

Technical Accomplishment: Publications

5 Full-Length Papers Accepted, after review, for ITHERM 2012

1. Barako, Gao, Marconnet, Asheghi, Goodson, “Solder-Bonded Carbon Nanotube Thermal Interface Materials,” Proceedings of *ITHERM*, San Diego, May, 2012.
2. Barako, Park, Marconnet, Asheghi, Goodson, “Infrared Imaging and Reliability Study of Thermoelectric Modules under Thermal Cycling,” *ITHERM*, San Diego, May, 2012.
3. Park, Barako, Marconnet, Asheghi, Goodson, “Effect of Thermal Cycling on Commercial Thermoelectric Modules,” *ITHERM*, San Diego, May, 2012.
4. Marconnet, Motoyama, Barako, Gao, Pozder, Fowler, Ramakrishna, Mortland, Asheghi, Goodson, “Nanoscale Conformable Coatings for Enhanced Thermal Conduction of Carbon Nanotube Films,” *ITHERM*, San Diego, May, 2012.
5. Gao, Kodama, Won, Dogbe, Pan, and Goodson, “Inhomogeneous Mechanical Properties of Vertically Aligned Multi-walled Carbon Nanotube Films,” *ITHERM*, San Diego, May, 2012.

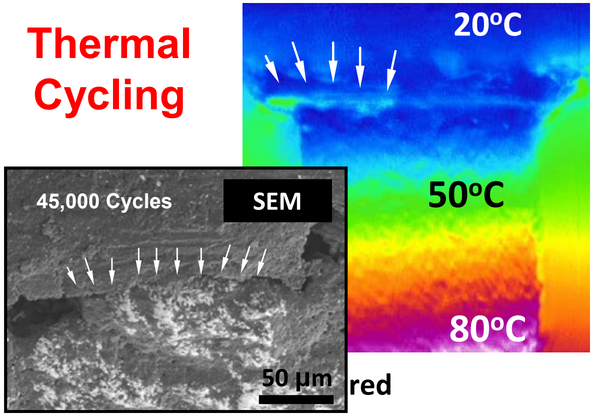
4. Won, Gao, Panzer, Dogbe, Pan, Kenny, Goodson, 2012, "Mechanical Characterization of Aligned Multi-Wall Carbon Nanotube Films," *CARBON*, Vol. 50, pp 347-355.
5. Marconnet, Yamamoto, Panzer, Wardle, Goodson, 2011, "Thermal Conduction in Aligned Carbon Nanotube-Polymer Nanocomposites with High Packing Density," *ACS Nano*, Vol. 5, pp. 4818-4825.
6. Marconnet, Panzer, Goodson, “Thermal Conduction Phenomena in Carbon Nanotubes and Related Nanostructured Materials,” invited and submitted, *Reviews of Modern Physics*.
7. Gao, Kodama, Dogbe, Pan, Goodson, “Nonhomogeneous Mechanical Properties of Vertically Aligned Multi-Walled Carbon Nanotube Films,” *CARBON,* accepted and in press.
8. Leblanc, Phadke, Kodama, Salleo, Goodson, “Electrothermal Phenomena in Zinc Oxide Nanowires and Contacts,” *Applied Physics Letters*, accepted and in press.
9. Garg, Bonini, Kozinsky, Marzari, "Role of Disorder and Anharmonicity in the Thermal Conductivity of Silicon-Germanium Alloys: A First-Principles Study,” *Physical Review Letters*, 106, 045901 (2011).
10. Volja, Kozinsky, Li, Wee, Marzari, Fornari, "Electronic, vibrational and transport properties of pnictogen substituted ternary skutterudites,” submitted to *Physical Review B*.

7 Archival Journal Papers Appeared or were Accepted

Technical Accomplishments: Stanford Overview

ThermoElectric Module/Pellet

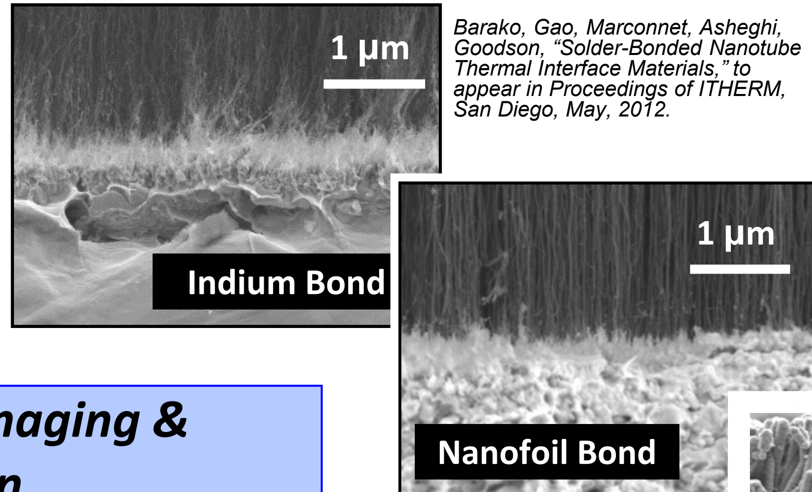
Thermal Cycling



Barako, Park, Marconnet, Asheghi, Goodson, "Infrared Imaging and Reliability Study of Thermoelectric Modules under Thermal Cycling," to appear in Proceedings of ITHERM, San Diego, May, 2012.

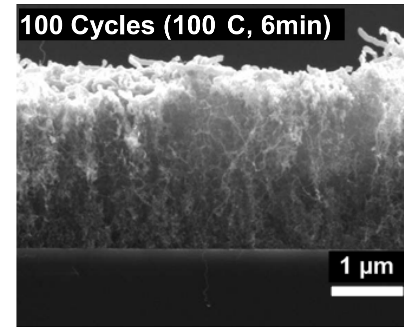
Nanostructured Interfaces

Solder-Bonded Nanotube Thermal Interface Materials



Barako, Gao, Marconnet, Asheghi, Goodson, "Solder-Bonded Nanotube Thermal Interface Materials," to appear in Proceedings of ITHERM, San Diego, May, 2012.

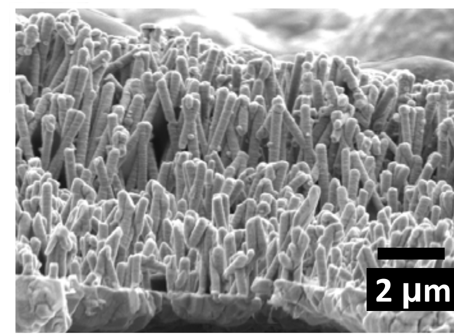
Thermal Cycling

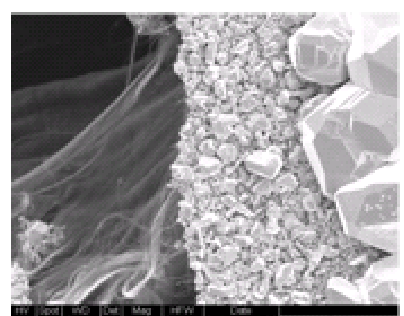


Gao, Panzer, Goodson et al., J. Electronic Materials, 2010

Electrodeposited Metal Nanowire TIMs

Michael Barako, Unpublished research

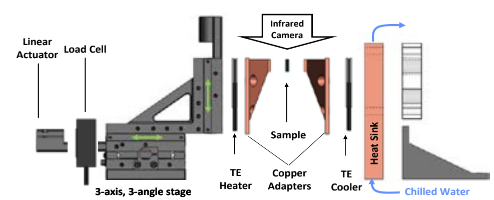


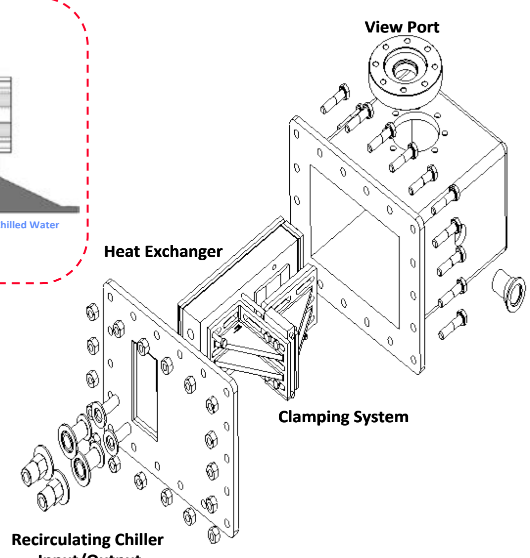


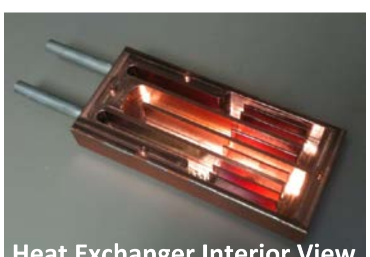
Nanoscale Conformable Coatings for Enhanced Thermal Conduction of CNT Films

Marconnet, Motoyama, Barako, Gao, Pozder, Fowler, Ramakrishna, Mortland, Asheghi, and Goodson, "Nanoscale Conformable Coatings for Enhanced Thermal Conduction of Carbon Nanotube Films," to appear in *Proceedings of ITHERM*, San Diego, May, 2012.

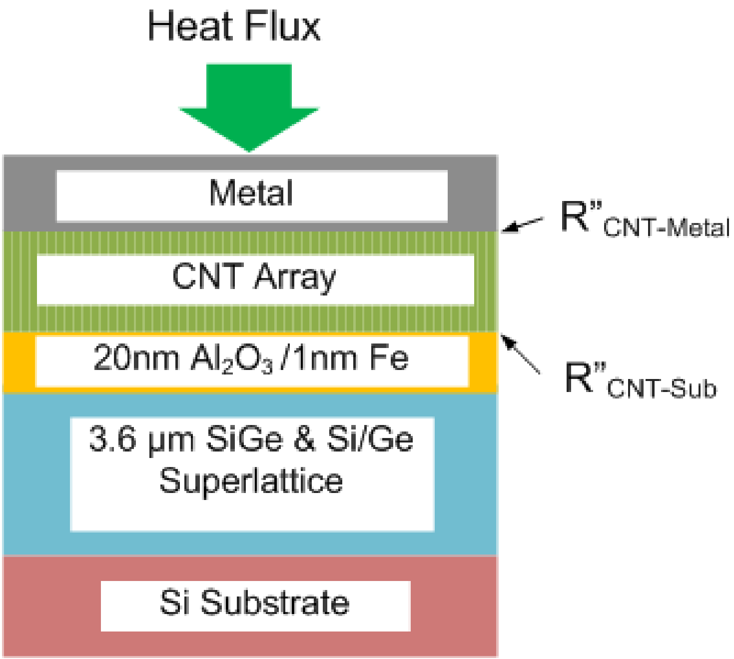
High Temperature IR Imaging & Characterization

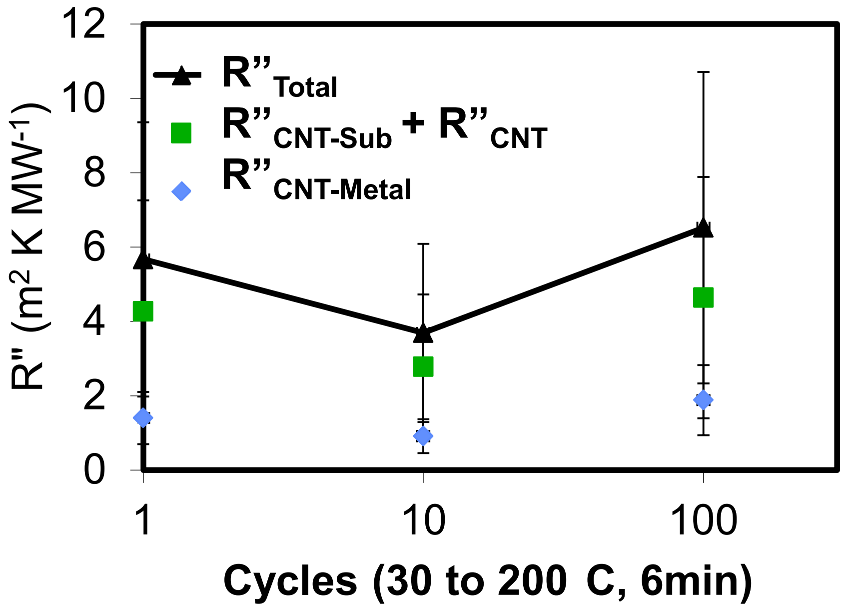




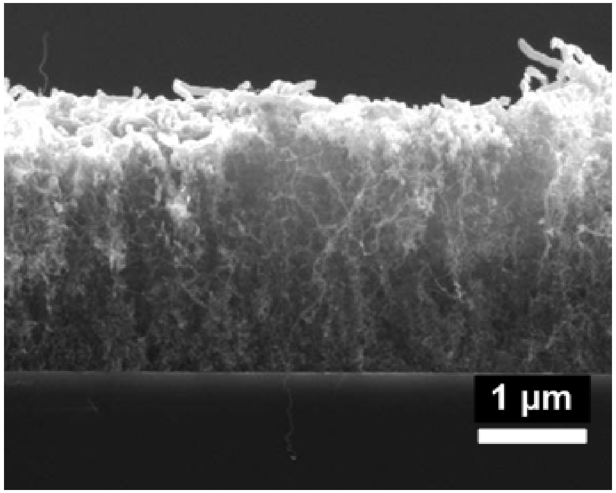


Technical Accomplishment : Interface Characterization on Thermoelectric with Thermal Cycling





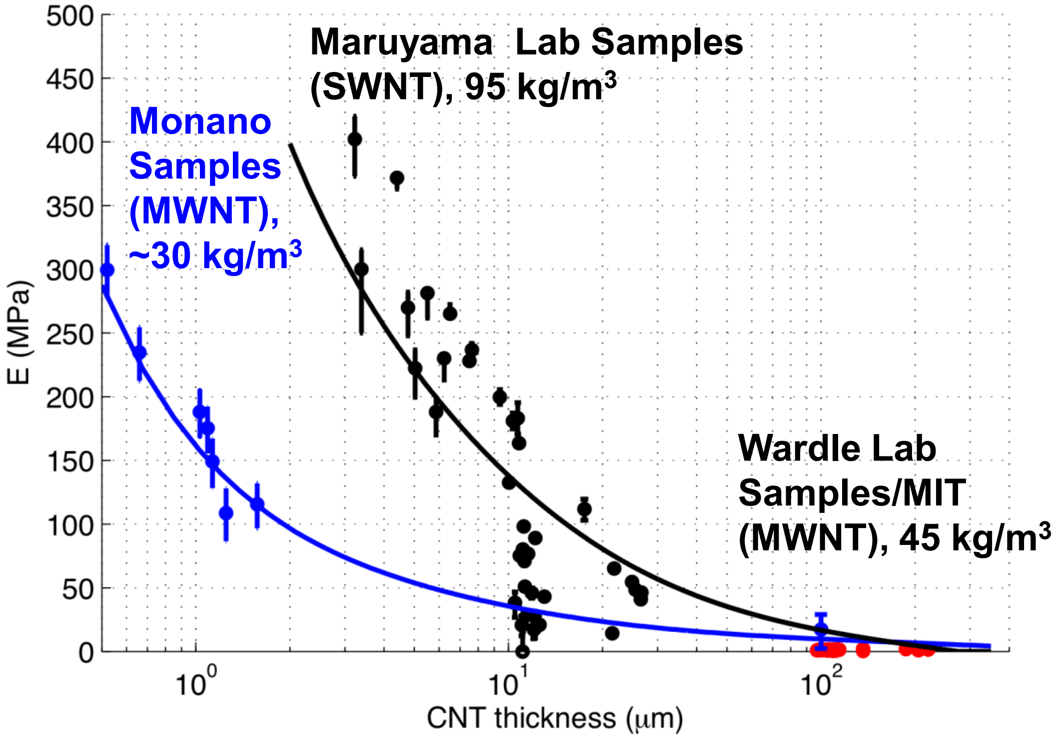
Resistances for 1.5, 2.5, and 40 micron thick CNT films varied between 0.035 and 0.055 cm^2 °C/W, with evidence of decreasing engagement with increasing film thickness.

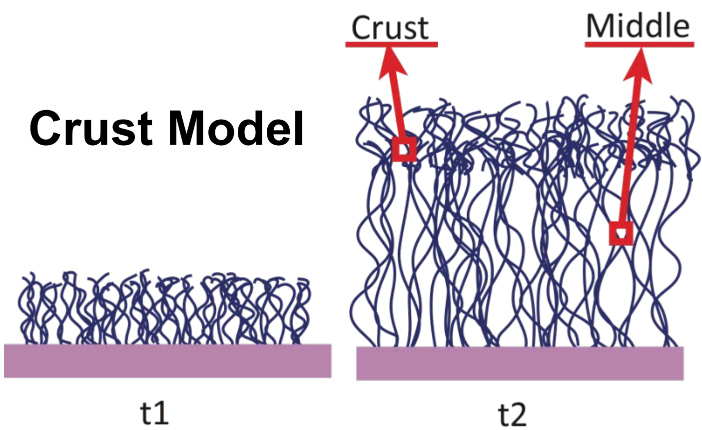


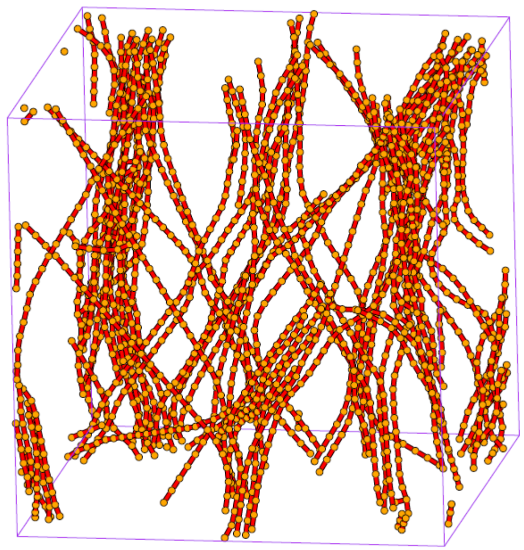
Technical Accomplishment: Mechanical Characterization of CNT Films

Won, Gao, Goodson, et al., "Mechanical Characterization of Aligned Multi-Wall Carbon Nanotube Films," *CARBON* (2012)

	Thickness (μm)	Modulus (MPa)	Density (kg/m³)
$SWCNT_{Top}$	1	600	110
$SWCNT_{Middle}$	0-25	0.5	95
$MWCNT_{Top}$	0.4	300	40
$MWCNT_{Middle}$	0-150	10	29
Polysilicon	5.8-8.7	155e3	2330







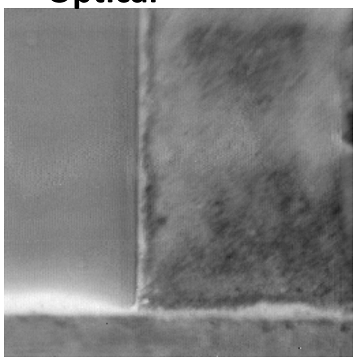
Zipping/Velcro Model

With W. Cai Group, Stanford

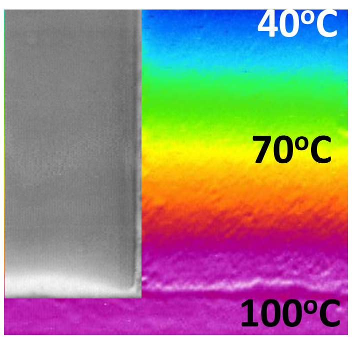
Technical Accomplishment: Infrared Thermometry Failure Analysis of TE Modules

Before Cycling

Optical

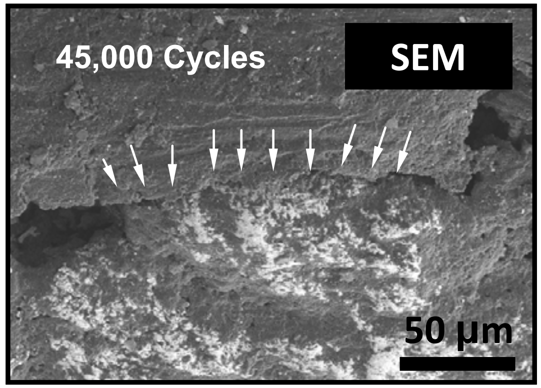


Infrared

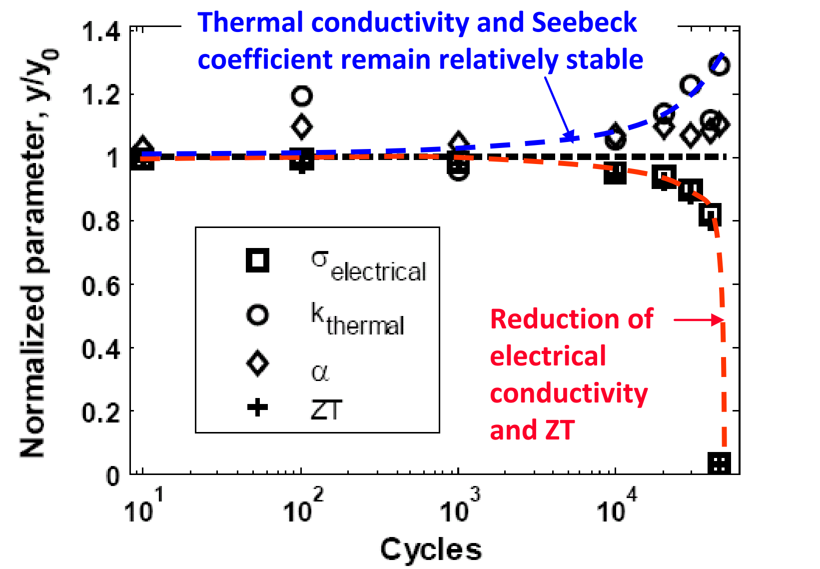


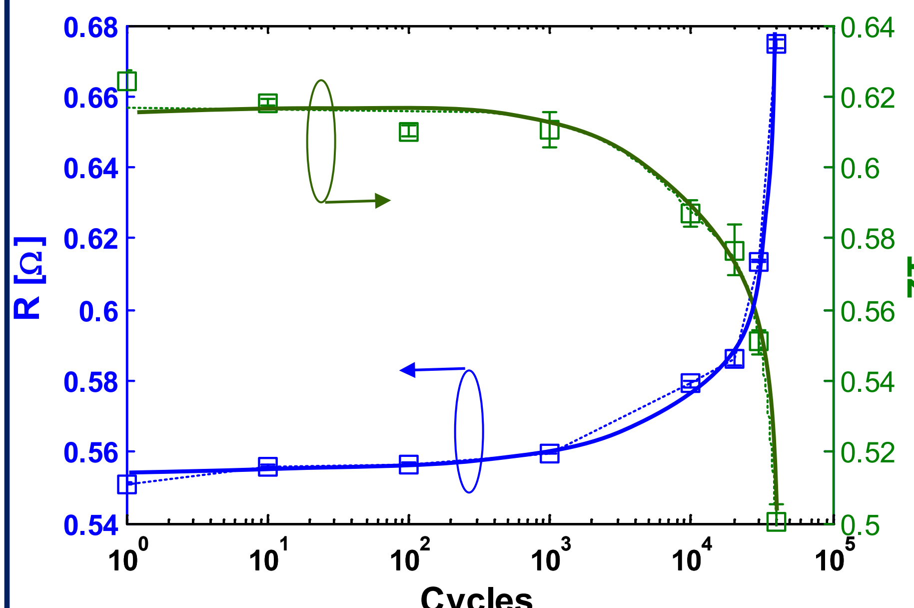
A modified Harman technique was developed to measure the TE figure of merit *ZT* and the electrical resistance *R*.

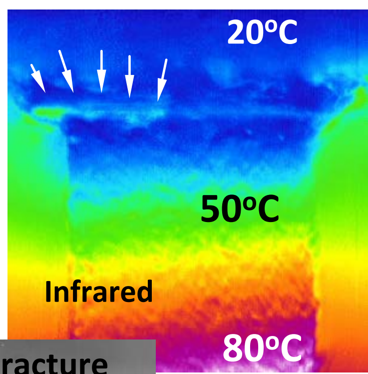
After 45,000 Cycles

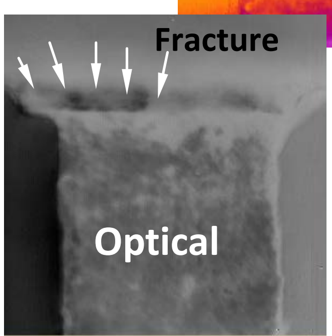


SEM courtesy of Yuan Gao





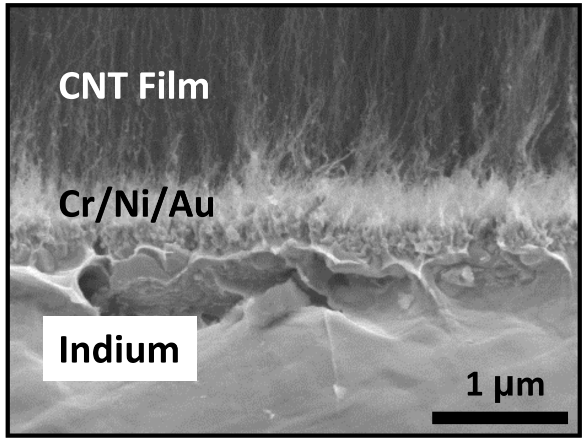




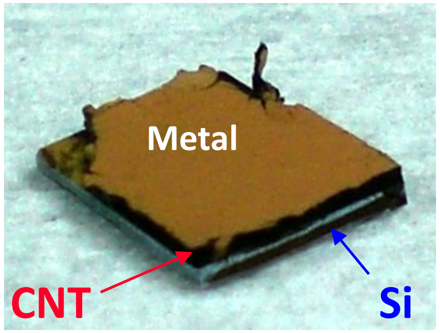
Technical Accomplishment: CNT-Indium Bonding

- Indium (In) foil† is obtained (25 μm thick).
- Cleaned and etched using:
  1. Acetone
  2. Isopropyl alcohol
  3. Deionized water
  4. Solder flux 5R

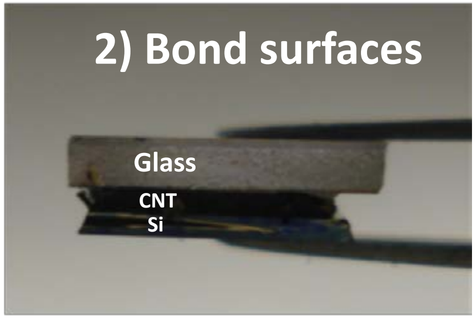
Barako, Gao, Marconnet, Asheghi, Goodson, "Solder-Bonded Nanotube Thermal Interface Materials," Proceedings of ITHERM, May, 2012.

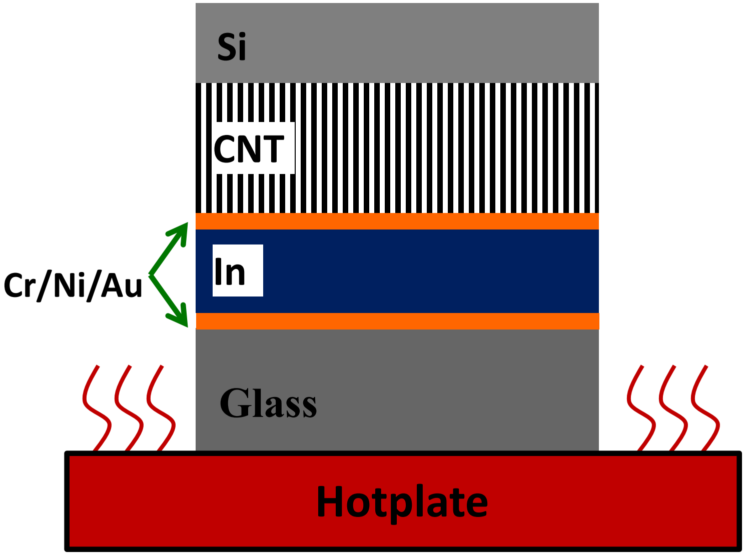


1) Metallize Substrates

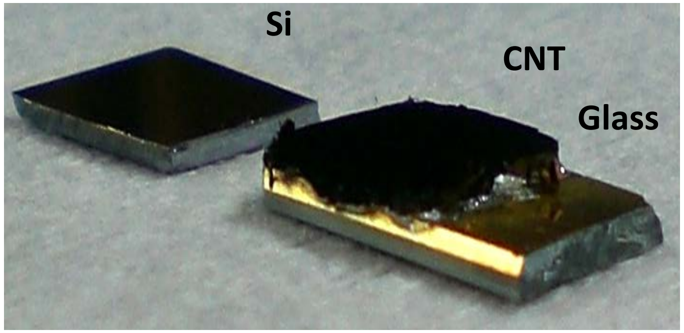


- The foil is compressed between the CNT film and the glass substrate with light pressure
- The stack is placed on a hot plate at 180°C for one minute. This melts and bonds the indium to the adjacent surfaces. (T_{melt} = 156.6°C)





3) Remove growth Si



† Indium foil by Indium Corp.

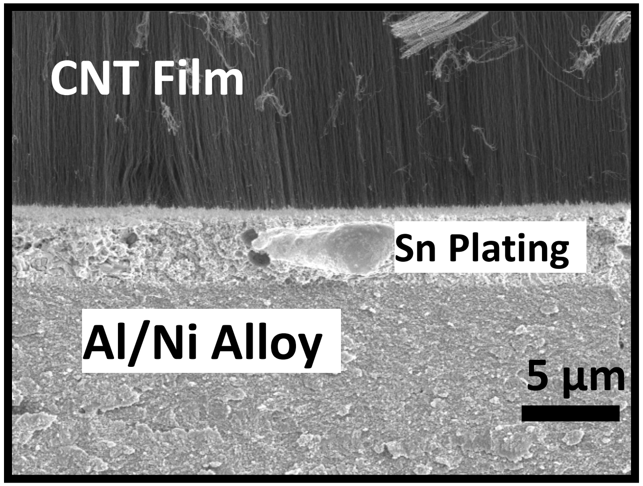
Technical Accomplishment: CNT Nanofoil Bonding

Barako, Gao, Marconnet, Asheghi, Goodson, "Solder-Bonded Carbon Nanotube Thermal Interface Materials," to appear in Proceedings of ITHERM, San Diego, May, 2012.

- Nanofoil‡ (NF) is a 40μm Al/Ni superlattice which ignites and exothermically alloys to adjacent surfaces

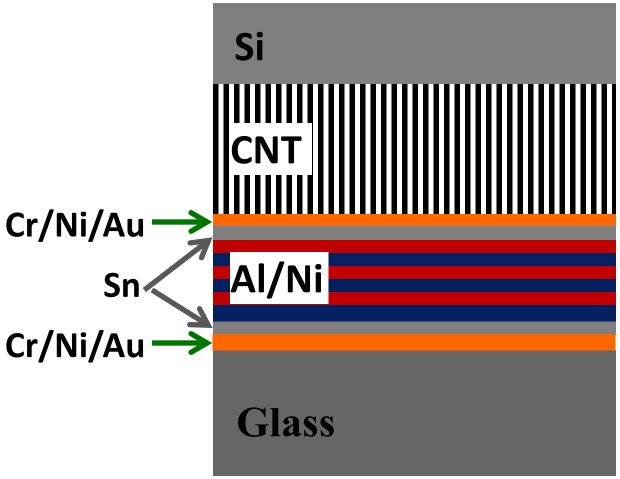
- NF is placed between two gold surfaces. Pressure is applied and the NF is ignited, bonding the two surfaces

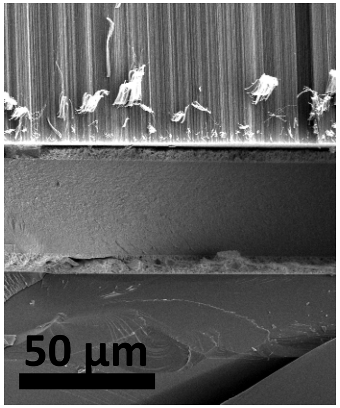
- Sn-plated NF bonds Au surfaces (forming Sn-Au bonds). The resulting intermetallic is stable up to 1000°C

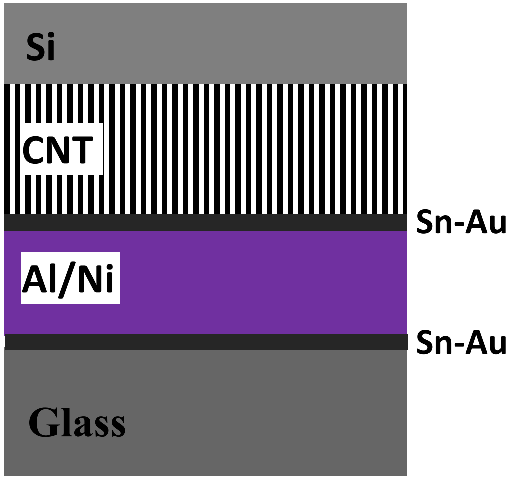


b) NF alloys to form Sn-Au bonds to adjacent surfaces

a) NF is placed between CNT and adjacent surface







‡ Nanofoil® by Indium Corp.

Technical Accomplishment: Pressure-Dependent Infrared Thermometry of CNT Interfaces

Thermal Conductivity

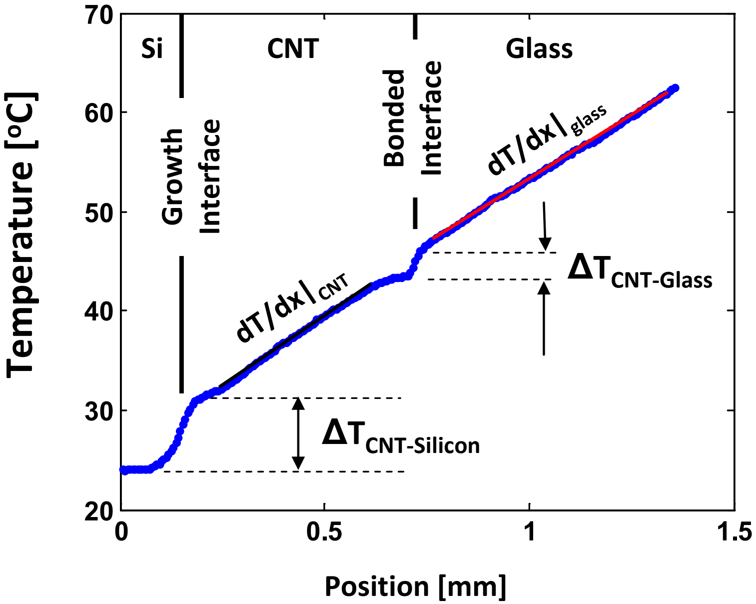
Using conservation of energy, Fourier's Law, and neglecting convection/radiation, we get:

$$\frac{k_{sample}}{k_{ref}} = \frac{\left.\frac{dT}{dx}\right|_{ref}}{\left.\frac{dT}{dx}\right|_{sample}}$$

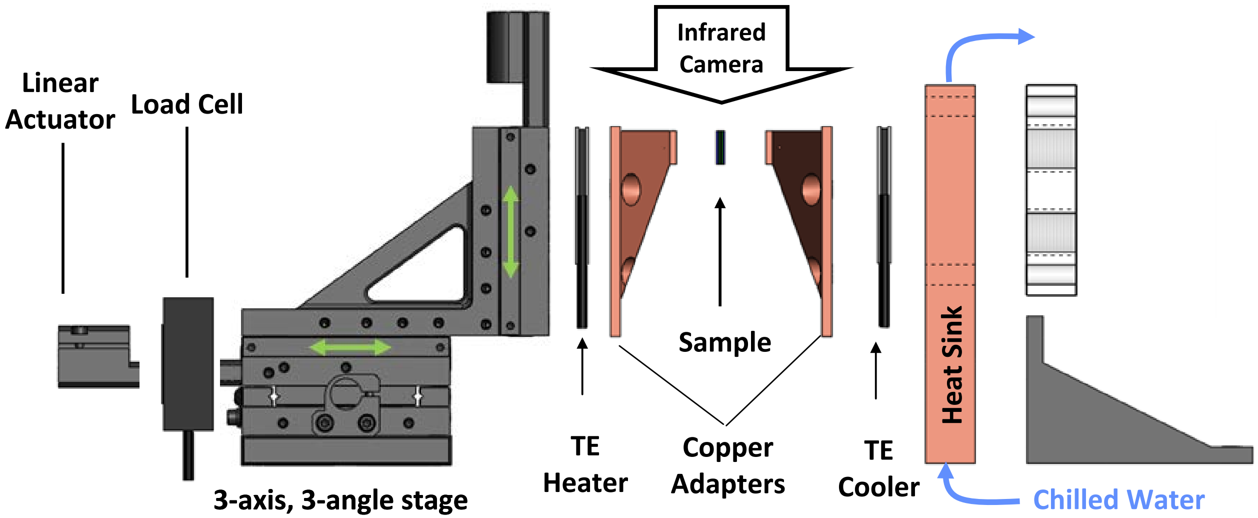
Thermal Boundary Resistance

Using the temperature drop at the interface and Fourier's Law

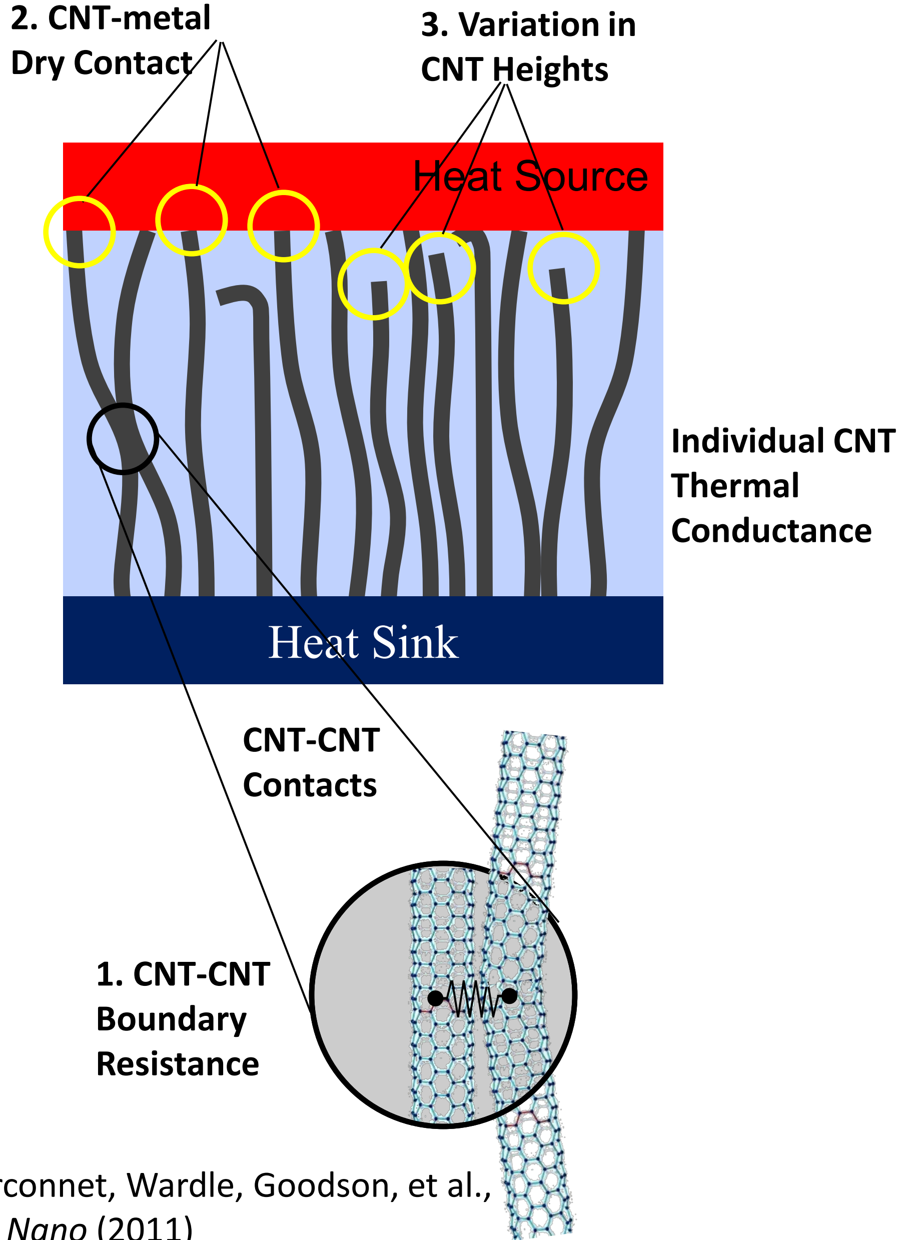
$$R''_{CNT-ref} = \frac{\Delta T_{\mathrm{int}}}{q''} = \frac{\Delta T_{\mathrm{int}}}{k_{ref}\left.\frac{dT}{dx}\right|_{ref}}$$

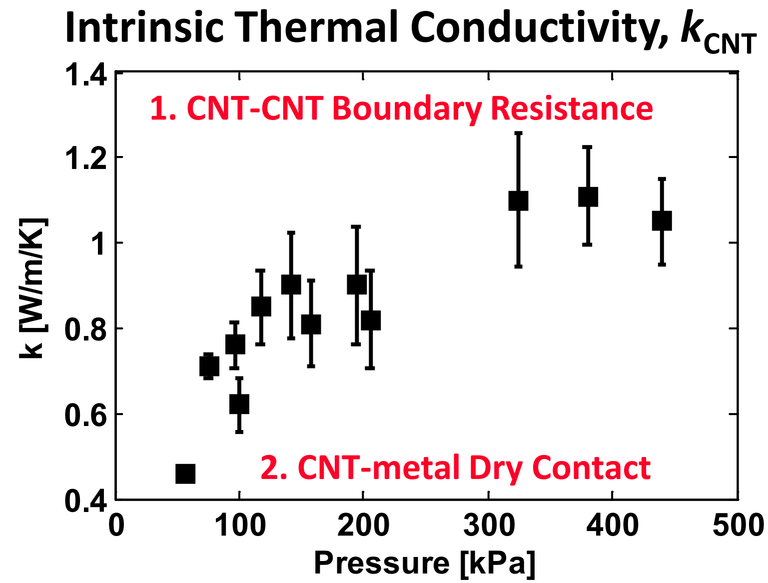


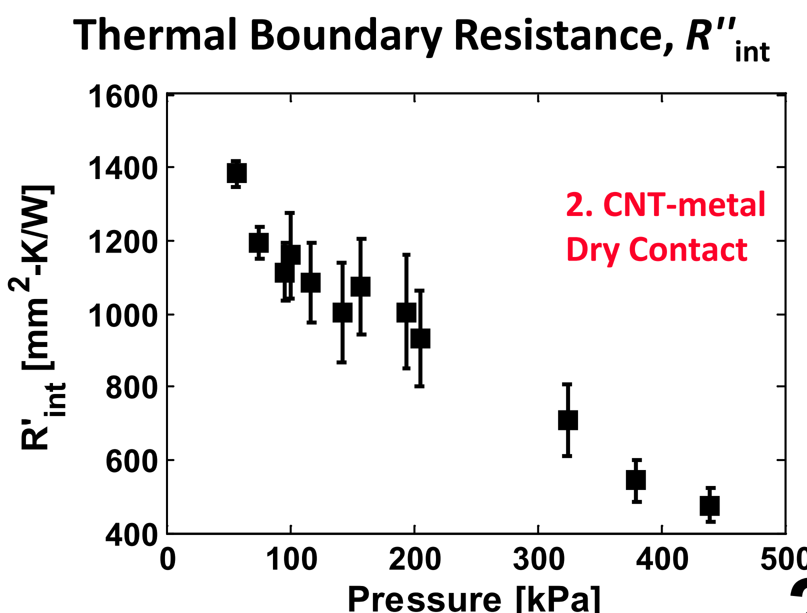
Compressive Measurement Apparatus



Technical Accomplishment: Pressure Dependence Before Bonding



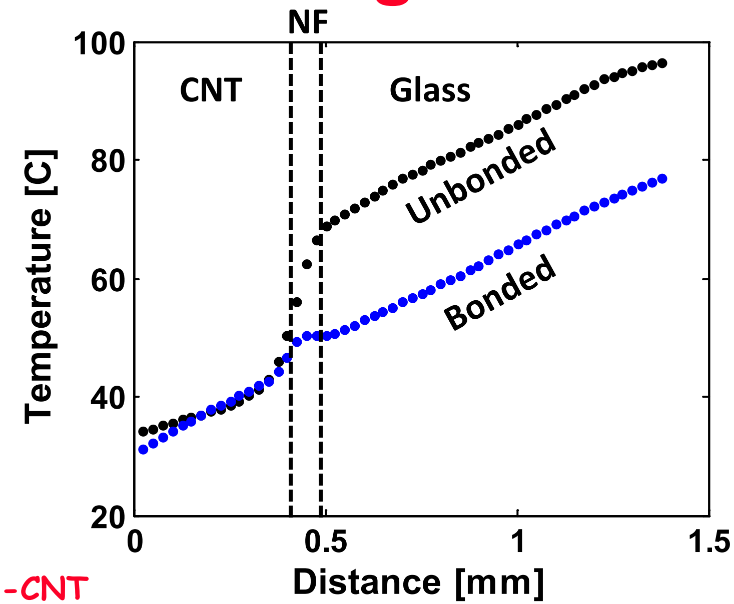




Marconnet, Wardle, Goodson, et al., *ACS Nano* (2011)

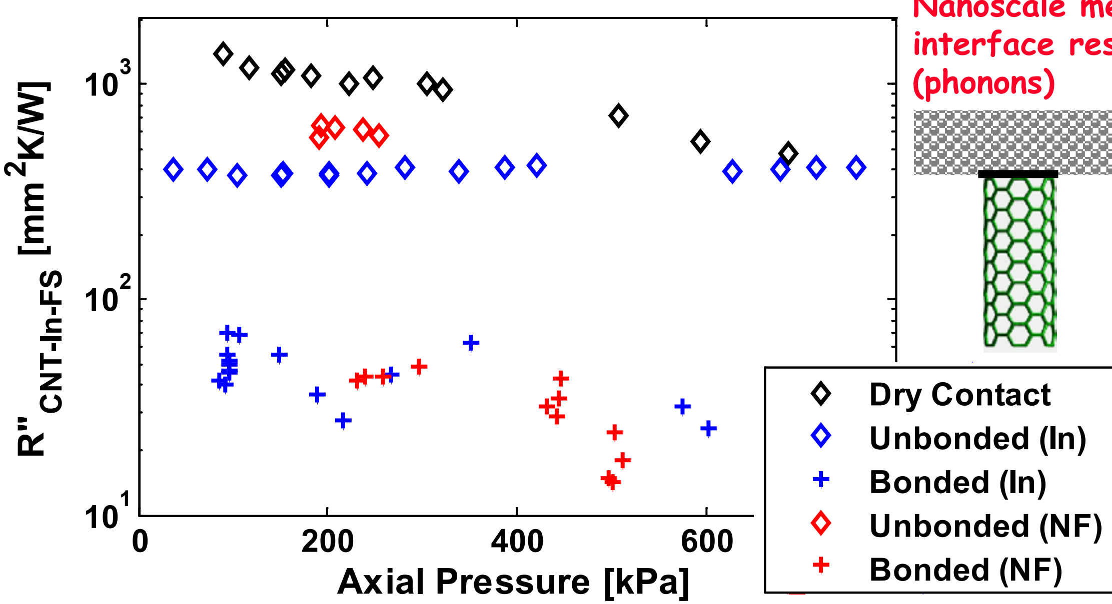
Technical Accomplishment: Pressure Dependence After Bonding

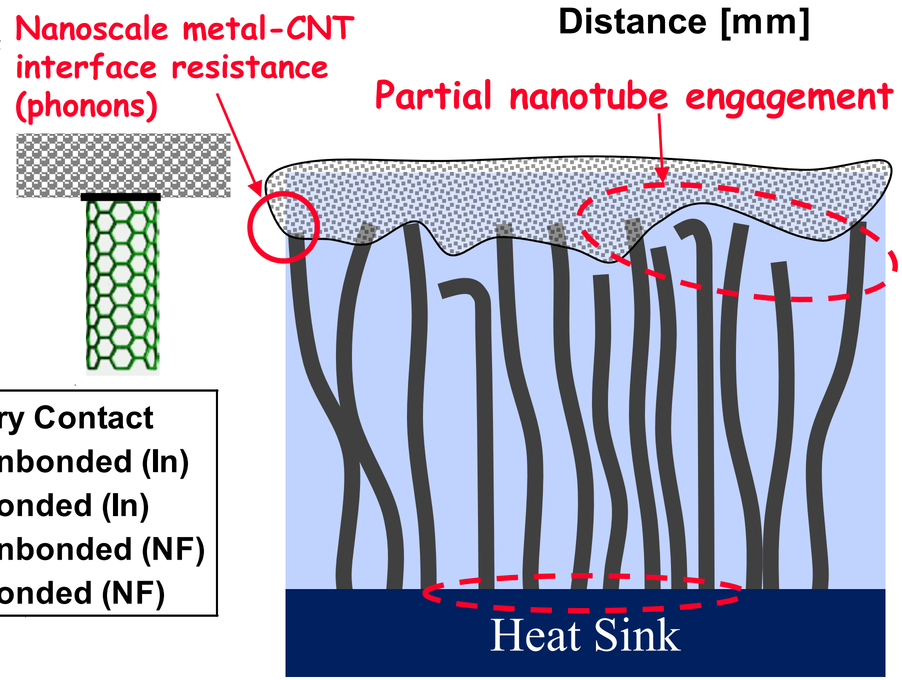
For constant q'', the interfacial temperature drop is reduced by an order of magnitude through solder bonding



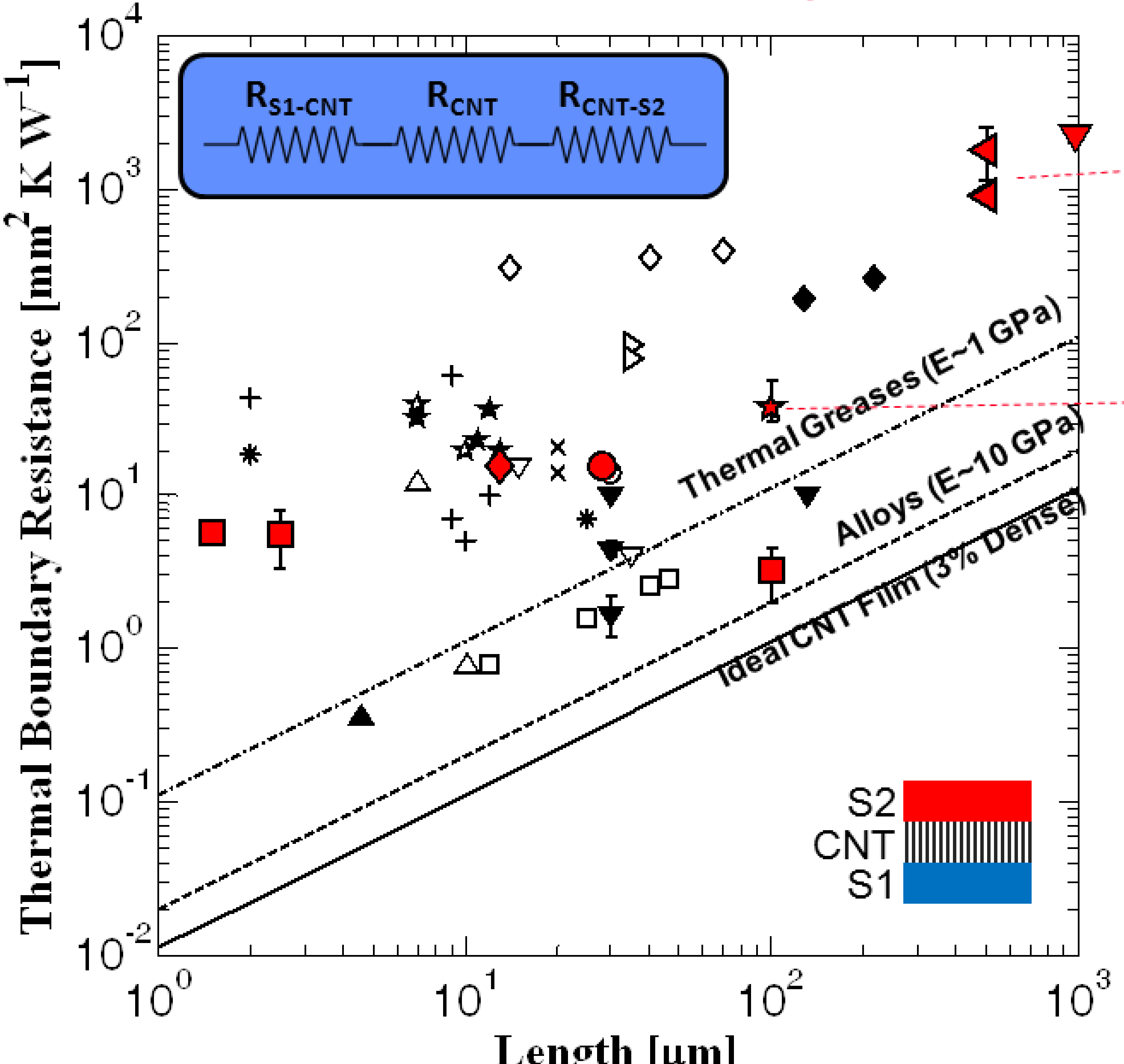
Indium wets to CNTs and engages more CNTs in conduction, increasing the bulk thermal conductivity of the film

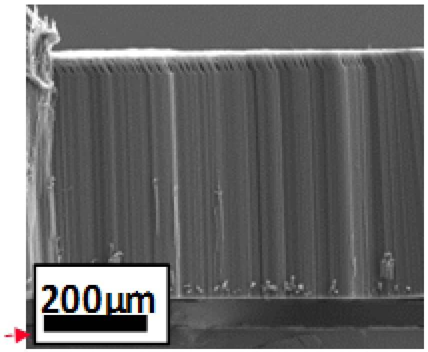
Thermal Boundary Resistance, R''_{int}

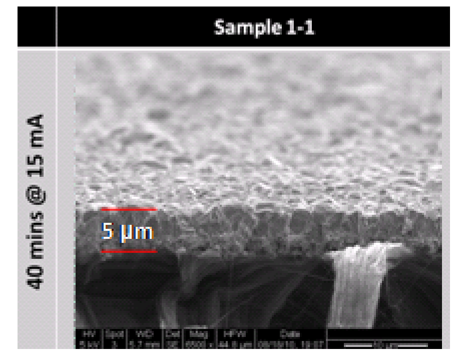




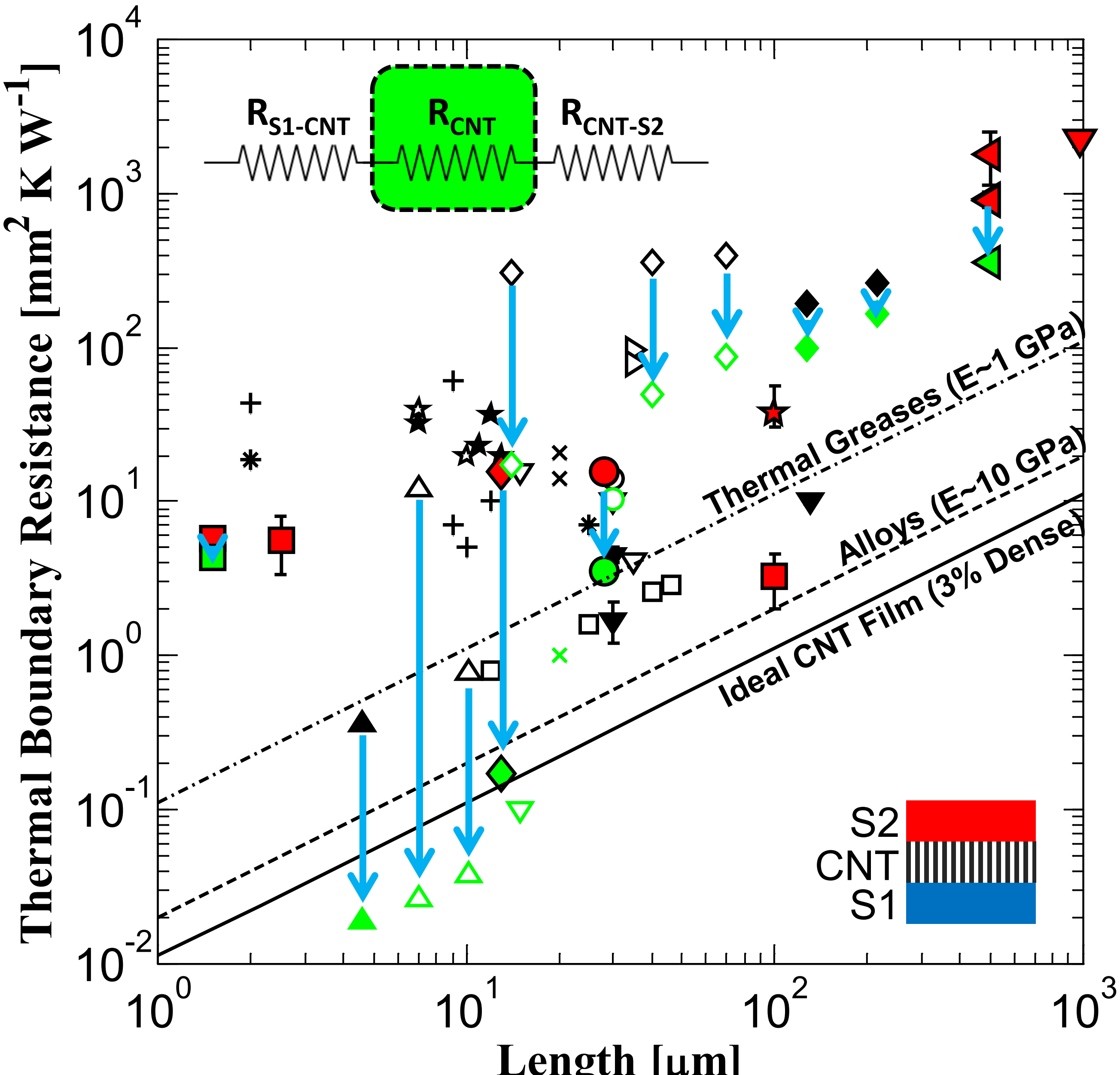
Technical Accomplishment:
Total Thermal Resistance (S1-CNT-S2)







Technical Accomplishment: *Intrinsic* Thermal Resistance

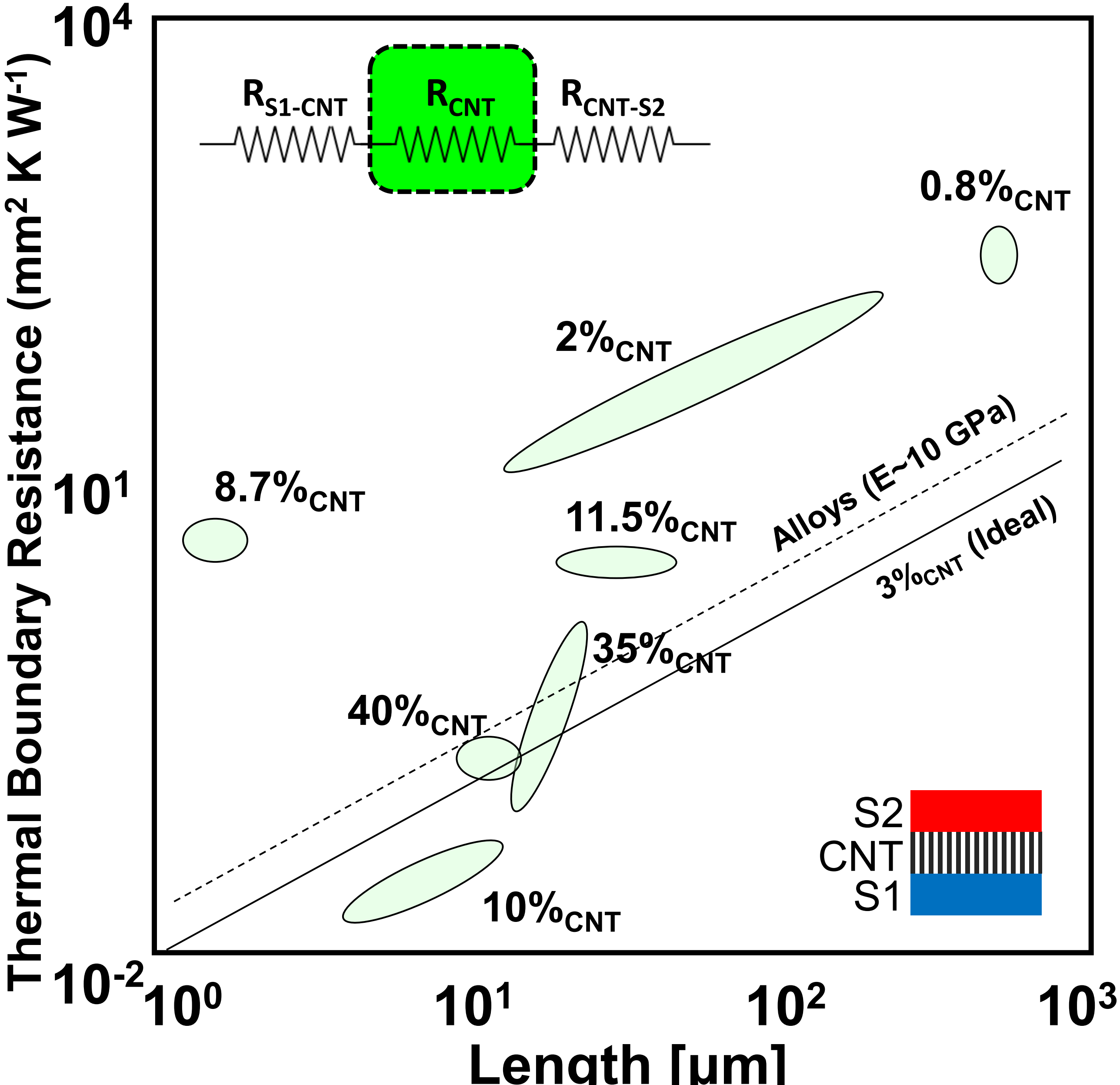


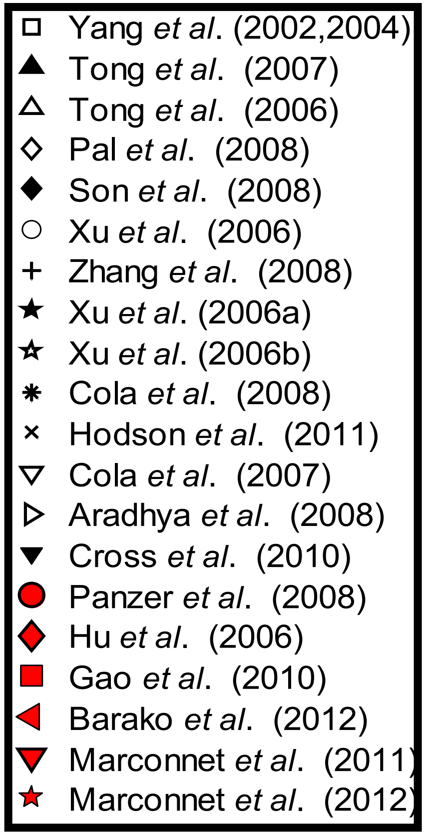
If the CNT-Substrate/ metalization interface resistance could be reduced, the intrinsic thermal resistance of the CNT films would outperform solders

The blue arrow shows the magnitude of R_S1-CNT and R_CNT-S2).

The green data points indicate the magnitude of the intrinsic R_CNT.

Technical Accomplishment: Impact of CNT Volume Fraction on Intrinsic Thermal Conductivity





Technical Accomplishment: Electrodeposited Metal Nanowire TIMs

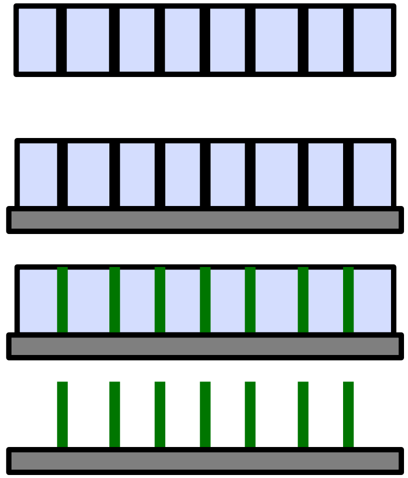
In collaboration with Prinz group, Stanford

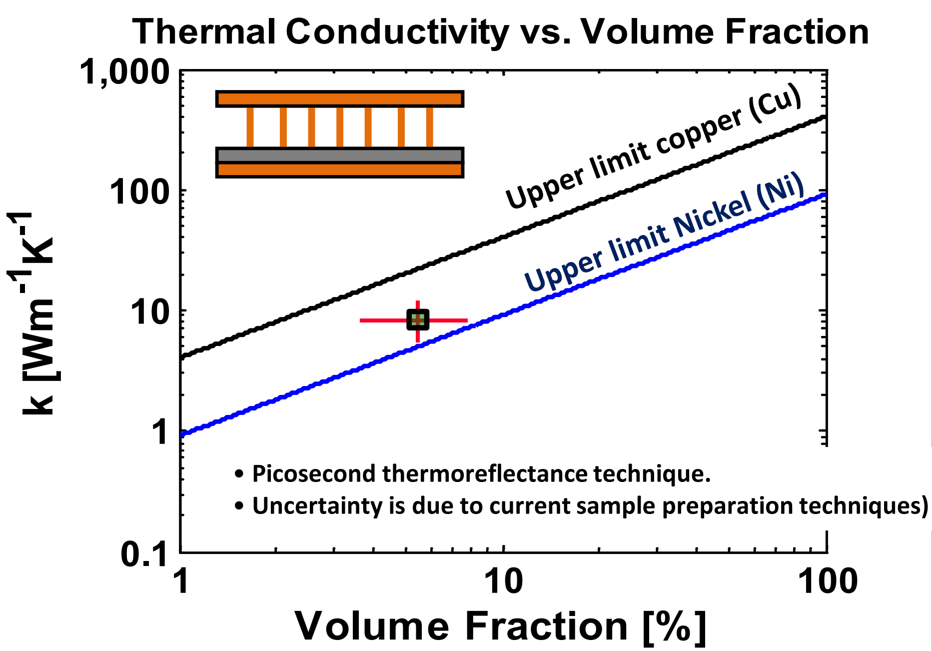
a) Polycarbonate membrane is etched to create cylindrical pores

b) Catalyst Pt/Pd is deposited on one side of the membrane

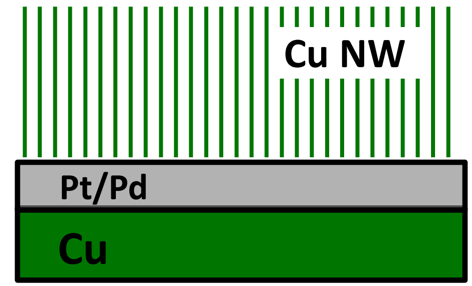
c) Metal is eletrodeposited into the pores

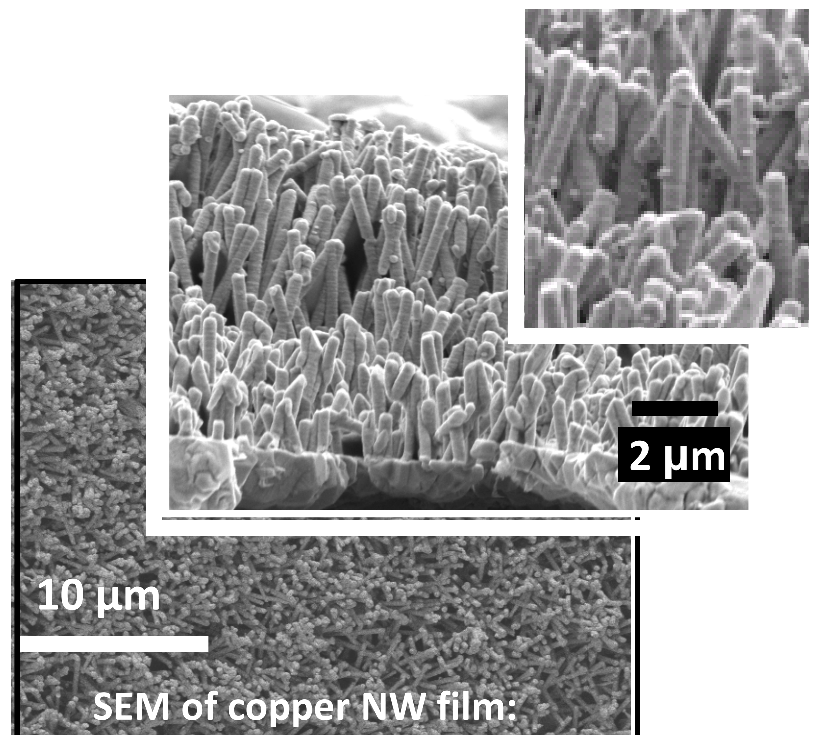
d) Membrane is etched away, leaving freestanding nanowires



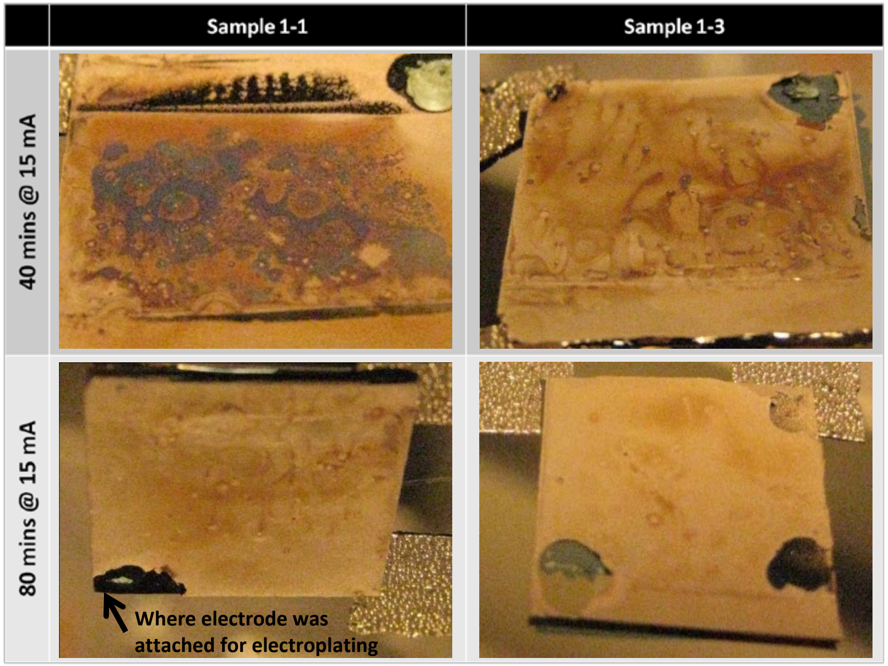


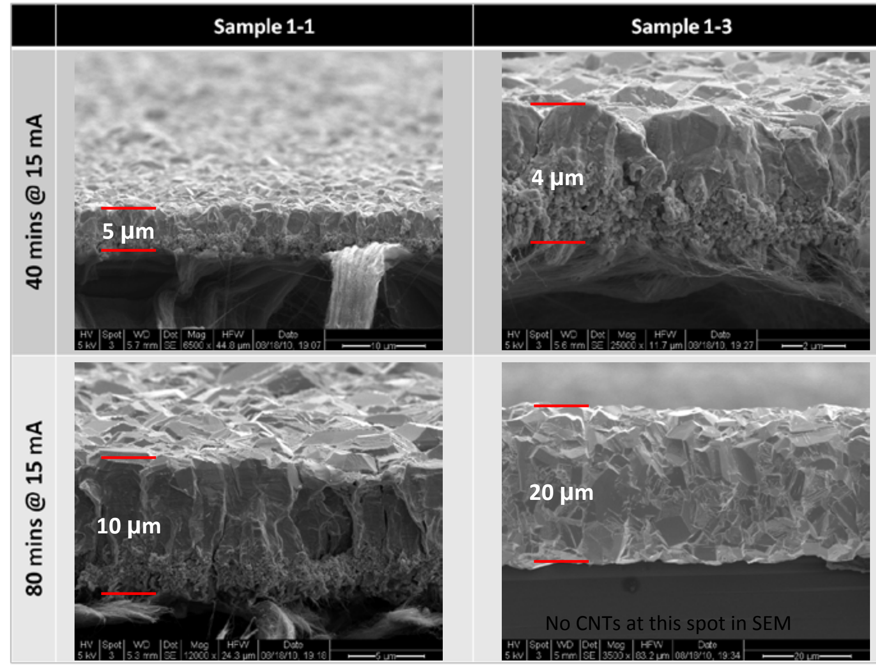
Nominal geometry:
- Cylindrical NWs
- 10 µm film thickness
- 200 nm diameter

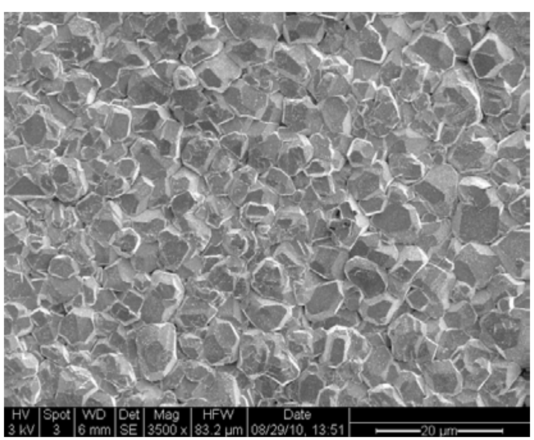


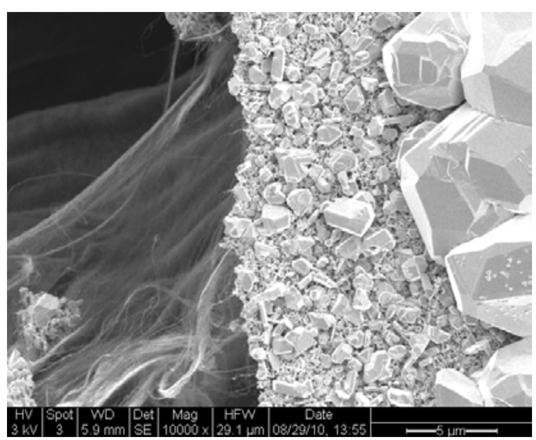


Technical Accomplishment 2011: Nanoscale Conformable Coatings for Enhanced Thermal Conduction of CNTs





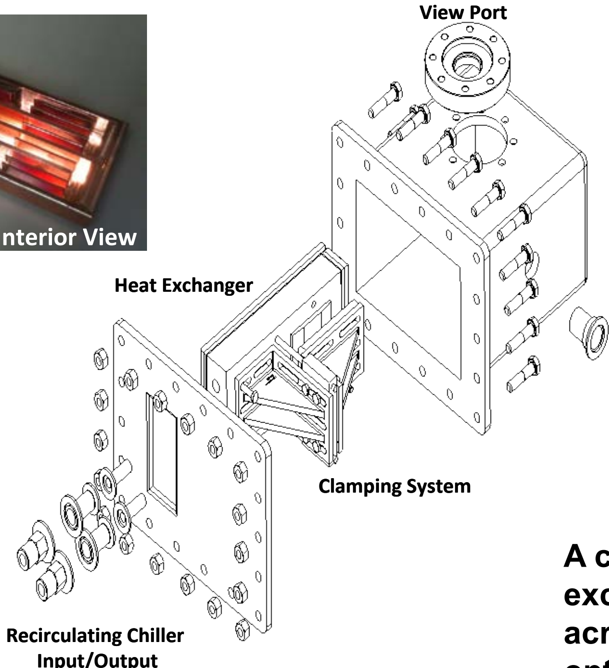


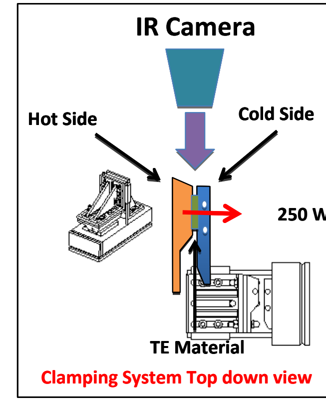


Uniform coating & Grain Size most of the area except where the electrode is attached

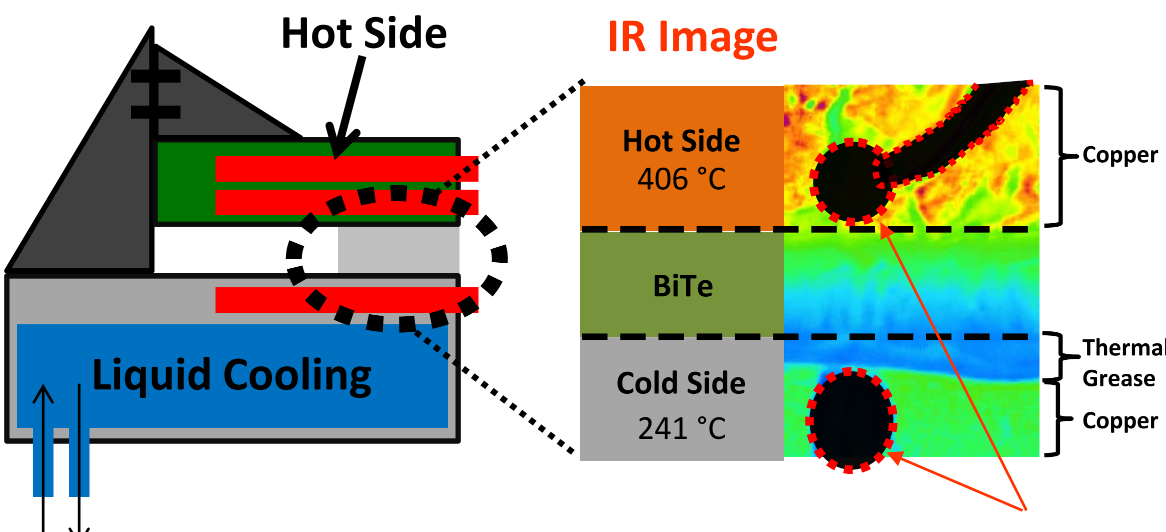
Marconnet, Motoyama, Barako, Gao, Pozder, Fowler, Ramakrishna, Mortland, Asheghi, and Goodson, "Nanoscale Conformable Coatings for Enhanced Thermal Conduction of Carbon Nanotube Films," to appear in Proceedings of ITHERM, San Diego, May, 2012.

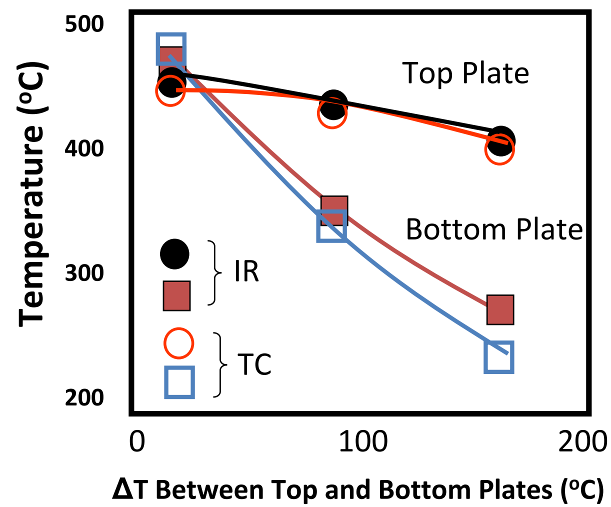
Technical Accomplishment: High Temperature Infrared Imaging





A custom-fabricated vacuum enclosure with integrated heat exchanger will be built to achieve >500 C temperature gradient across a TE sample and facilitate simultaneous electrical and optical measurements.

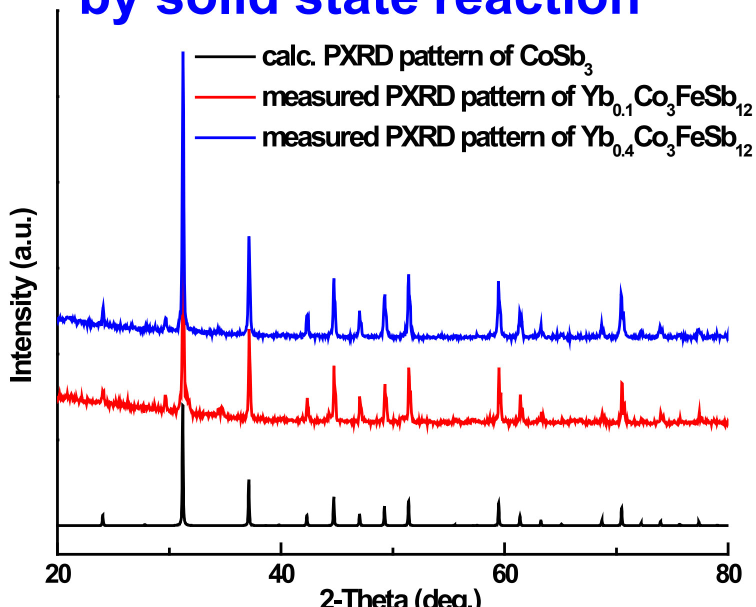




Technical Accomplishment:
Bulk TE Materials for Automotive Applications

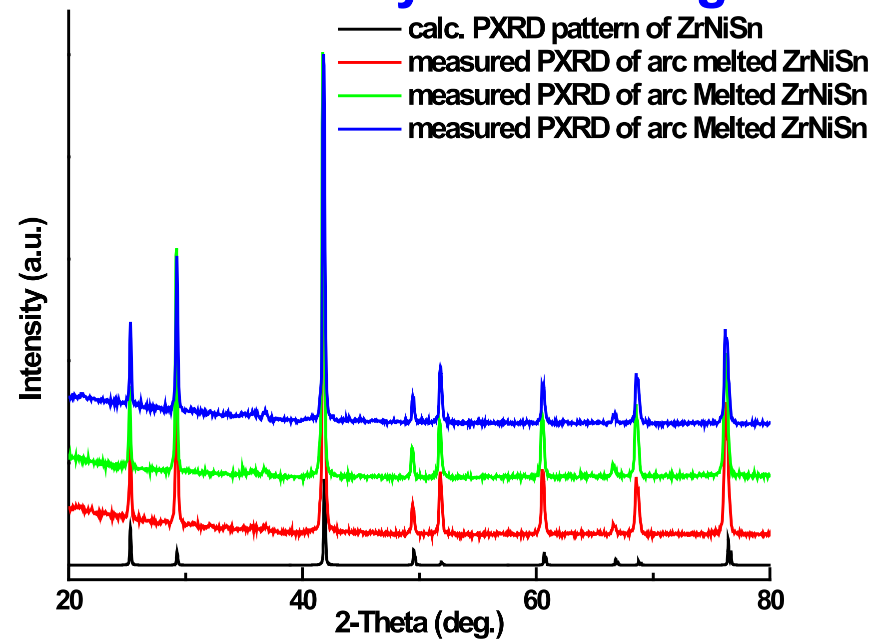
- p-type partially filled and Fe-substituted Skutterudites: $Yb_xCo_{4-y}Fe_ySb_{12}$
- Double filled and Fe-substituted Skutterudites: $Ba_xYb_yCo_{4-z}Fe_zSb_{12}$
- n- and p-type Half-Heusler alloys
- Bi_2Te_3-alloys for High Resolution IR Thermometry (in collaboration with Marlow Industries, Inc.)
- Survey of other material systems with potential for enhanced thermoelectric properties

Yb-filled Fe-substituted $CoSb_3$ by solid state reaction



Thermopower of hot pressed $Yb_{0.4}Co_3FeSb_{12}$ ~ 60μV/K at room temp.

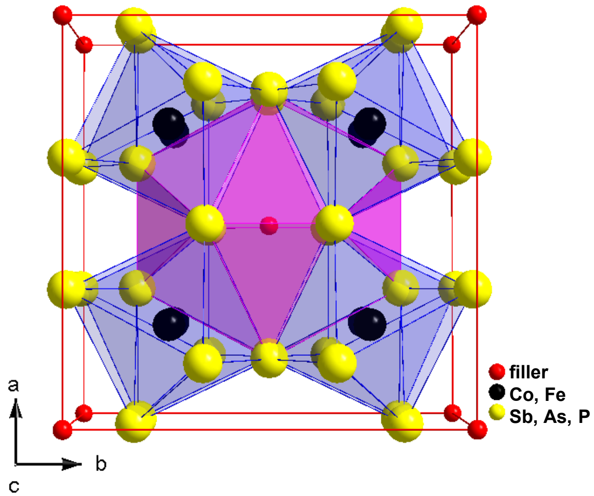
ZrNiSn by Arc Melting



In collaboration with GM R&D for melt-spun processing in investigating amorphous and fine-grained Half-Heusler alloys.

Technical Accomplishment:
Bulk TE Materials for Automotive Applications

Prof. G. Nolas, Dr. Yongkwan Dong, University of South Florida



Glen Slack initiated PGEC concept with skutterudites:

- ✓ Fillers should be loosely bonded to the cage-forming atoms.
- ✓ Fillers should have large atomic displacements.
- ✓ Fillers act as independent oscillators ("rattlers").
- ✓ Interaction of rattlers with the normal modes should lower lattice thermal conductivity.
- ✓ Phonon-scattering centers ("rattlers") should not greatly affect electronic properties.

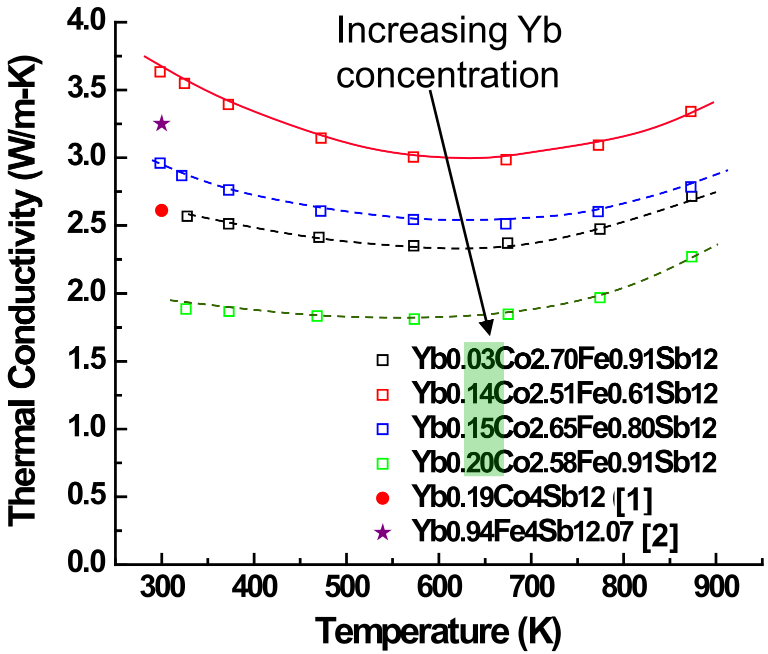
- ➢ Ytterbium (Yb) partially-filled skutterudites
  - Partial filling optimizes lattice thermal conductivity reduction[1]
  - Yb intermediate valence in $CoSb_3$ maximizes filler concentration while minimizing added carriers[2]
- ➢ P-type partially filled skutterudites (high temp measurements at NIST & Clemson U.)
- ➢ Amorphous intermetallic alloys[3] (in collaboration with General Motors)
- ➢ Bi_2Te_3-alloys for High Resolution Infra-Red Thermometry (in collaboration with Marlow Ind.)
- ➢ Survey of other material systems with potential for enhanced thermoelectric properties

1. G.S. Nolas, et al, Phys. Rev. B 58, 164 (1998)
2. G.S. Nolas, et al, Appl. Phys. Lett. 77, 1855 (2000)
3. G.S. Nolas and H.J. Goldsmid, Phys. Stat. Sol. 194, 271 (2002)

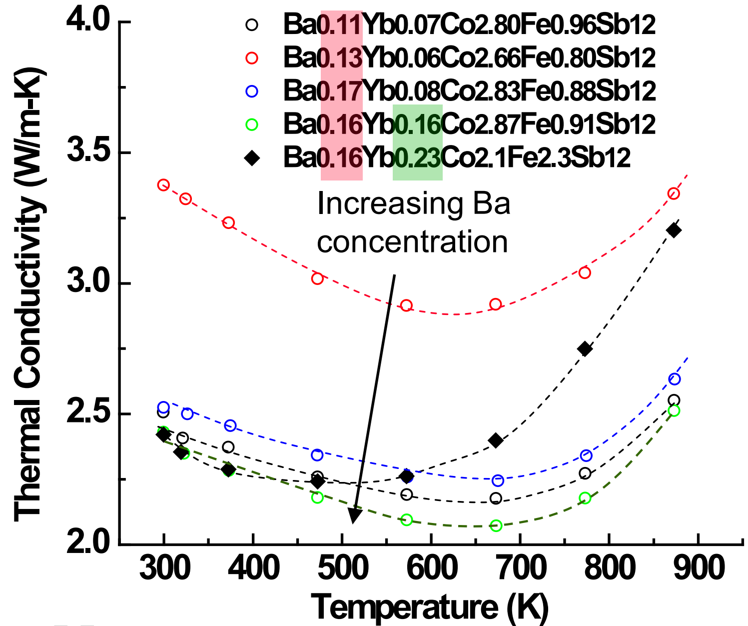
Technical Accomplishment: Bulk TE Materials for Automotive Applications

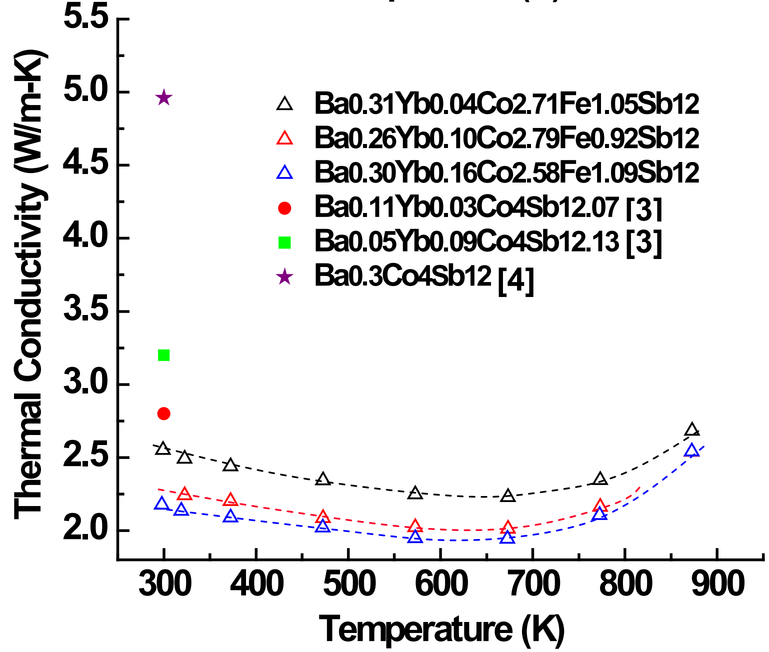
Thermal Conductivity of Yb-filled Skutterudites

Partial filling optimizes lattice thermal conductivity reduction



p-type Ba + Yb filled Skutterudites

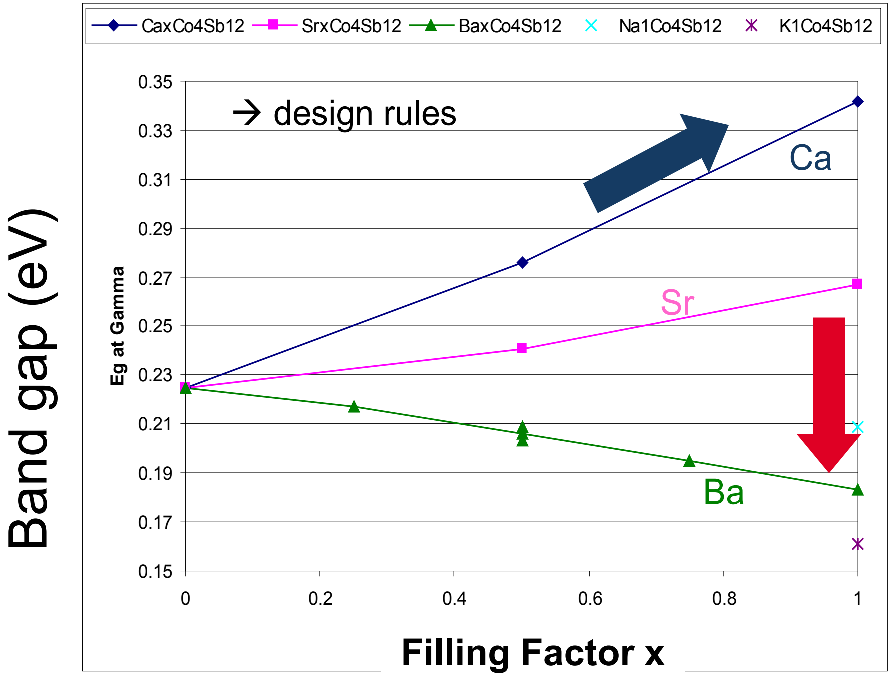




1. G. S. Nolas, et al, Appl. Phys. Lett. 77, 1855 (2000)
2. P. F. Qiu, et al, J. Appl. Phys. 109, 063713 (2011)
3. X. Shi, et al, Appl. Phys. Lett. 92, 182101 (2008)
4. L. D. Chen, et al, J. Appl. Phys. 90, 1864 (2001)

Technical Accomplishment 2011: Effects of Fillers in skutterudites

- The effect of filling distorts the structure **locally**.
  - Soft Sb rings accommodate the distortion.
- Electrons from filler open **band gap**, while volume expansion closes the gap.
  - Band gap is also sensitive to local distortion



➔ Filler vibration is localized and strongly hybridized with Sb atoms. Effect of **force constants** more important than filler mass.

$$M_{\mathrm{Ba}} > M_{\mathrm{Sr}} > M_{\mathrm{Ca}},$$

but

$$\omega_{\mathrm{Ba}} > \omega_{\mathrm{Sr}} > \omega_{\mathrm{Ca}}.$$

Technical Accomplishment: Computational Composition Engineering

Ternary-substituted skutterudites may hold more potential for n-type

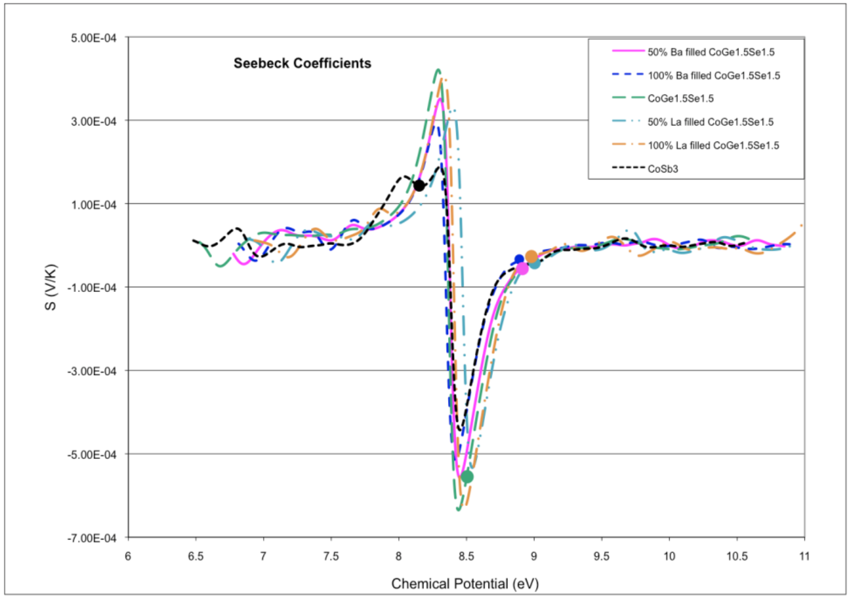
XCo_4B_{12} B = Sb → (Ge,Sn)/ (S,Se,Te)

Higher Seebeck coeffs than $CoSb_3$

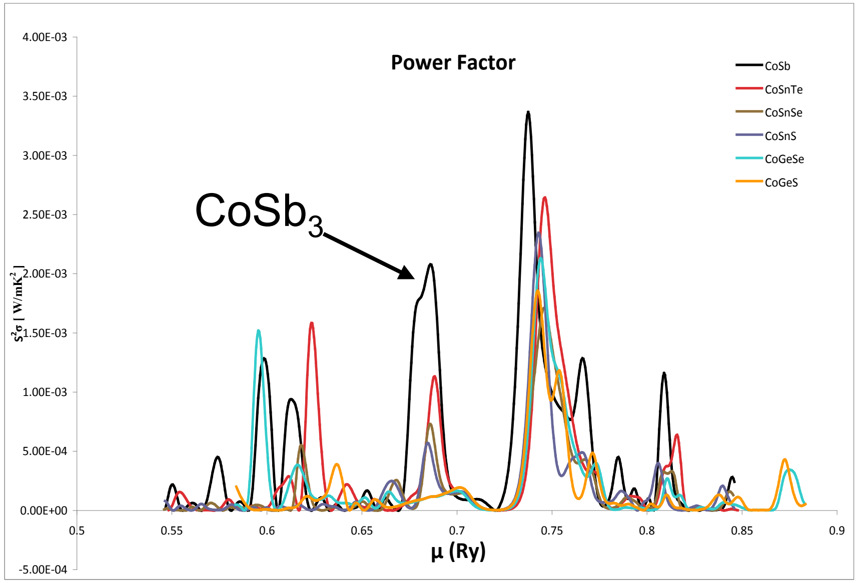
Filling of ternary skutterudites weakly affects the Seebeck maxima

Changes the carrier concentration significantly

Seebeck coeff

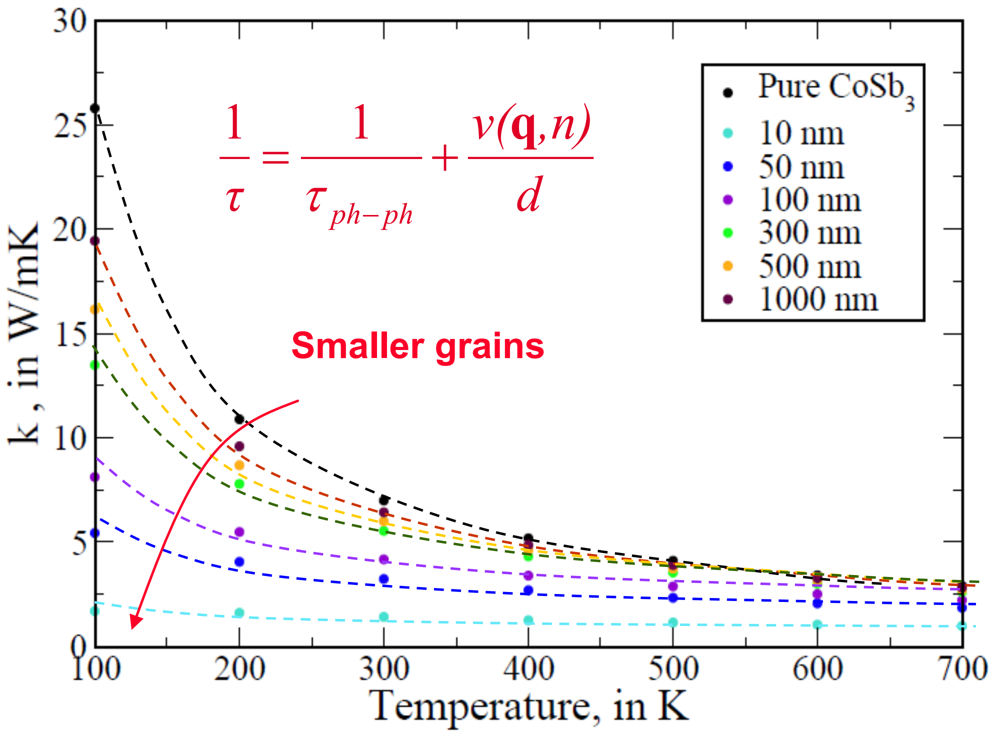


Power factor



Technical Accomplishment: Nanostructure Design for Thermal Transport

- New method developed for ab-initio thermal conductivity prediction
  - Grain boundary scattering term included in thermal conductivity
- Effect of scattering noticeable at 300K for 500nm grains
- Grain boundary scattering much less effective at high T for skutterudites

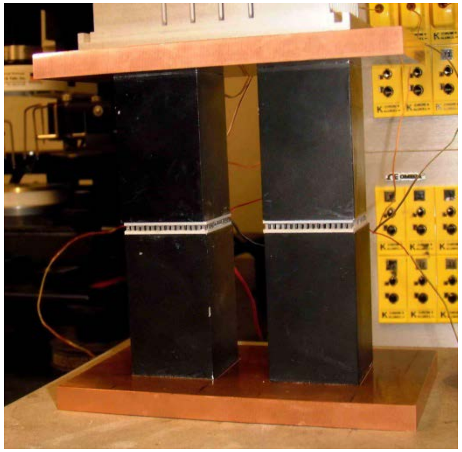


Accomplishment: Outreach & Engagement

Industry Initiatives in Science and Math Education (IISME) – Summer 2011

Mentorship of a public high school teacher for summer research experience and curriculum development using thermoelectrics

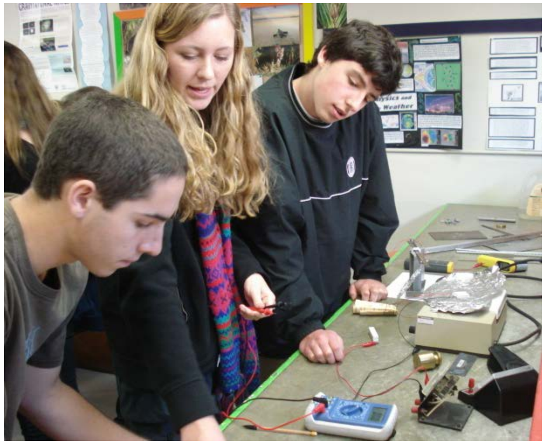
- ✓Designed engineering course which is now taught at a public high school
- ✓Experienced first-hand application of thermoelectric modules



Undergraduate Thermoelectrics Lab – Fall Quarter

Stanford's heat transfer course (ME131A) includes a thermoelectrics laboratory experience.

- ✓Designed in conjunction with IISME teacher
- ✓Lab exercise uses infrared microscopy with thermoelectric modules



K-12 Educational Outreach – Fall 2011-present

We are now partnered with a public high school to provide materials and mentors for a TE design lab

- ✓Introduces high school students to thermoelectric modules and their applications each semester
- ✓Hands-on design lab to engage students in engineering

Collaboration & Coordination

1- Interface
2- System-level
3- Durability
4- Materials
5- Heat sink
6- Metrology

Samples

Information

Stanford

- Prepares CNTs samples on TE materials
- Transport property measurements of CNT-TE pellet combination, thermomechanical reliability tests on interface (300-800 K)
- Process development for CNT TIM tape

1, 2, 3, 5

Bosch

- Ab-initio simulations of transport properties of TE materials and interfaces.
- System-level simulation and optimization

1, 3, 4, 6

1, 3, 4

USF

- Develops high-T, high efficiency TE materials
- Transport properties (ρ, S and κ) and Hall measurements (10 - 300K)
- Structural, morphological and thermal (DTA/TGA) analyses

4, 6

NIST

- Transport properties (ρ, S and κ) and Hall measure- ments (1.8-390K)
- Specific heat, Power Factor measurement at 300 K.
- Custom-designed precision TE properties measurement system (300 – 1200 K)

Proposed Future Work

- *Bulk TE Materials*: Develop p-type partially/double filled Fe-substituted Skutterudites, n- and p-type half heusler alloys for melt-spun processing, thermal stability tests of materials and joints.
- *CNT Thermal Tape Development and Characterization*: Bonding extension to 600°C, thermal stability investigation.
- *Nanostructured Metal Thermal Interface Materials*: Investigate thermal, mechanical, and electrical properties of metal nanowires and meshes, optimization of materials, geometries, and surface treatments for operation at 600°C.
- *High-T $(ZT)_{eff}$ Characterization Facility Implementation*: Vacuum chamber development with IR transparent window, validation using Bi_2Te_3-alloys
- *Ab-Initio Simulations*: Band gap calibration for skutterudite and half-Heusler families, focussed computatios on phase stability, Seebeck coefficient, and transport properties.

Summary Slide

- With this award, DOE & NSF are enabling an academic-corporate team to focus on the key practical challenges facing TEG implementation in vehicles: interfaces, system-relevant metrology, and materials compatibility

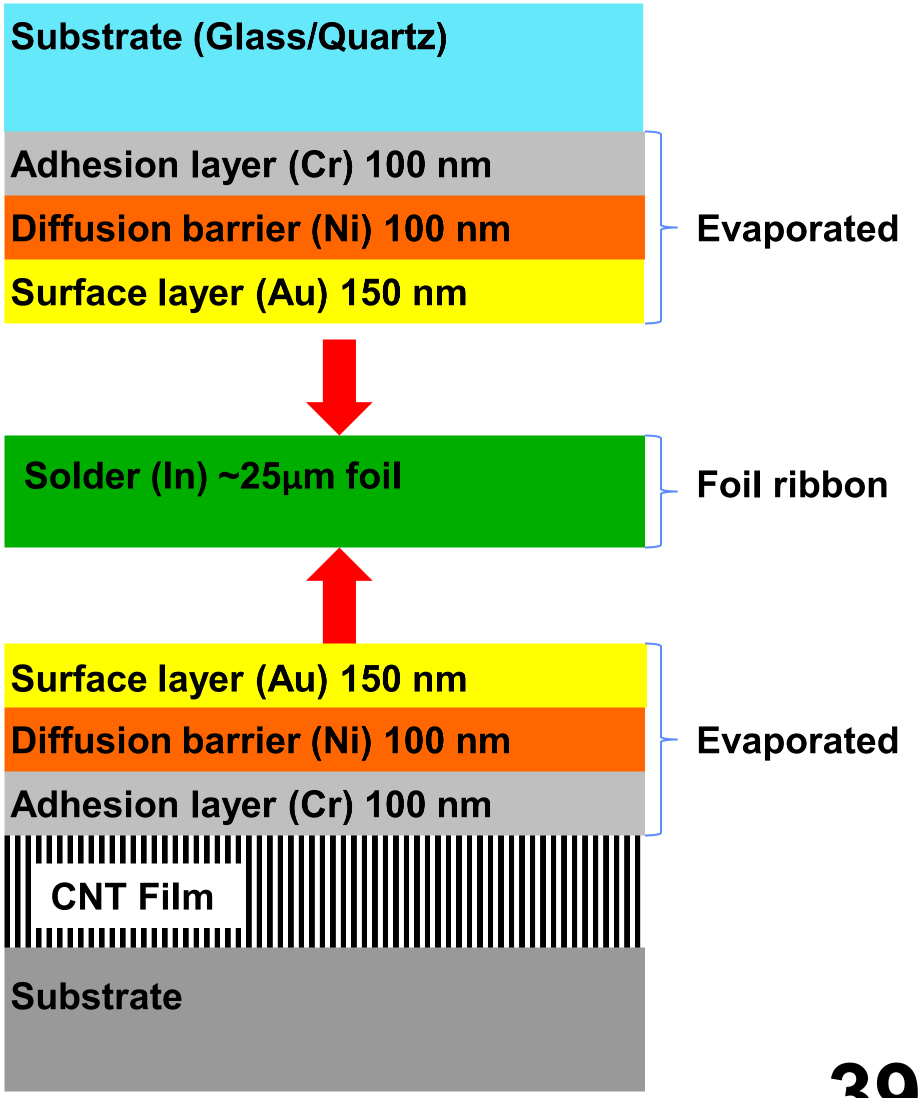
- We are developing metrology for fundamental properties of nanostructured interfaces, as well as $(ZT)_{eff}$ metrology for half-Heusler and skutterudite thermoelectrics considering interfaces. Simulations include atomistic and ab initio results for TE materials and interfaces, and system & heat exchanger level optimization with the corporate partner.

- Key 2011 results include: (a) process development of CNT tape and several bonding options (Stanford) (b) detailed mechanical characterization of CNT films (Stanford), (c) IR characterization of TE pellets and corresponding interfaces under thermal cycling (Stanford), (d) interface modeling & optimization (Bosch) and (e) process development (arc melting, melt spun) for bulk TE materials (USF)

Technical Backup Slides

Technical Accomplishment: CNT Metallization & Bonding Procedure

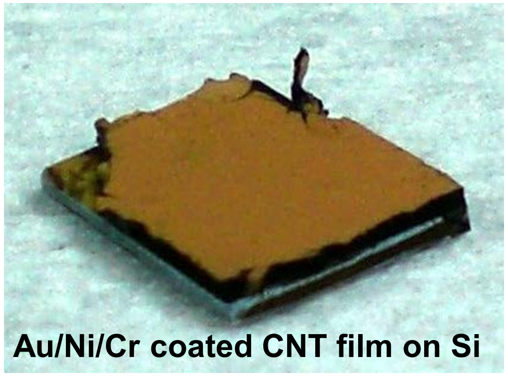
- Bonding the CNT films to relevant substrates is a major challenge as not all materials are compatible with the CNT growth procedure.
- Recent progress utilizing a combination of metallizations allows CNT films grown on sacrificial silicon wafers to be successfully transferred to a range of substrates using thin indium foils as binding layers.
- This is a key step towards developing the free standing CNT tape for thermal interface applications.



Technical Accomplishment: CNT Bonding Procedure

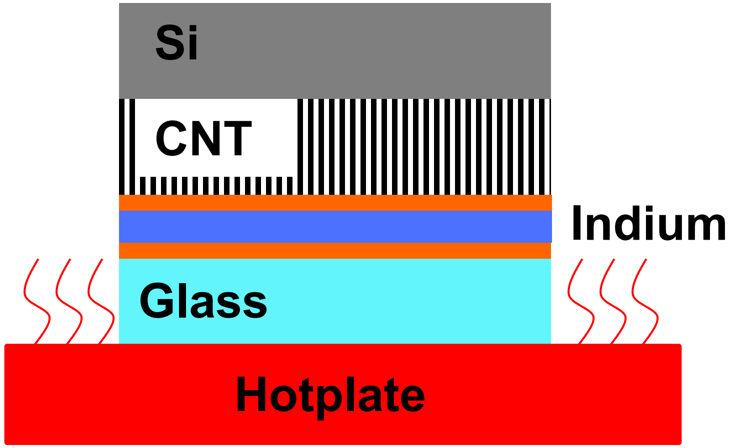
1) SAMPLE PREPARATION

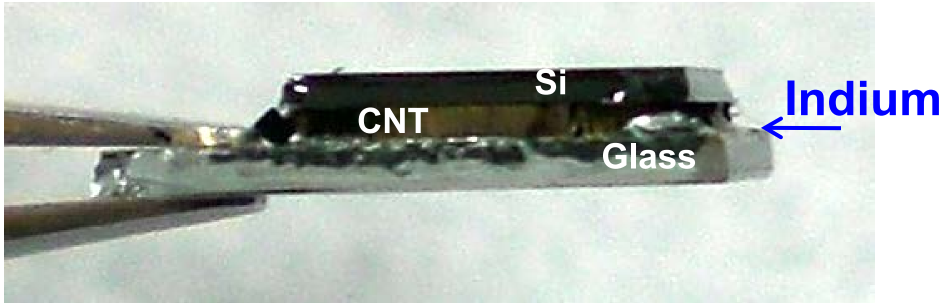
a) Evaporate Au/Ni/Cr on CNT and glass substrates



b) Clean indium foil or apply flux

2) THERMAL BONDING

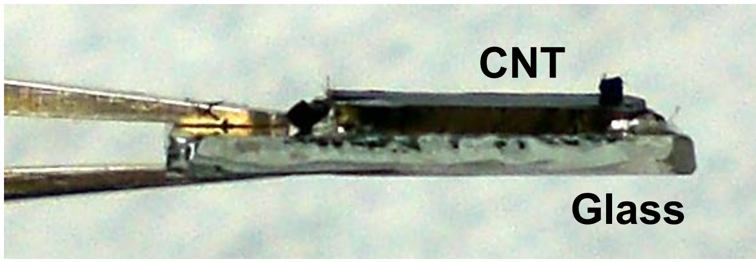


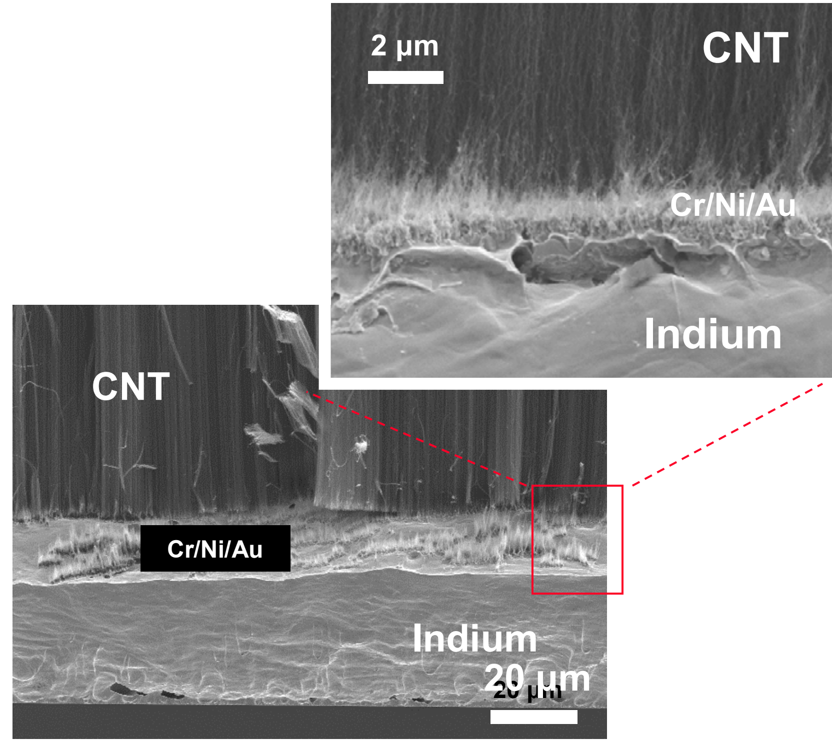


CNT film bonded to glass, before removal of Si substrate

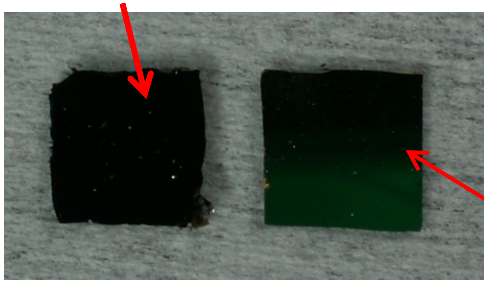
Technical Accomplishment: CNT Bonding Procedure

3) CNT FILM RELEASE

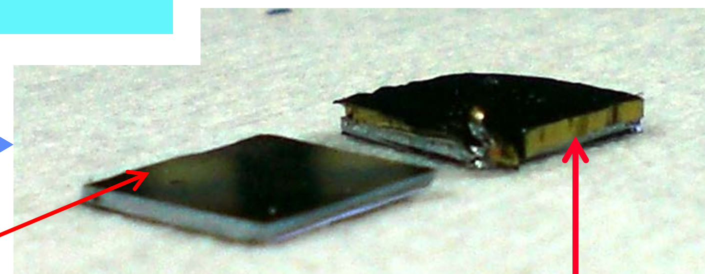




CNT bonded to Si

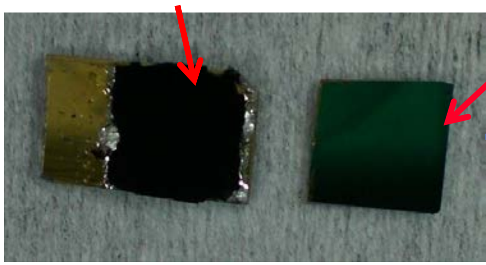


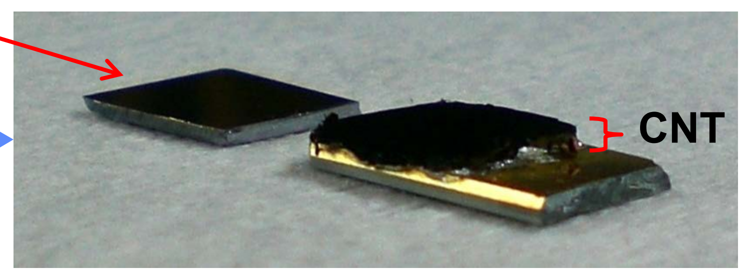
Original CNT substrate, with no CNT remaining



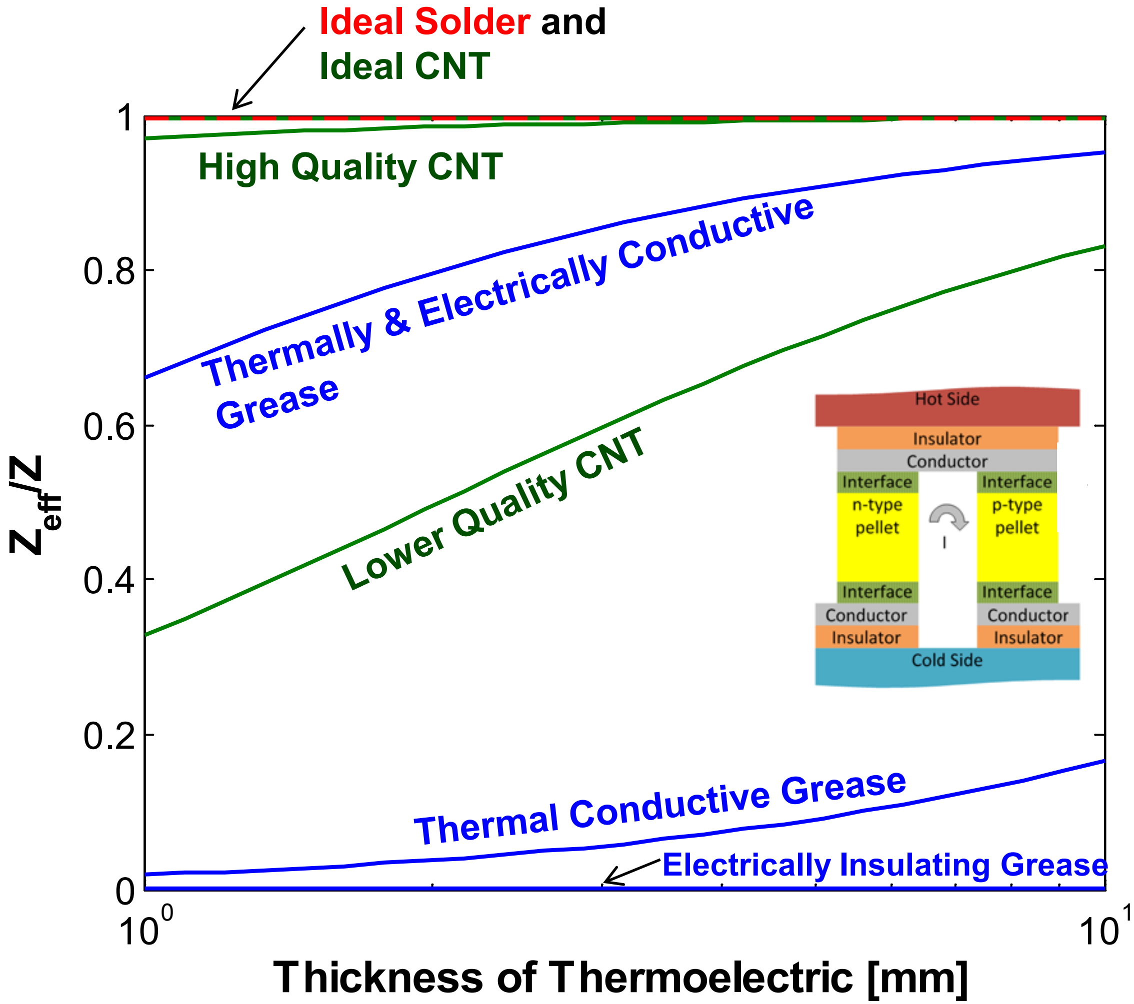
CNT (side is covered with Au from metallization)

CNT bonded to glass





Relevance: Effect of Interface Resistances on Thermoelectric Device Properties



Interface Material	R''$_{th}$ [W/m²/K]	R''$_e$ [Ω m²]
Solders And Ideal CNT	~10^{-7}	~10^{-12}
High Quality CNT	~10^{-6}	~10^{-10}
Lower Quality CNT	~10^{-5}	~10^{-8}
Thermally & Electrically Conductive Grease	~3×10^{-6}	~3×10^{-9}
Thermal Conductive Grease	~8×10^{-6}	~3×10^{-7}
Electrically Insulating Grease	~8×10^{-6}	>10^{-5}

Using model of Xuan, *et al.* International Journal of Heat and Mass Transfer **45** (2002).

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Nanotape could make solder pads obsolete

R. Colin Johnson
1/24/2011 12:01 AM EST

PORTLAND, Ore.—Solder pads could soon be made obsolete by a new nanotape material created by the Semiconductor Research Corporation (SRC) and Stanford University.

By sandwiching thermally conductive carbon nanotubes between thin metal foils, nanotape transfers heat away from chips better than solder but with a lightweight flexible material that is cheaper and and more compliant, according to researchers.

"Today, solder is made very thick to provide mechanical compliance,

Comment
2/11/2011 6:09 PM EST

"…Stanford is also working with the National Science Foundation (NSF) on a project with the **Department of Energy Partnership on Thermoelectric Devices for Vehicle Applications**. Here, the nanotape will facilitate the recovery of electrical power from hot exhaust gases using thermoelectric…"

http://www.eetimes.com/electronics-news/4212401/Nanotape-could-make-solder-pads-obsolete