NSF-DOE Thermoelectrics Partnership:

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

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R. Bosch LLC

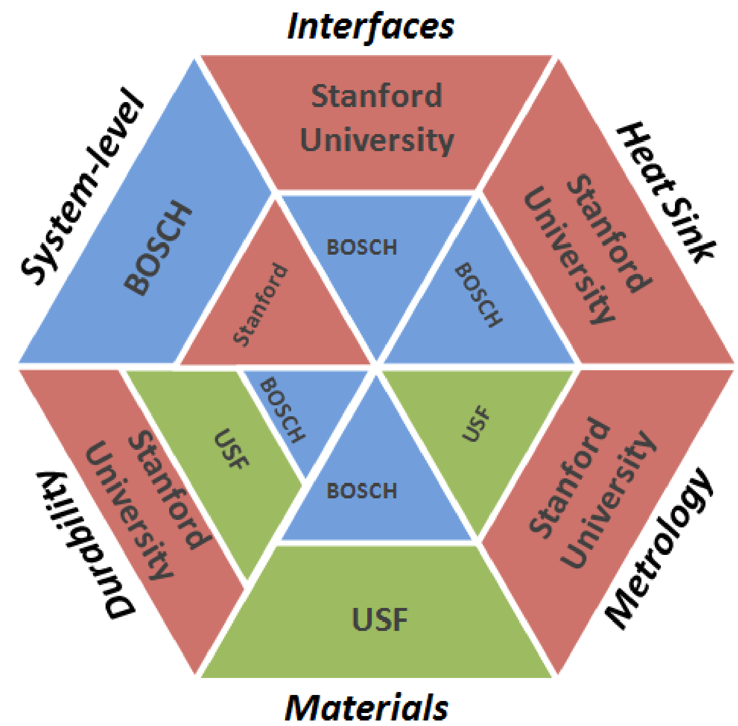
Novel Materials Laboratory
University of South Florida

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

Project Leadership
Prof. Ken Goodson, Stanford Mechanical Engineering
Prof. George Nolas, USF Department of Physics
Dr. Boris Kozinsky, Energy Comp. & Modeling, Bosch
Prof. Mehdi Asheghi, Stanford Mechanical Engineering
Dr. Winnie Wong-Ng, NIST Functional Properties Group

Staff
Dr. Yongkwan Dong, USF Department of Physics
Dr. Matt Panzer, Stanford Mechanical Engineering

Students:
Yuan Gao, Lewis Hom, Saniya Leblanc, Amy Marconnet



Leveraged Support:
Northrop Grumman, AMD/SRC, ONR, AFOSR
Fellowships from NSF, Sandia National Labs, Stanford DARE

Program Managers: John Fairbanks, Tom Avedisian (DOE). Arvind Atreya (NSF)

Novel Materials Laboratory
University of South Florida

BOSCH

Key Challenges for Thermoelectrics in Combustion Systems

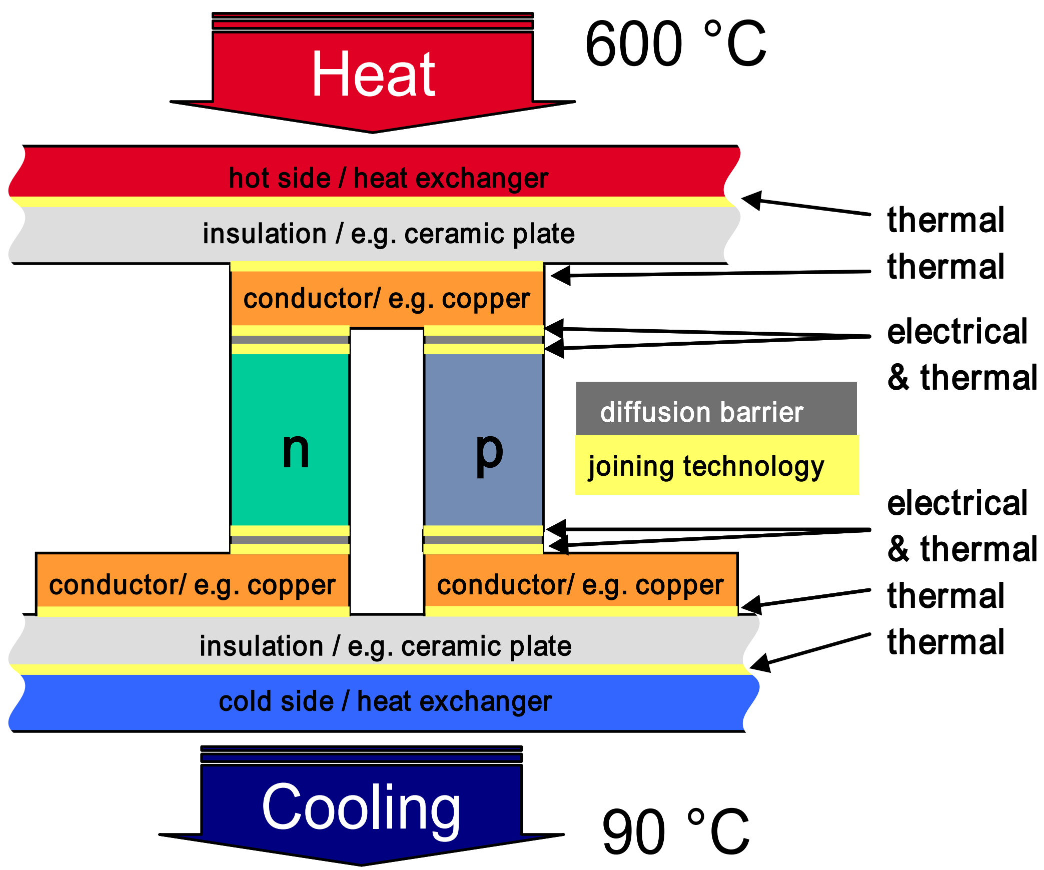
Improvements in the intrinsic ZT of TE materials are proving to be very difficult to translate into efficient, reliable TEG systems.

Major needs include…

…Low-thermal-resistance interfaces with tailored electrical properties, which are stable under thermal cycling.

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

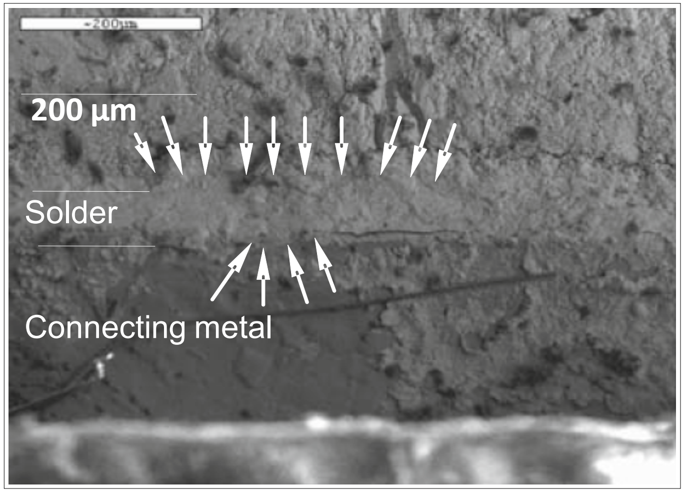
…Characterization methods that include interfaces and correlate better with system performance.



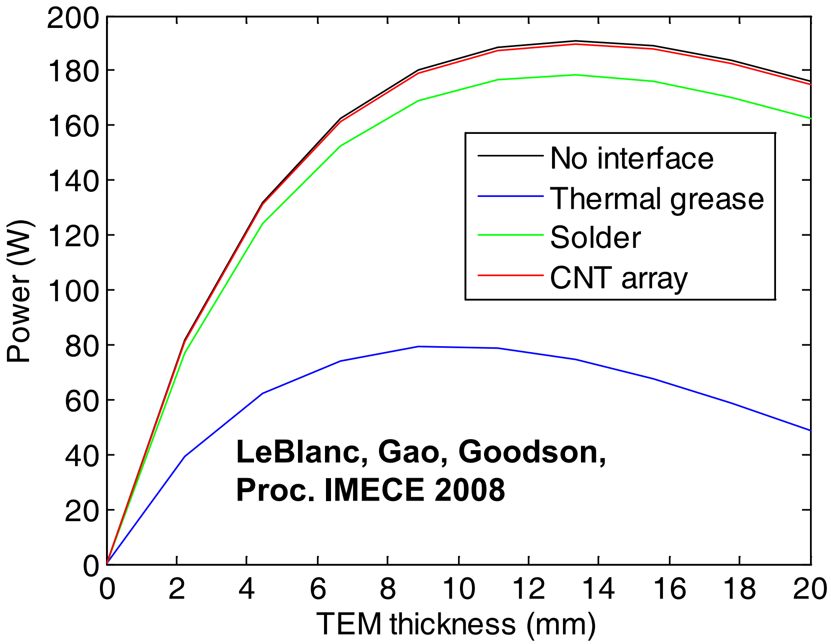
Thermoelectric Interface Challenge

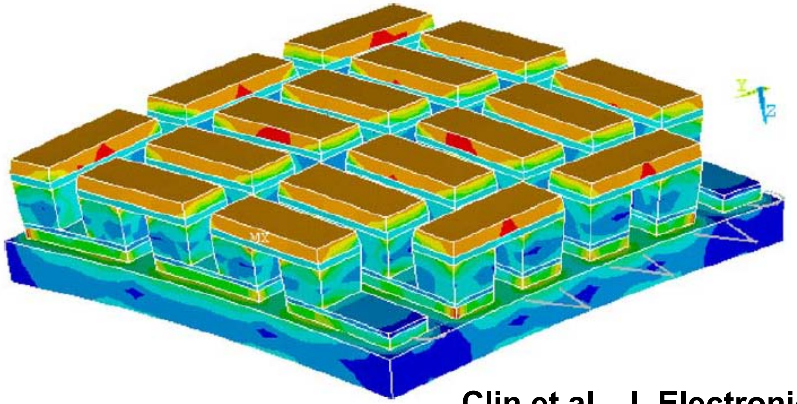
"Nanostructured Interfaces for Thermoelectrics,"
Gao, Marconnet, Leblanc, Shakouri, Goodson et al., Proc ICT 2009, J. Electronic Materials, 2010
Pettes, Hodes, Goodson, Trans. Advanced Packaging, 2009

- Combustion systems experience enormous stresses at interfaces due to large temperature differences.
- Interfaces must offer low thermal resistance, targeted electrical performance, mechanical compliance.



Hatzikraniotis et al., Proc.
Mater. Res. Soc. Symp., 2009.





Clin et al., J. Electronic Materials, 2009

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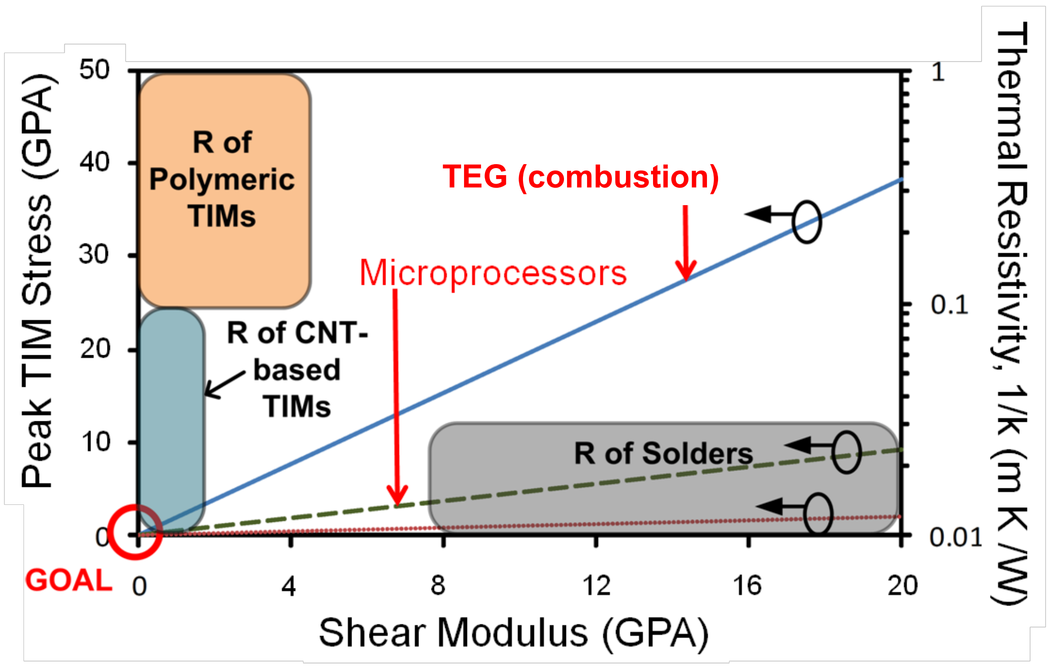
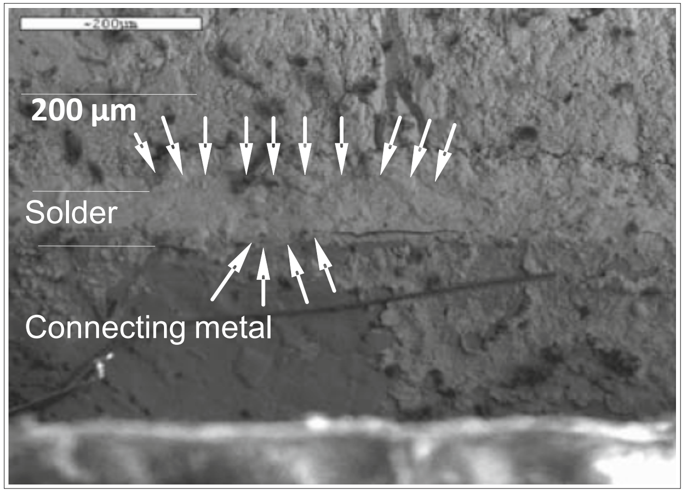
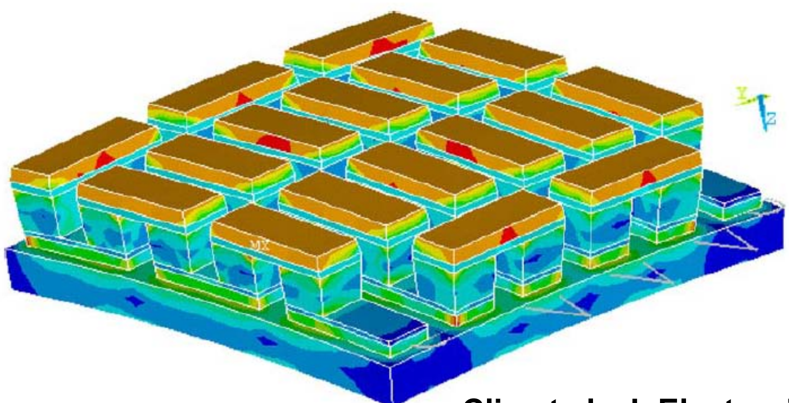




Hatzikraniotis et al., Proc. ***Mater. Res. Soc. Symp., 2009.***



Clin et al., J. Electronic Materials, 2009

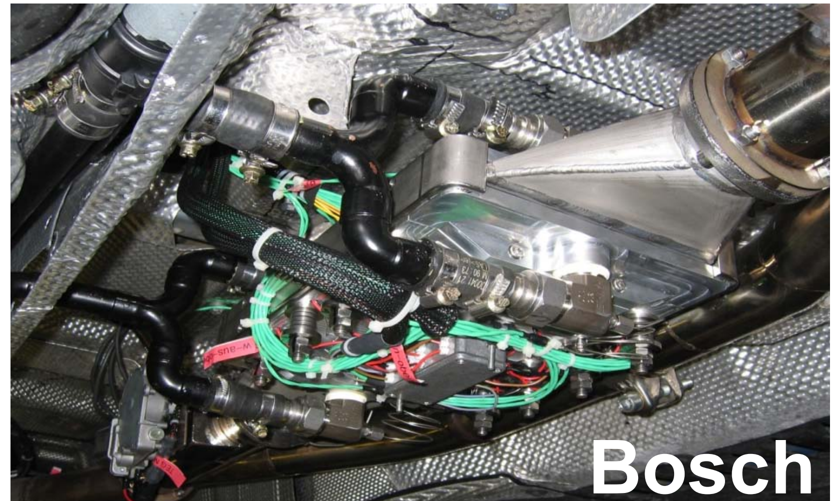
Automotive Thermoelectric Modules with Scalable Thermo- and Electro-Mechanical Interfaces

GOALS

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



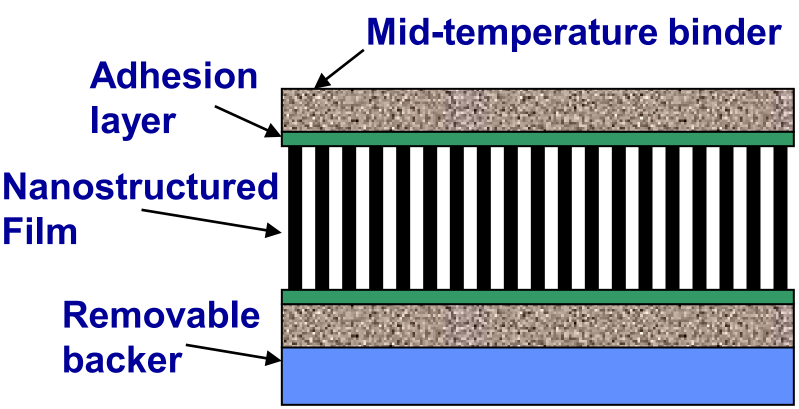
Prototype TEG in exhaust system

METHODS

Multiphysics simulations ranging from ab-initio (band structure) to system scale.

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

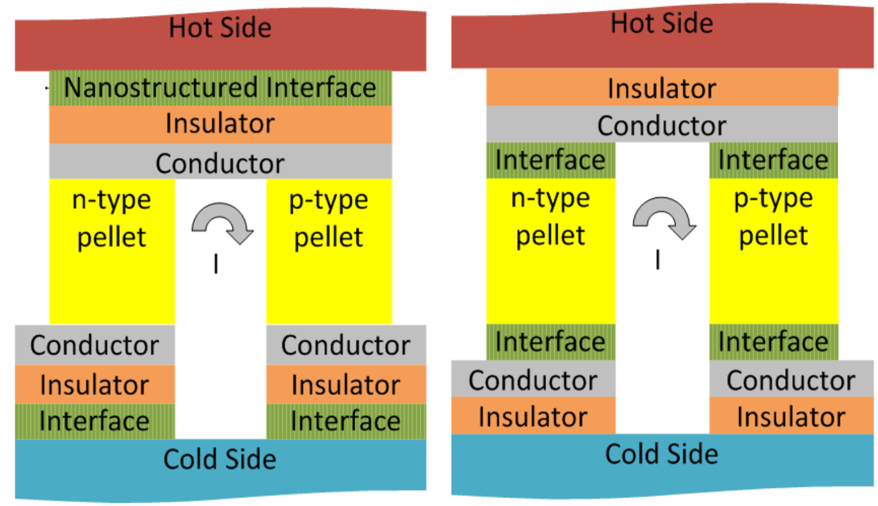
System impact assessment considering the interplay of thermal, fluidic, mechanical, electrical, and thermoelectric phenomena.



Hu, Fisher, Goodson, et al., J. Heat Transfer (2006)
Panzer, Dai, Goodson, et al., Patent Pending (2007)

Research Overview

U.S. Department of Energy
Energy Efficiency and Renewable Energy



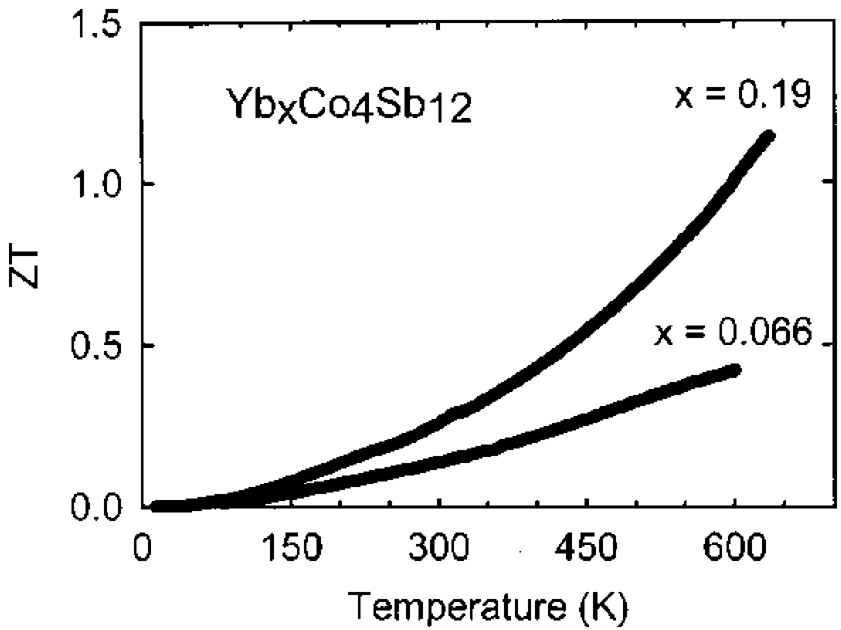
Interfaces 100%	Nanostructured films & composites, metallic bonding Ab initio simulations and optimization	Stanford Bosch
Metrology 100%	$(ZT)_{eff}$ with independent k&c_p, thermal cycling High temperature ZT	Stanford USF/NIST
Materials 100%	Filled skutterudites and half Heusler intermetallics Ab initio 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
Outreach	TE for vehicles competition, UG Lab, K-12 outreach	Stan&USF

Bulk TE Materials for Automotive Applications

Nolas et al., MRS Bulletin (2006).
Nolas, Kaeser, Littleton, Tritt, APL 77, 1855 (2000), Nolas, JAP 79, 4002 (1996)
Lamberton, G.S. Nolas, et al. APL 80, 598 (2001). Nolas, Cohn, and Slack, PRB (1998)

- ***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 and ZT.



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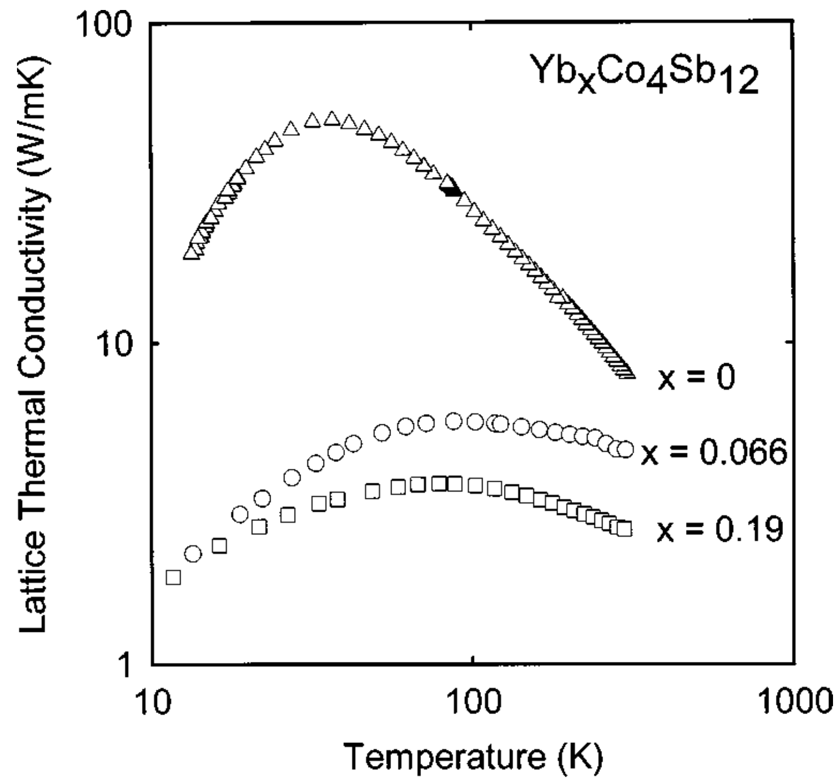

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Bulk TE Materials for Automotive Applications

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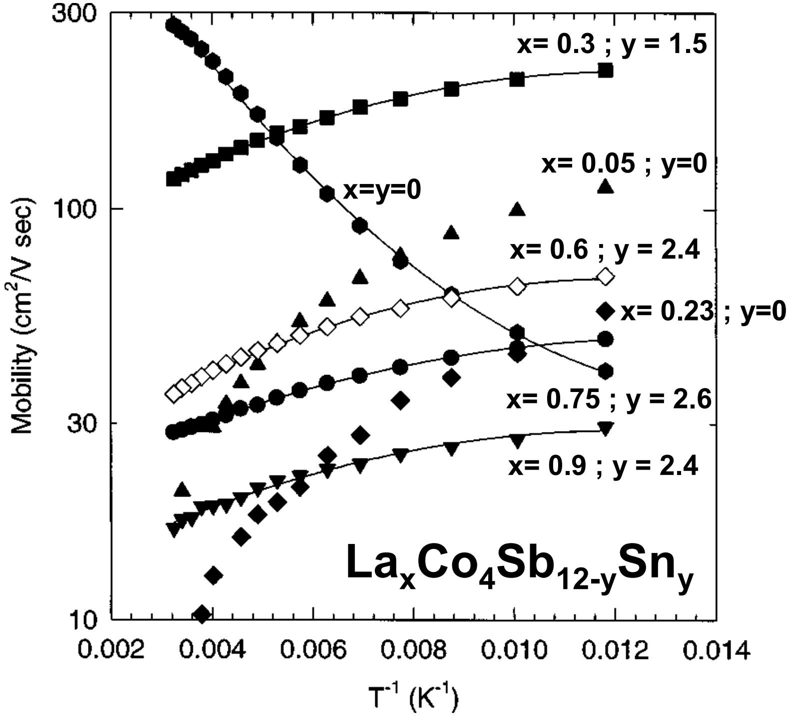
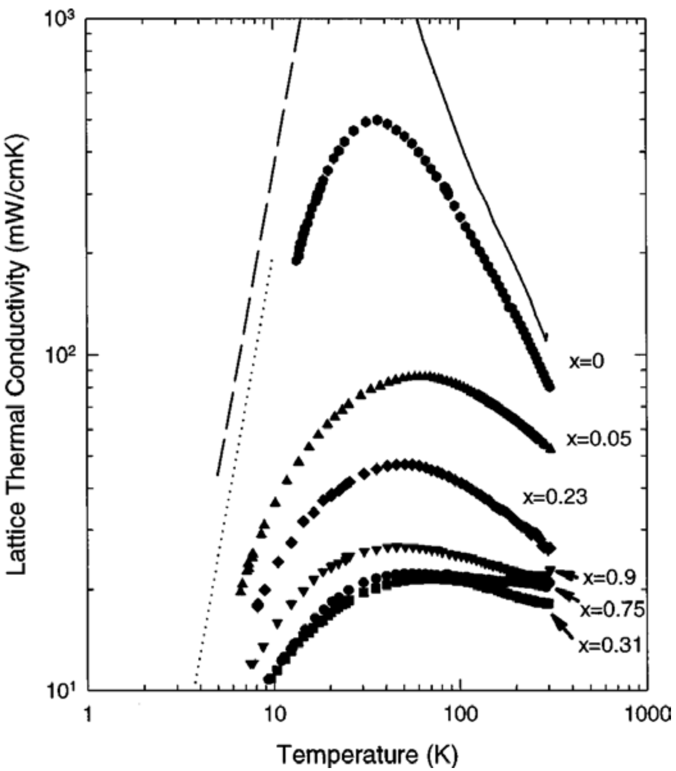
- ***Skutterudites with partial filling using heavy, low valence "guest" atoms***

Partial Filling – Optimization of mobility & thermal conductivity





- ***Half-Heusler alloys: from small grain size towards the disordered state***

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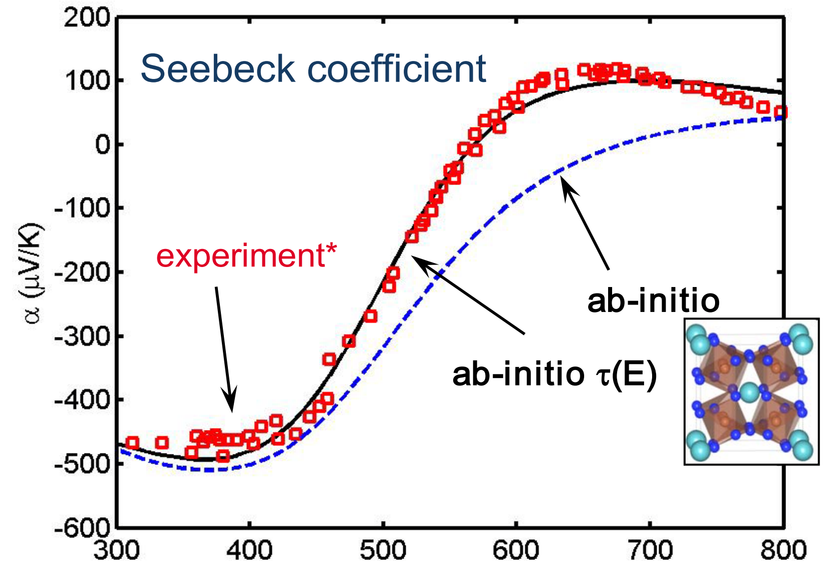
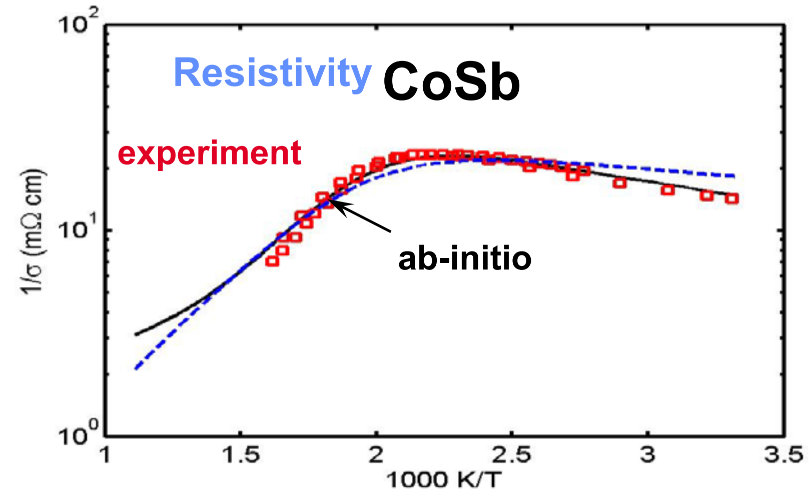
Functional Simulation & Optimization of Materials

Dr. Boris Kozinsky, Energy Modeling, Control, and Computation, Bosch LLC

Wee, Kozinsky et al, Phys. Rev. B 81 (2010)

- **Ab-initio/BTE computations will assist the optimization of TE material stoichiometry.**
- **Past work at Bosch predicted the effect of Ba filling on $CoSb_3$ skutterudites using DFPT.**
- **Collaborative optimization with Nolas group will focus on filled skutterudites, mobility, seebeck, and interfaces with metallics.**

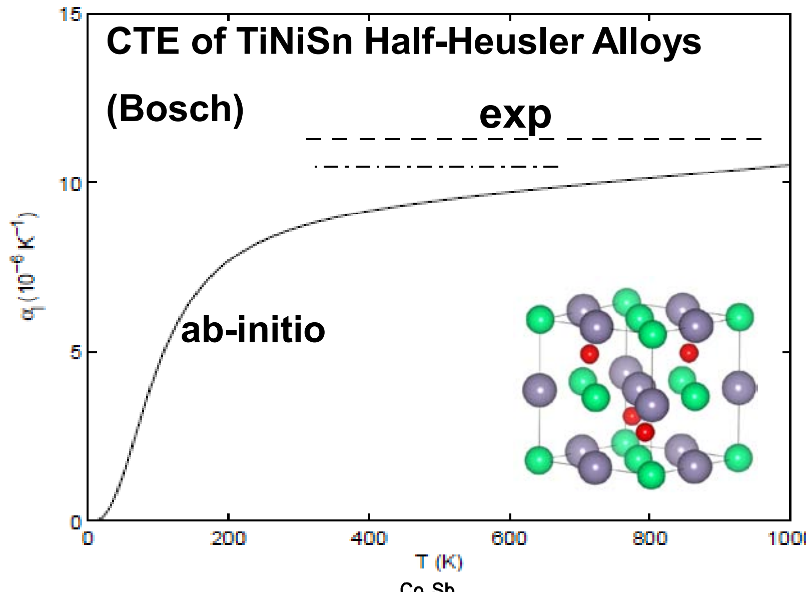


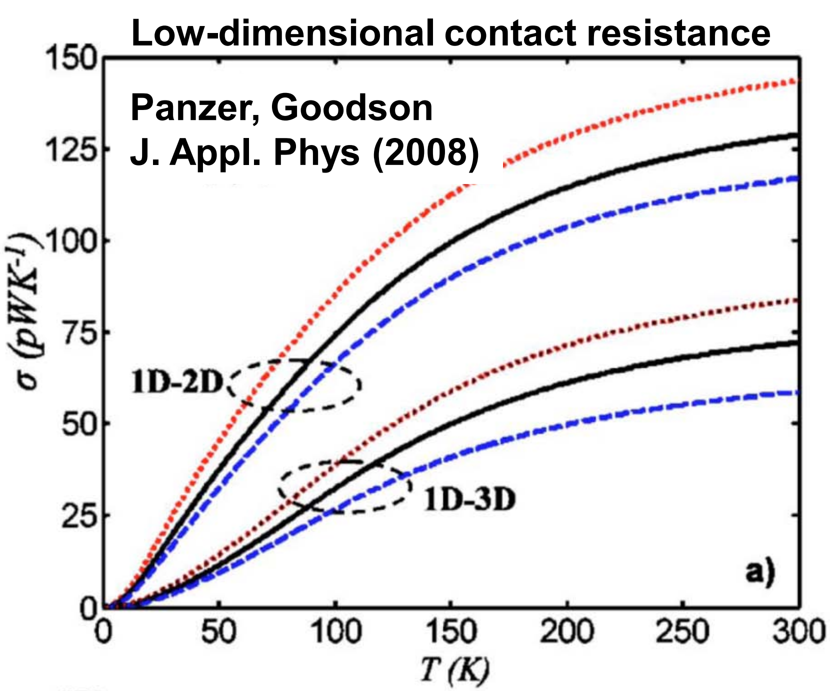


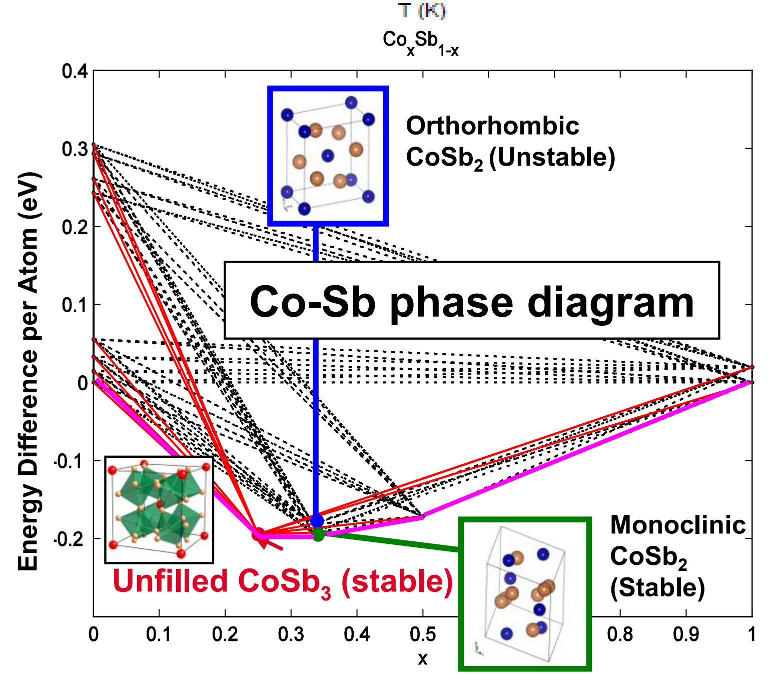
Interface Modeling & Optimization

Kozinsky, Physical Review Letters (2006). Panzer, Goodson et al. JAP (2008)

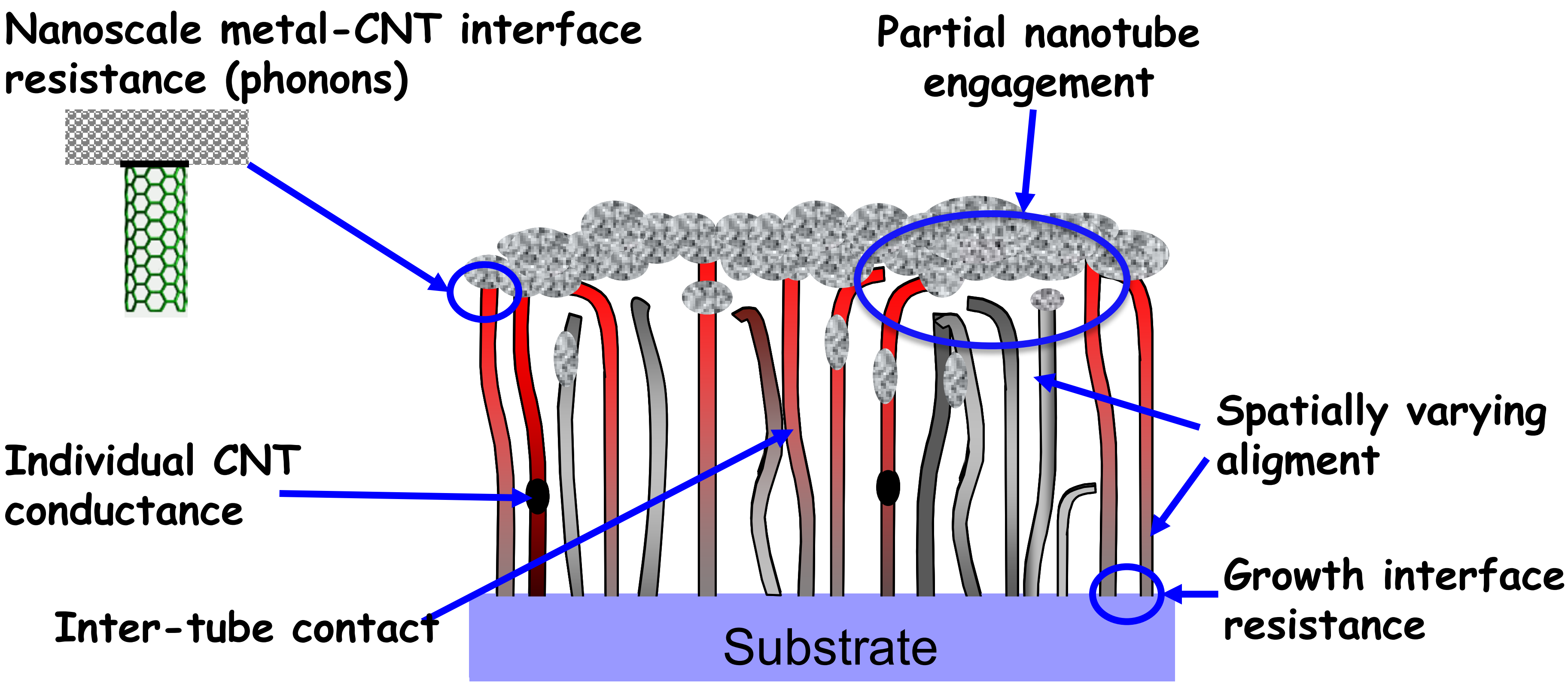
- Simulations examine thermodynamic stability of TE material phases and assess potential for interdiffusion.
- Simulations examine interface electrical conduction and optimize resistance considering band structure.
- Mechanical & thermal simulations will focus on the expansion coefficients and transport through low-dimensional contacts.







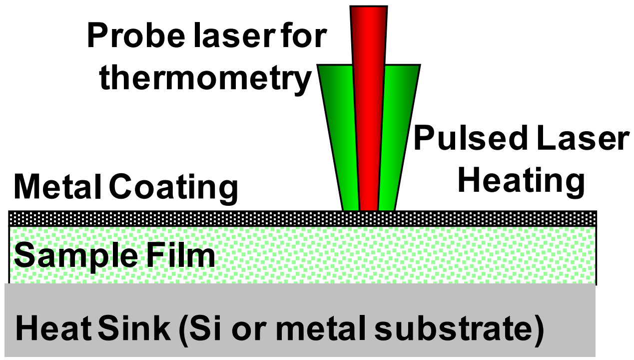
Conduction Physics in CNT Films



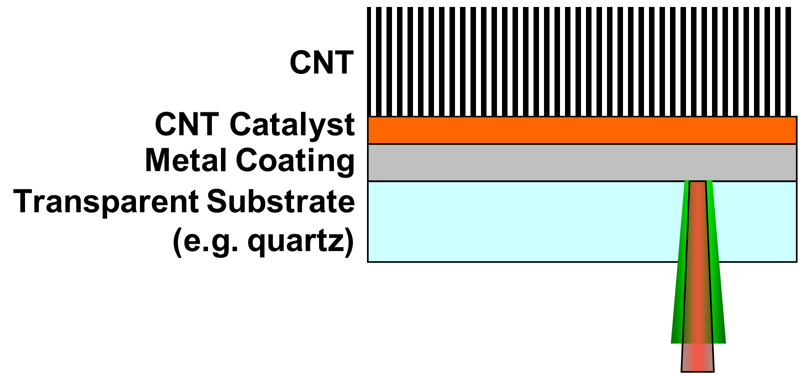
Pop,Dai,Goodson et al.	*Physical Review Letters*	(2005)
Pop,Dai,Goodson et al.	*Nano Letters*	(2006)
Hu,Fisher,Goodson et al.	*Journal of Heat Transfer*	(2006,07)
Panzer,Dai,Goodson et al.	*Journal of Heat Transfer*	(2008)
Panzer,Goodson	*Journal of Applied Physics*	(2008)
Gao,Shakouri,Goodson et al.	*Journal of Electronic Materials*	(2010)
Panzer,Murayama,Goodson et al.	*Nano Letters*	(2010)

Thermal and Mechanical Characterization of Aligned CNT Films

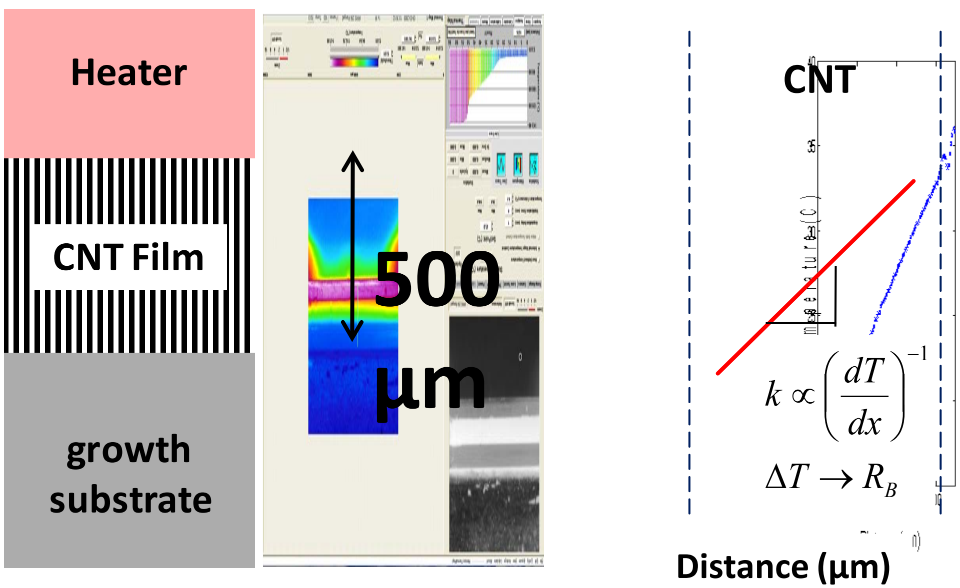
Nanosecond Thermoreflectance



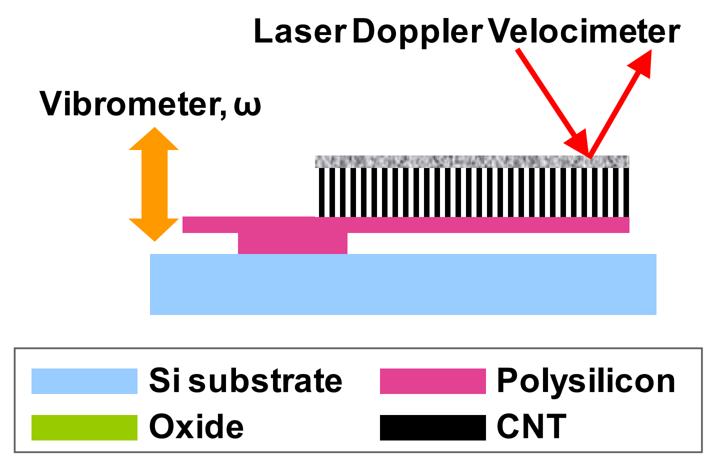
Picosecond Thermoreflectance



Cross-sectional IR Microscopy

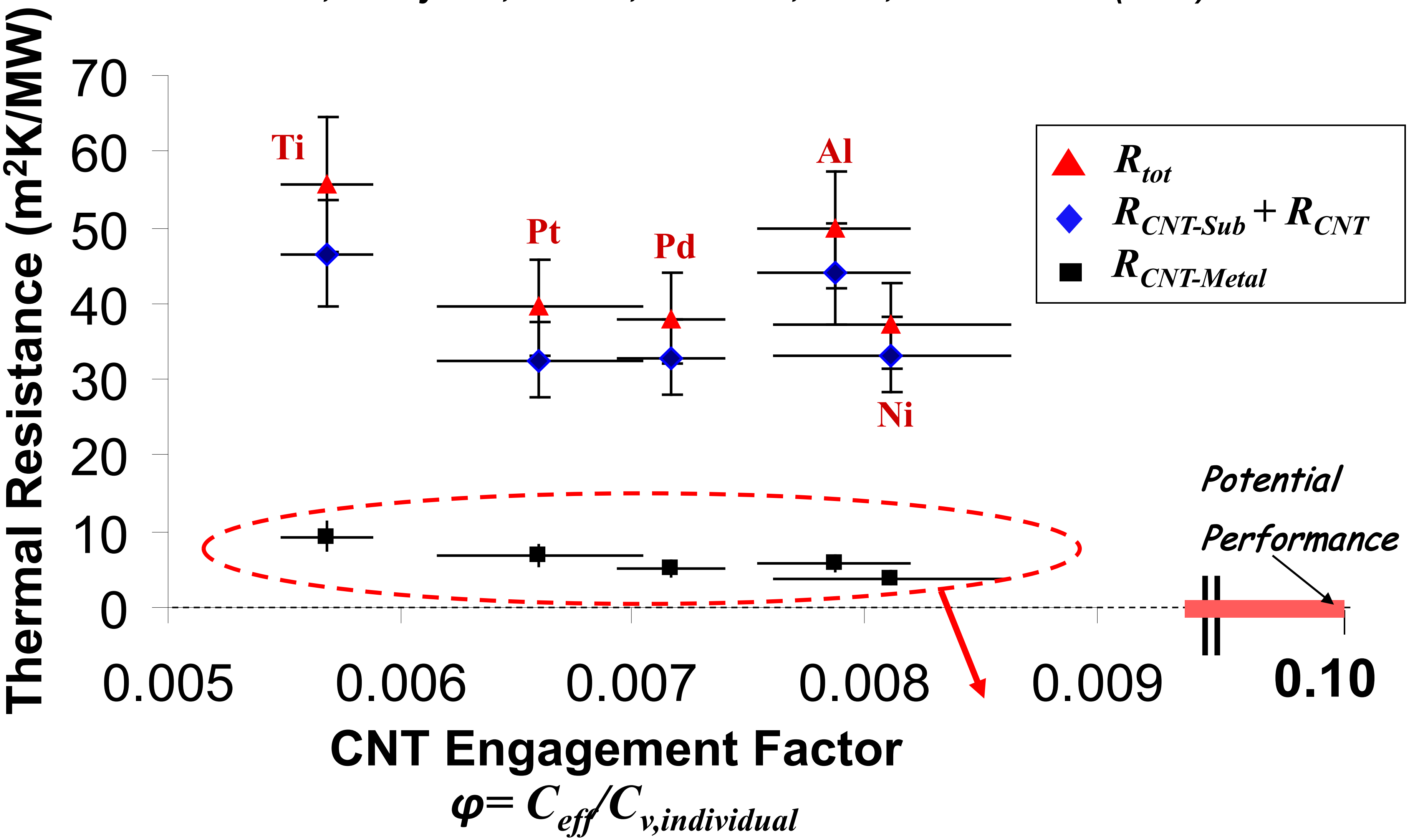


Mechanical Characterization



Metallization and CNT Thermal Resistance using Nanosecond Thermoreflectance

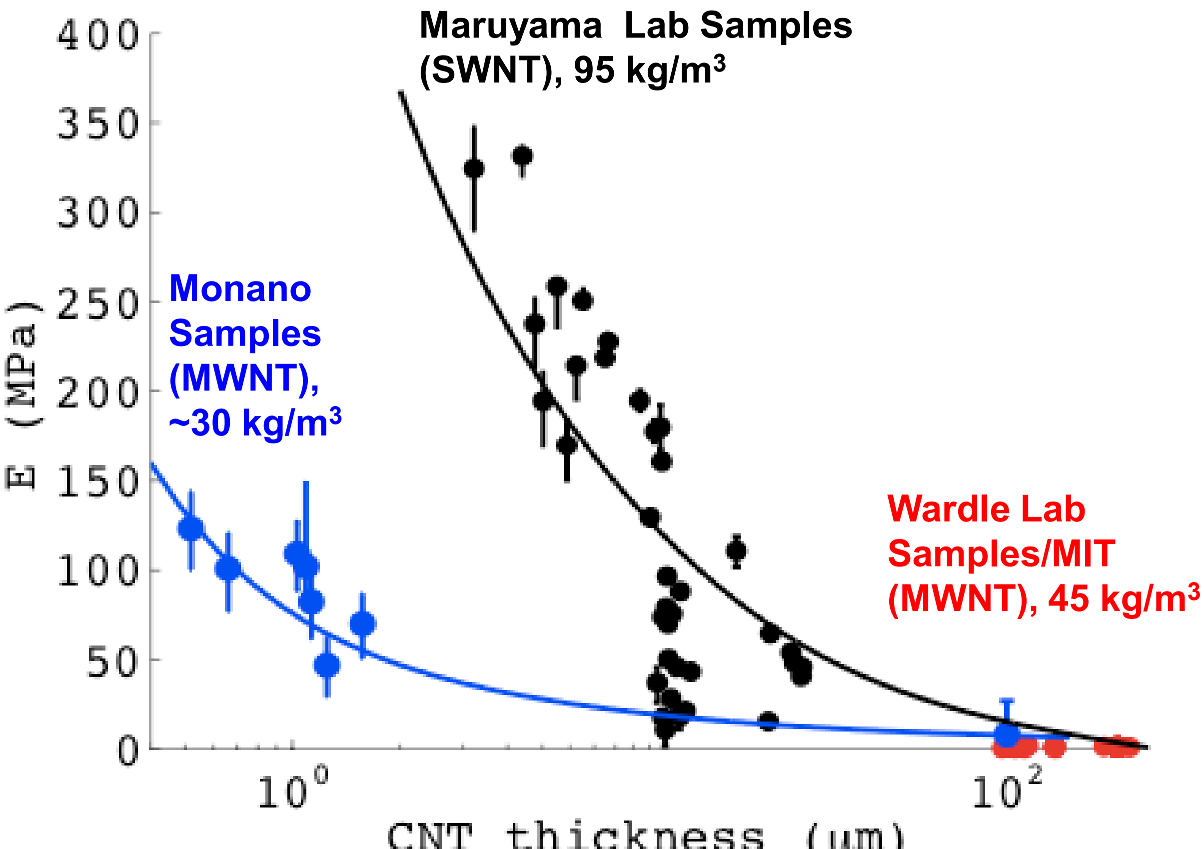
Panzer, Murayama, Wardle, Goodson, et al., Nano Letters (2010)

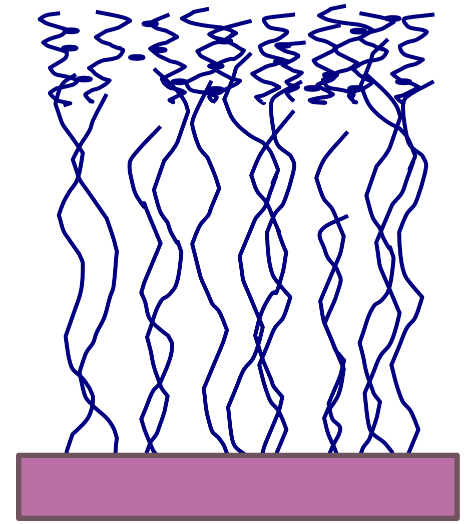


Mechanical Behavior of CNT Films

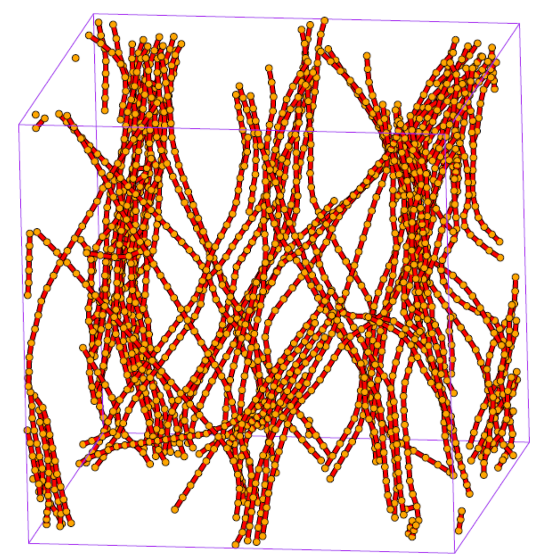
Students: Yoonjin Won, Yuan Gao, Matt Panzer. Collaborators: Prof. Wei Cai, Stanford ME

	Thickness (μm)	Modulus (MPa)	Density (kg/m^3)
CNT_{Top}	0.4	140	>29
CNT_{Middle}	0-150	7	29
Si	8.7	155e3	2330



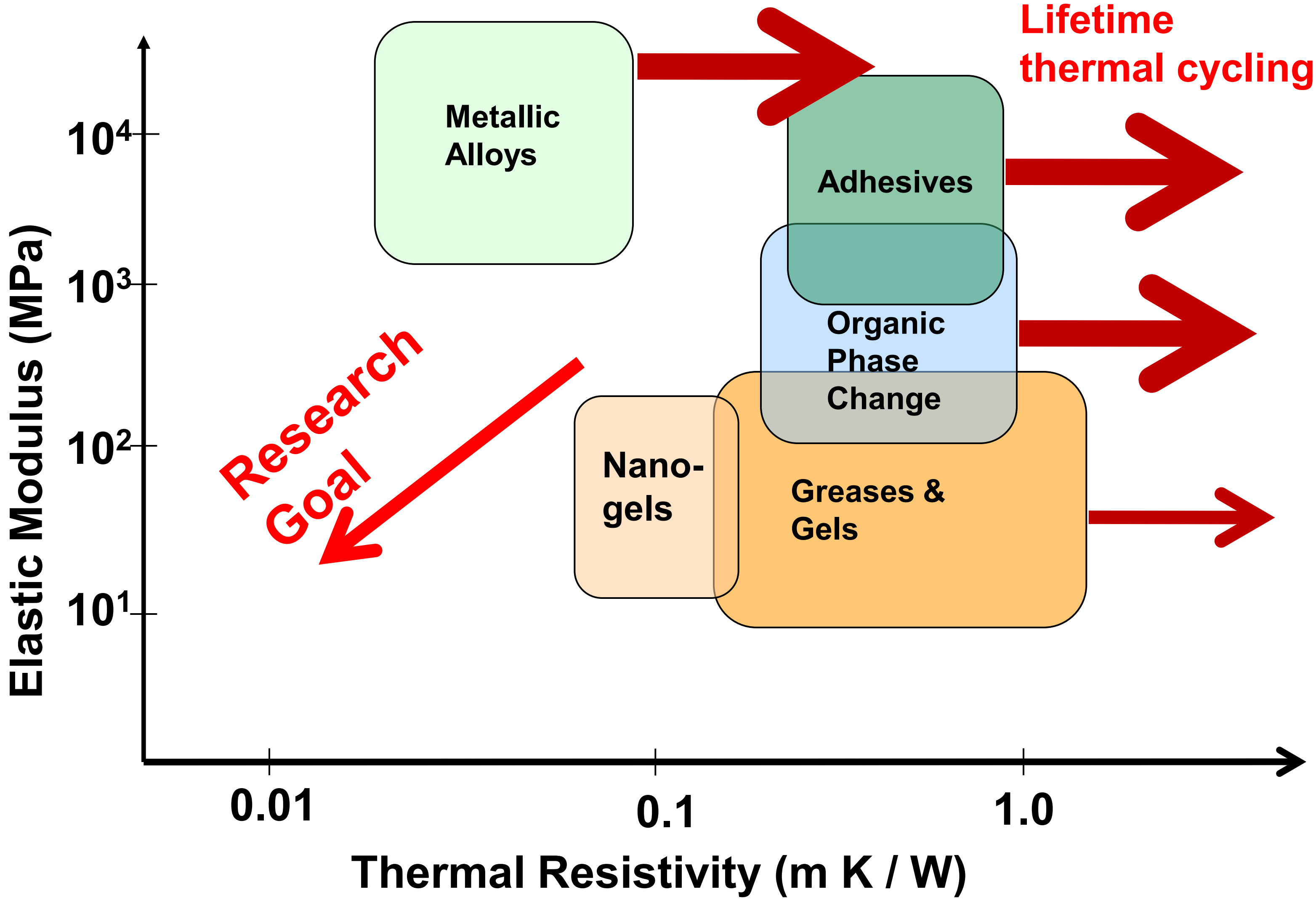


Crust Model



Zipping/Velcro Model

Thermal & Mechanical Requirements at Interfaces



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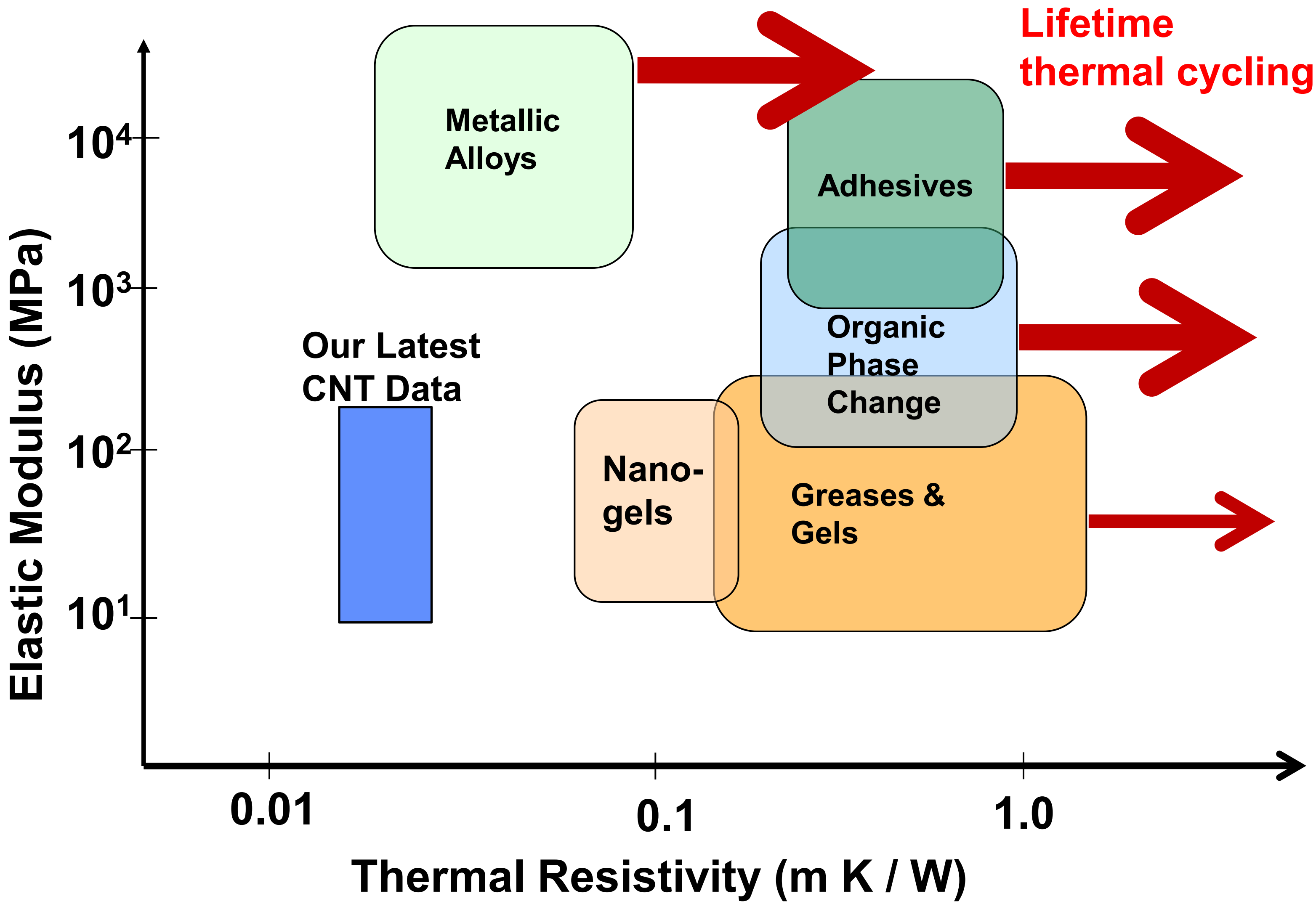
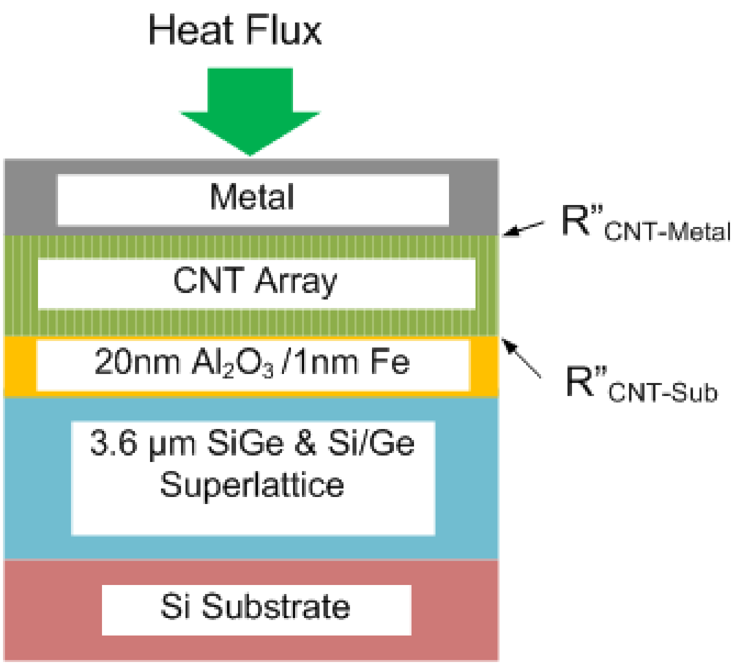
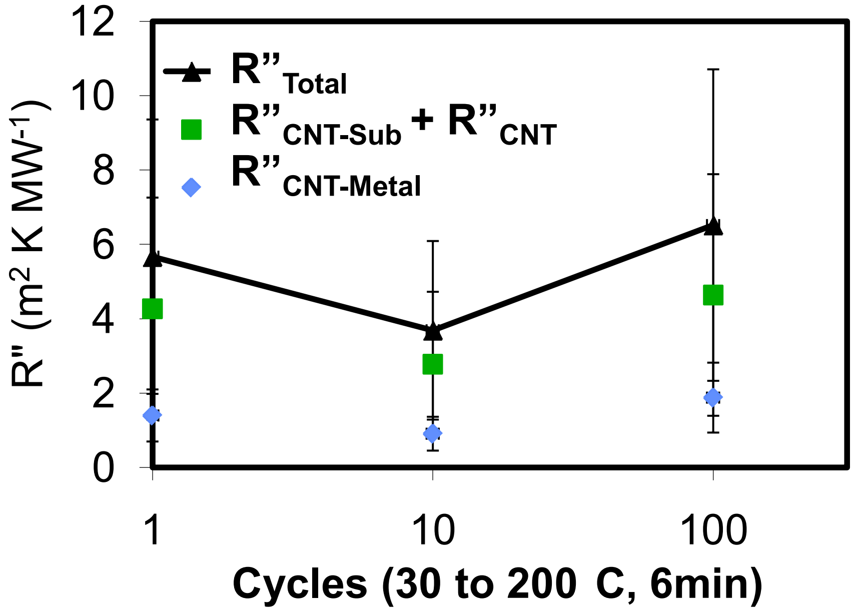
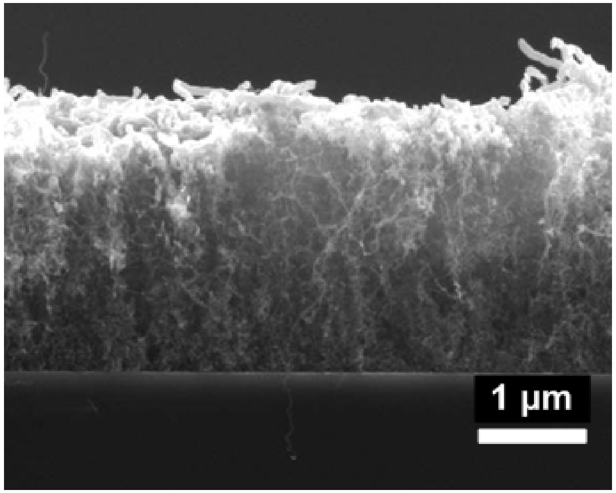


Thermal Cycling of CNT-SiGe Composite

Gao, Leblanc, Marconnet, Shakouri, Goodson et al., "Nanostructured Interfaces for Thermoelectrics," Proc. ICT 2009. J. Electronic Materials (2010).

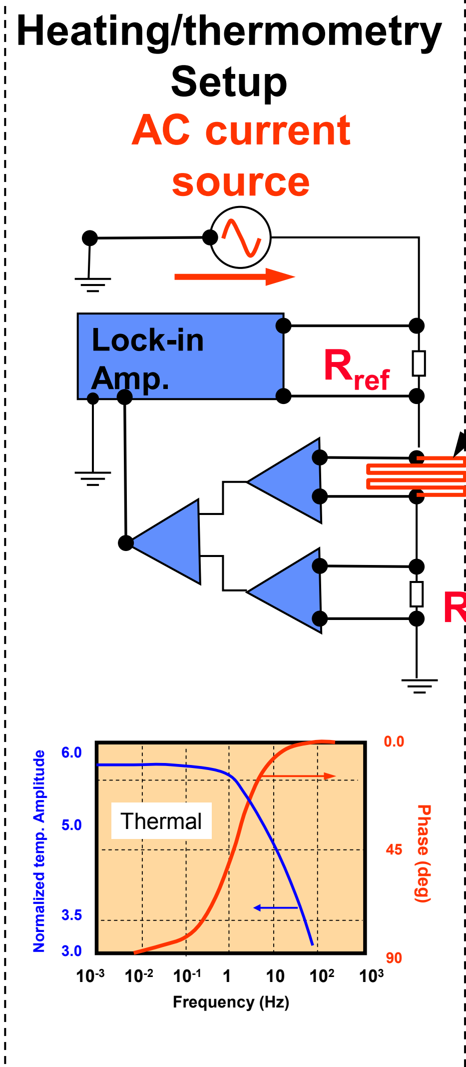


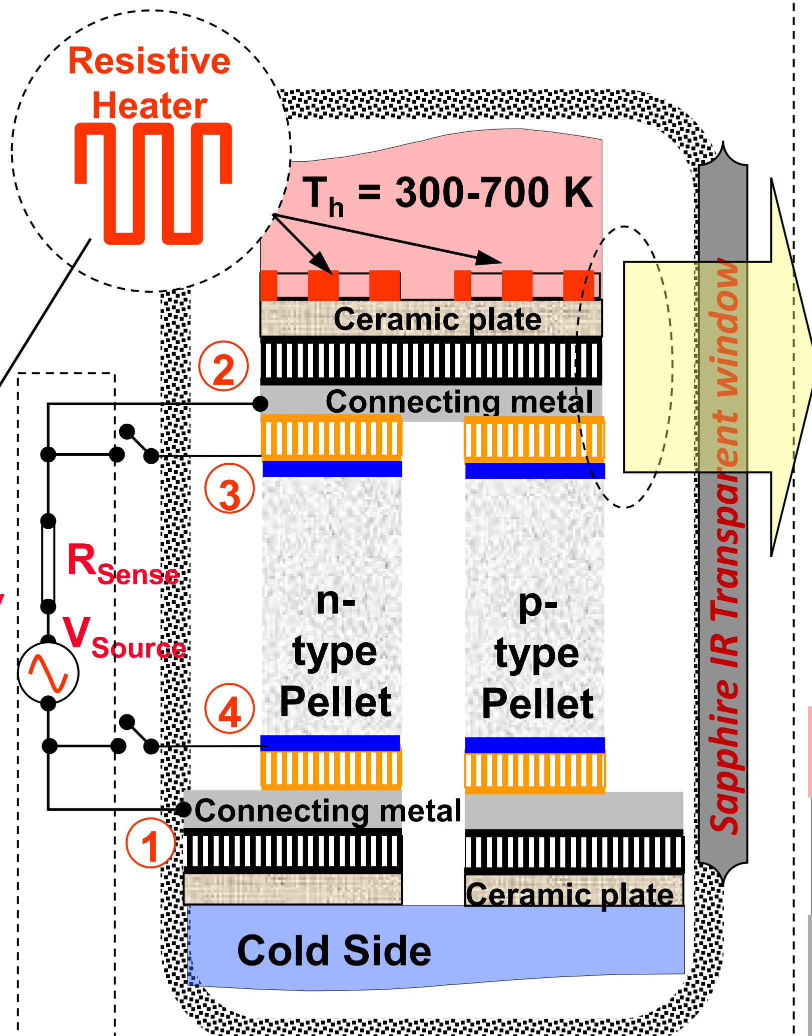




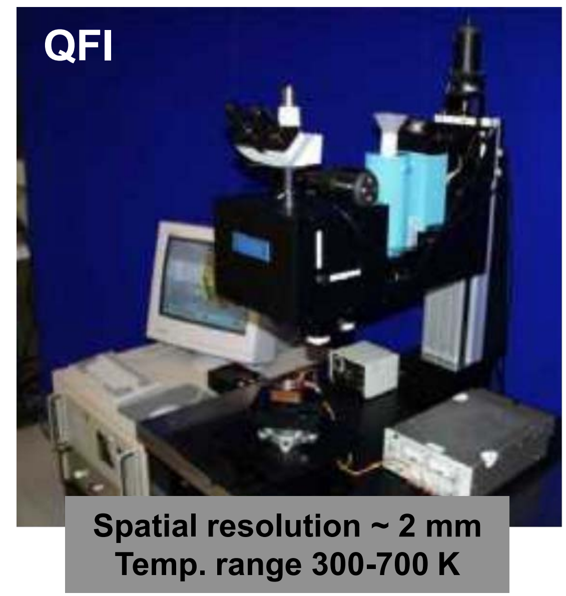
Resistances for 1.5, 2.5, and 40 micron thick CNT films varied between 0.035 and 0.055 cm^2 ^{o}C/W, with evidence of decreasing engagement with increasing film thickness.

$(ZT)_{eff}$ Characterization with Electrical Heating & Cross-Sectional IR Thermometry





IR microscope system



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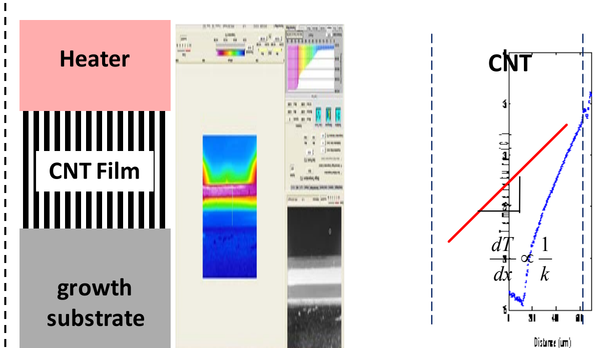
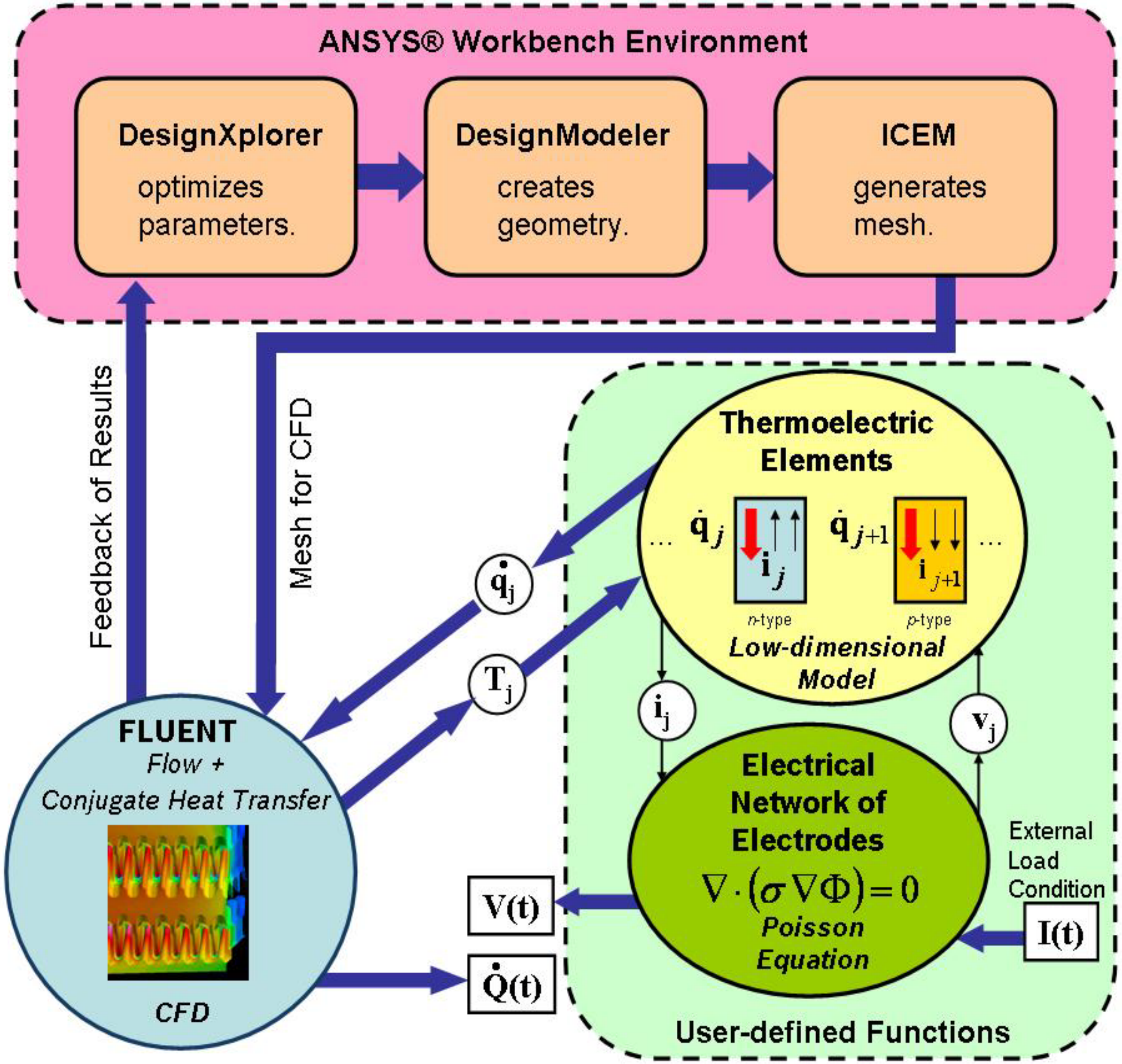


HX and System-Level Simulations



- Bosch-lead system simulations explore impact of improved parameters on system efficiency
- Multiphysics simulations of thermal/thermoelectric transport in TE material, and interface transport incorporating ab initio results.
- HX design and optimization accounts for novel pressure drop designs including Stanford Vapor Escape technology

Educational Engagement

Thermoelectrics for Vehicles Challenge: Multi-University Competition

Long-term vision: Teams of undergraduates work with commercial TE components and heat sinks to extract waste heat from demo vehicle exhaust.

✓Connects classroom education and research & development.

✓Links students with industry, graduate & faculty advisors.

Undergraduate Thermoelectrics Lab

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

✓ Connects theory and practical applications.

✓ Recruits undergraduates for research experiences in thermoelectrics with graduate student mentoring.

K-12 Educational Outreach

High school students and teachers will conduct energy-conversion research in Stanford's Microscale Heat Transfer Laboratory.

Interactions and Flow of Samples & Information

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