alphabet energy

we make waste heat valuable

# Multiphysics Simulation of a Thermoelectric Conversion System

Jordan Chase / COMSOL Boston 2016
jordan@alphabetenergy.com

# We make waste heat valuable


**OUR MISSION:** Deliver the worlds largest thermoelectric power generation / conversion systems

- Founded in 2009 at UC Berkeley, by a material science PhD student, Dr. Matt Scullin
- Headquartered in Hayward, California
- Raised $40$^+$ million in venture capital funding
- 35 full-time employees

# There's a lot of waste heat in the world

FACTORIES

CARS & TRUCKS

MINING

OIL & GAS

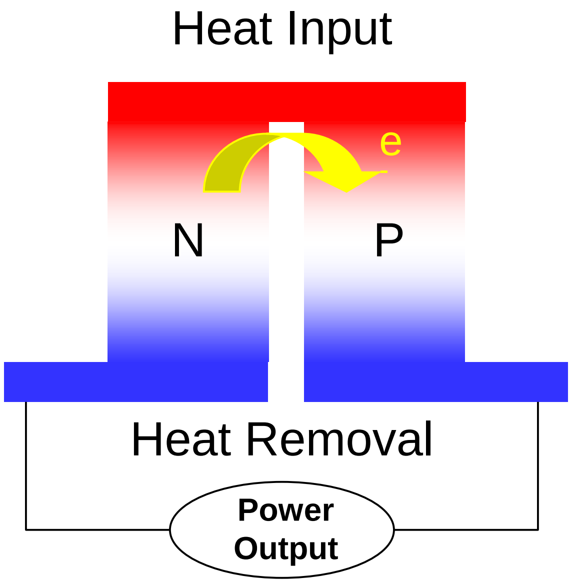
DEFENSE

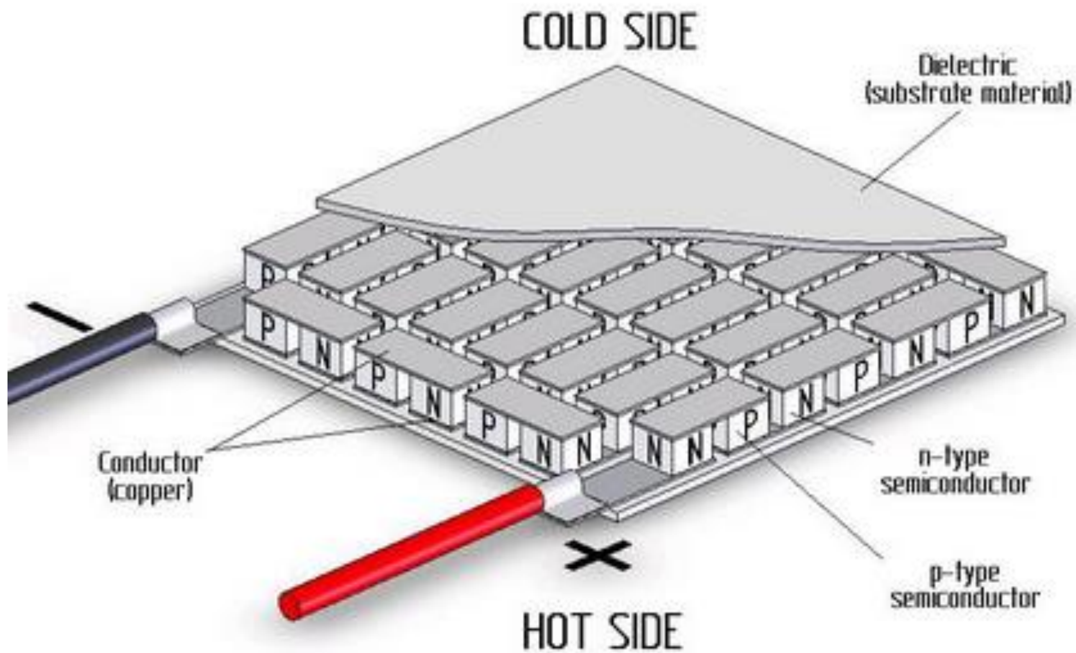
# Physics Principles

the thermoelectric effect

## Power Generation

(Seebeck effect [μV/K])




**Thermoelectric Figure of Merit:**

$$Z = \frac{\alpha^2}{\rho\lambda}$$

$\alpha$ - Seebeck Coefficient
$\rho$ - Electrical Resistivity
$\lambda$ - Thermal Conductivity

http://cratel.wichita.edu/blogs/eecsseniordesignfall2012spring2013/category/prototype-ii/final-report-prototype-ii/

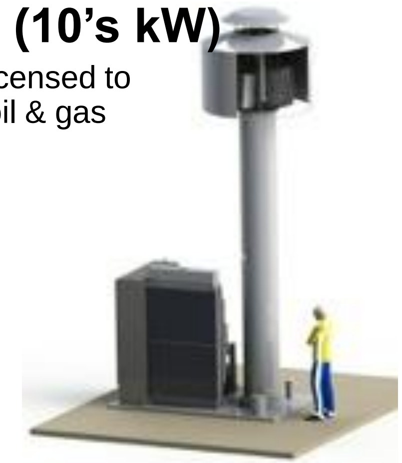
alphabet energy

# From material to turnkey systems

our products address all scales of modular power generation

## Turnkey Generators (10’s kW)

Turnkey generator technology licensed to Partners in target verticals like oil & gas



PGC™ For Flare Stacks

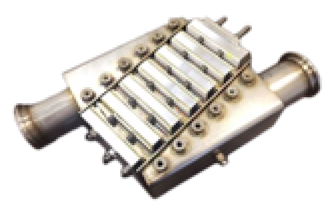
E1™ (20-foot container)
For 1MW engines

Sub-system simulation

## PowerModule™ (kW)

Primary product that Alphabet Energy ships to a range of industries


For industry

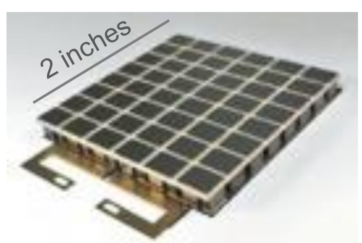


For automotive

Device Simulation

## PowerCard™ (W)

Thermoelectric device contract manufactured by major scale-up partners




## Tetrahedrite

Thermoelectric materials made by Alphabet Energy

# Today's Focus

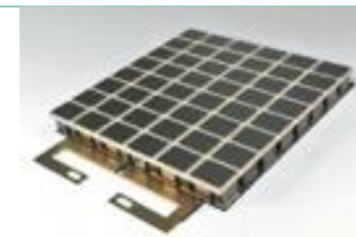
outline of presentation

## Sequential Thermal Steps in Material Fabrication

Integration of high CTE, high modulus metals with their thermoelastic opposites to form ohmic contacts and promote electronic and mechanical reliability…

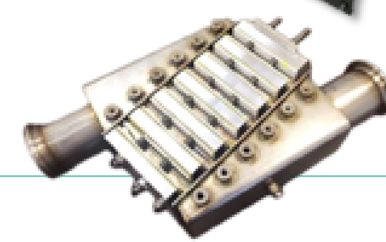
## Thermoelectric Performance of a PowerCard™ (W)

Assembling an idealized device package that survives fabrication without pulling itself apart and exhibits low degradation in-situ under idealized operating conditions…



## Unit Cell Performance of a PowerModule™ (kW)

Maintaining homogenous operating conditions for an array of thermoelectric devices while the nature of heat exchangers is to cause in-plane temperature gradients and thereby anisotropic deformation



# Residual Thermal Stress

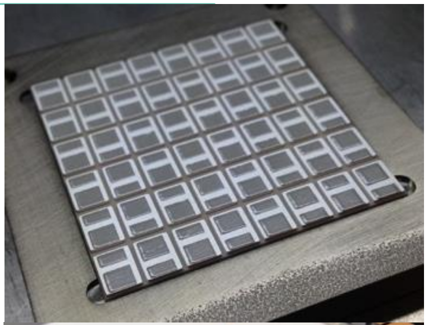
sequential thermal steps in material/fabrication

## General Methodology

Discretize fabrication process into individual steps within Comsol:

1. Firing of hot shunts (conductors) onto dielectric substrate
2. Depositing of metals onto thermoelectric materials
   - Ohmic contacts
   - Diffusion barriers
   - Thermoelastic buffers
3. Thick-film brazing of metallized TE elements onto the substrate
4. Soldering of hot-side subassembly onto the flex circuit
5. Loading the device with in-situ conditions
   - Compressive force
   - Temperature gradient / Heat flux
   - Direct current

Quantitative assessment is difficult; primary intent is qualitative study of reducing the induced stress.



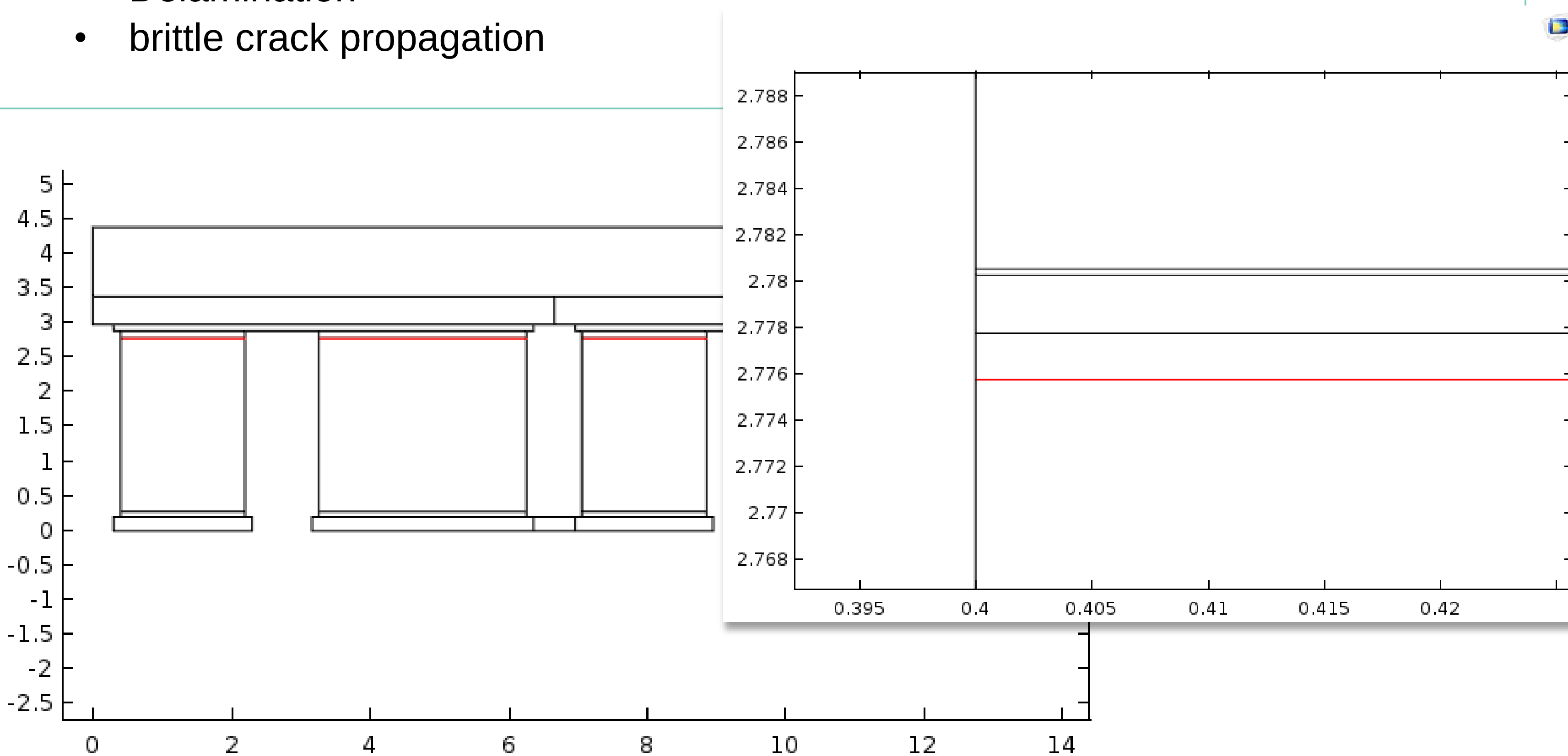
# Model Output

## 2D solid mechanics w/ thermal stress

**Motivation**

If the interfacial stresses reach a critical value, one may build hypothesis around failure mechanisms such as:

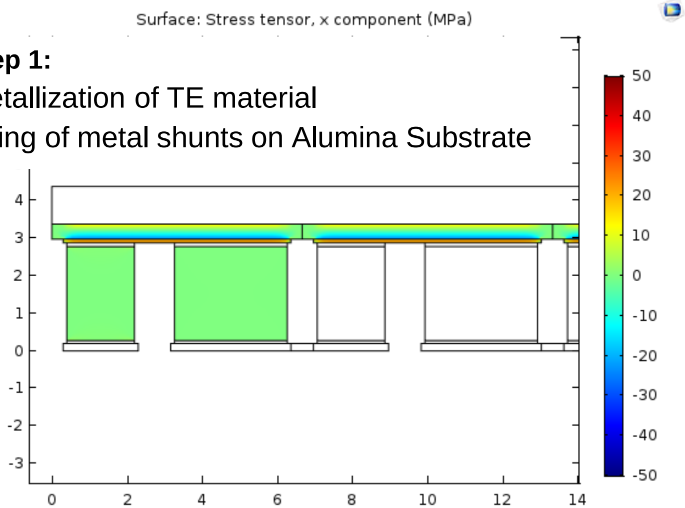
- Delamination
- brittle crack propagation



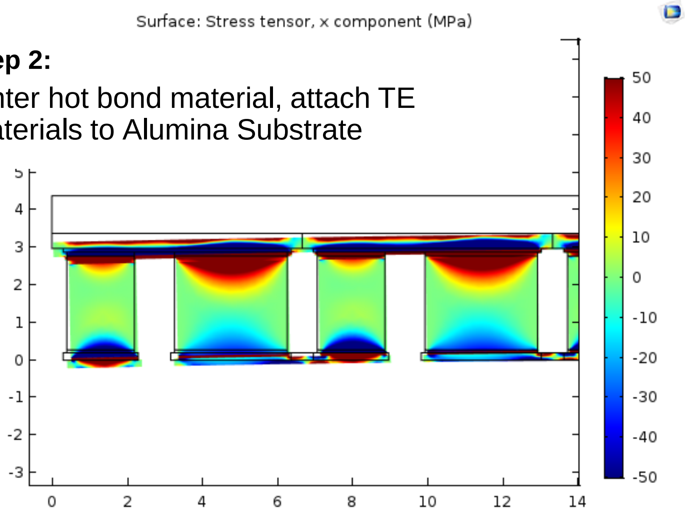
# Results

## 2D solid mechanics w/ thermal stress

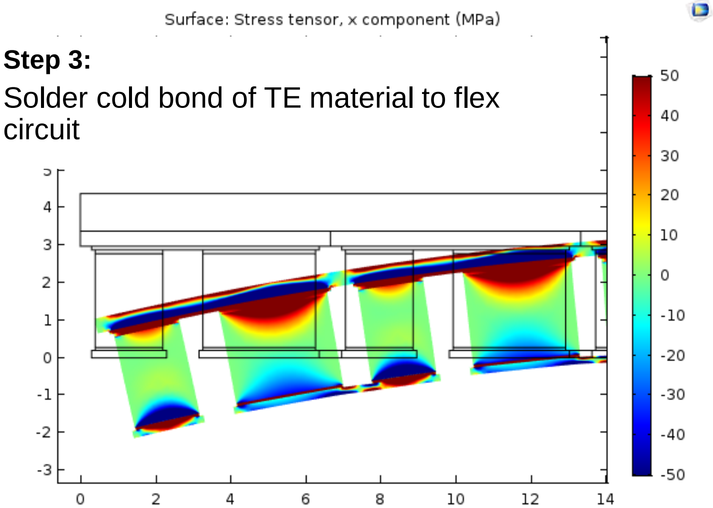
**Step 1:**
Metallization of TE material
Firing of metal shunts on Alumina Substrate



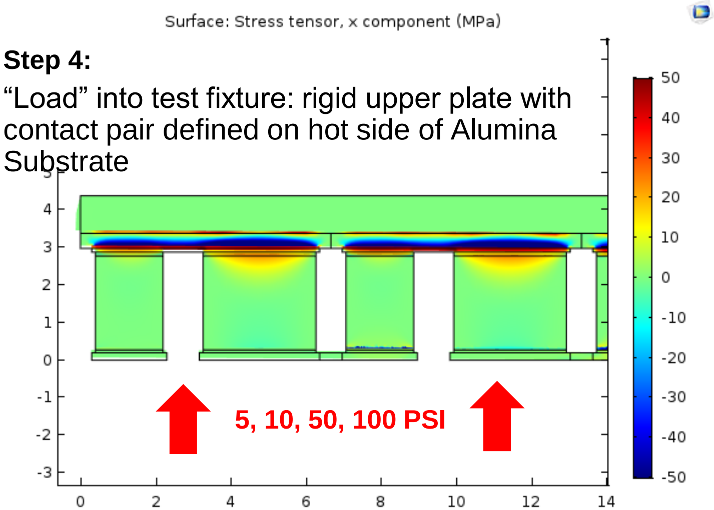

**Step 2:**
Sinter hot bond material, attach TE materials to Alumina Substrate



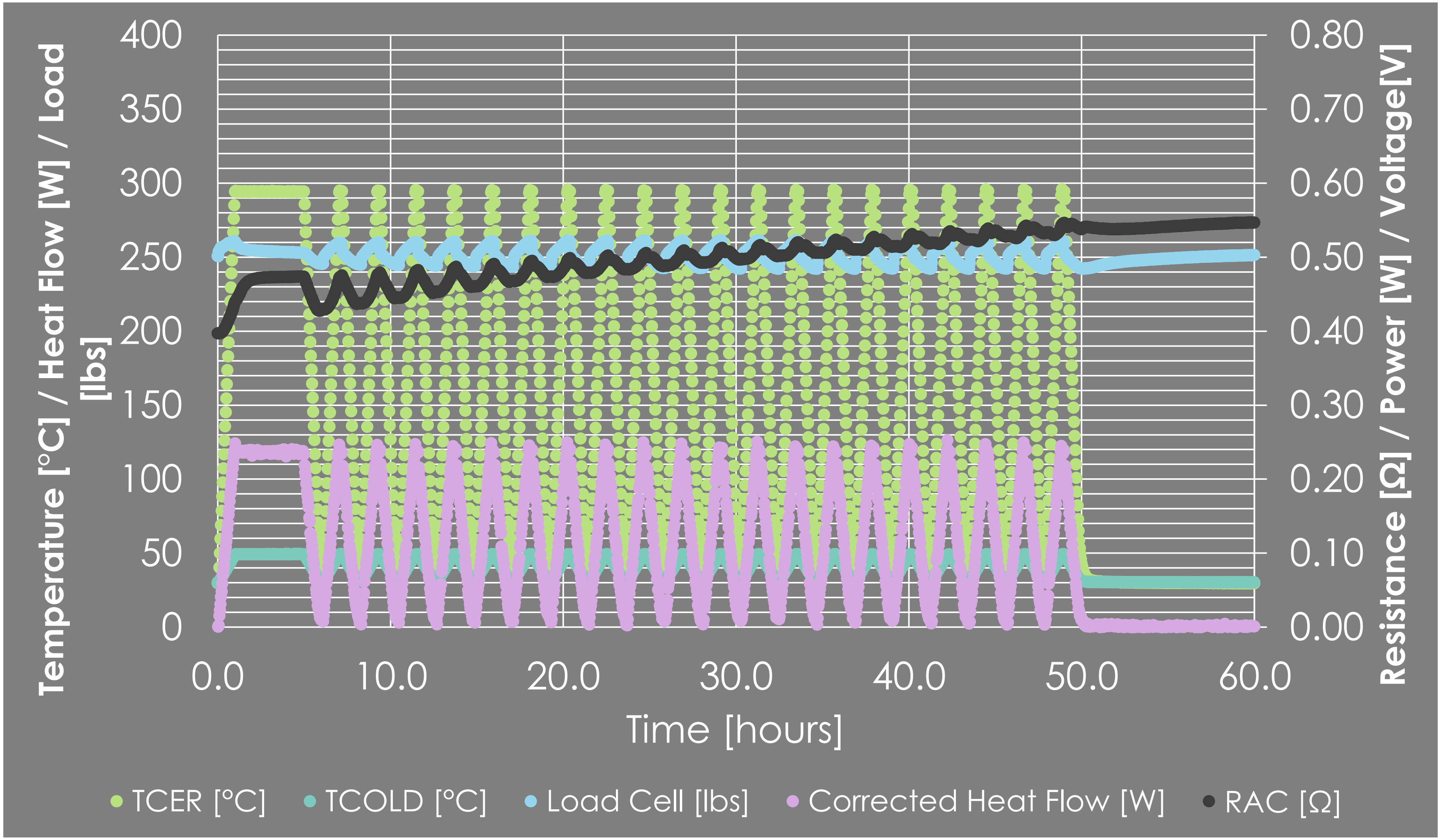

**Step 3:**
Solder cold bond of TE material to flex circuit




**Step 4:**
“Load” into test fixture: rigid upper plate with contact pair defined on hot side of Alumina Substrate

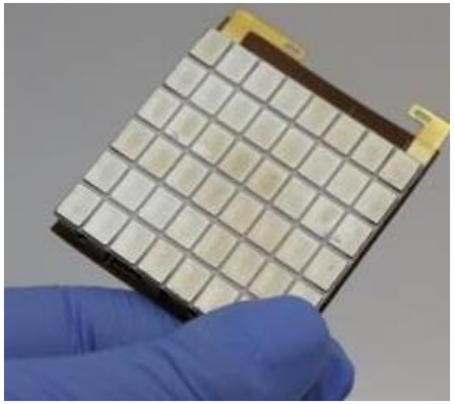


# Test Data Example



# Thermoelectric Performance

of a PowerCard™ ($10^2$ $W_e$)



## General Methodology

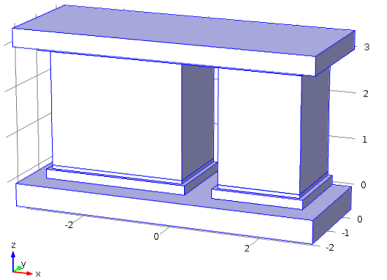
Parameterize the geometry of the thermoelectric device

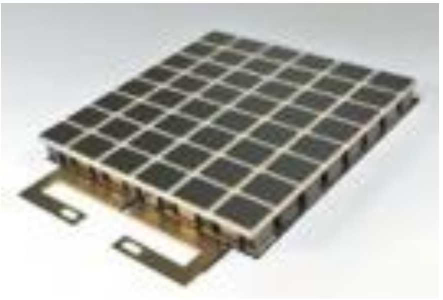
- Thermal resistance: L/W/H of TE elements, fill fraction
- Ohmic losses: thickness of hot and cold electrical shunts
- Thermal parasitics: thickness of substrates, addition of thermal interface materials, thermal bypass phenomena

## Boundary Conditions

This simplified model employs isothermal boundary conditions, thus fixing the heat flux through the part and disallowing in-plane temperature gradients.

- Hot Junction Temperature
- Cold Junction Temperature
- Ground
- Current Density





# Model Output

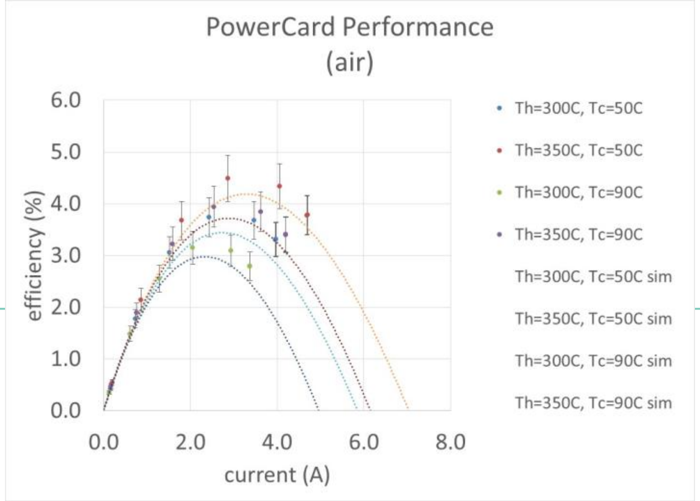
## 3D thermoelectric effect

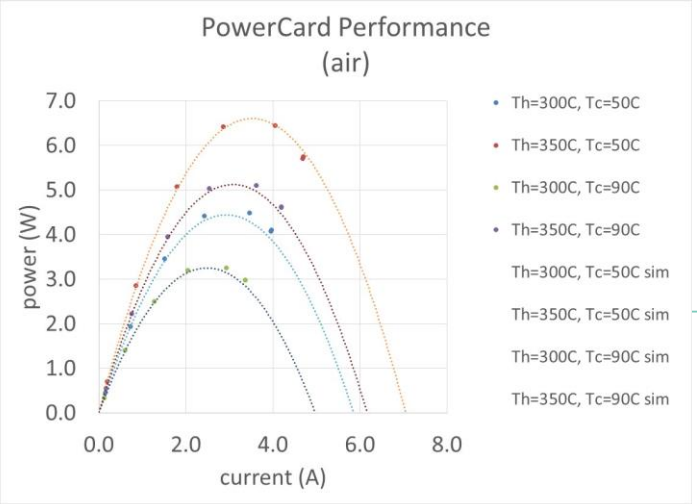
### Motivation

In order to establish the quality of the fabrication process, there must be an understanding of the expected, beginning-of-life characteristics of the device.

Metrics used include internal electrical resistance; since peak power comes at the load-matched operating conditions and is a property that is possible to measure continuously as a function of time and temperature.

Similarly, in order to quantify reliability and degradation rates, the expected PowerCard performance allows us to measure what damage may be inherent to the fabrication process or subsequently realized in-situ.



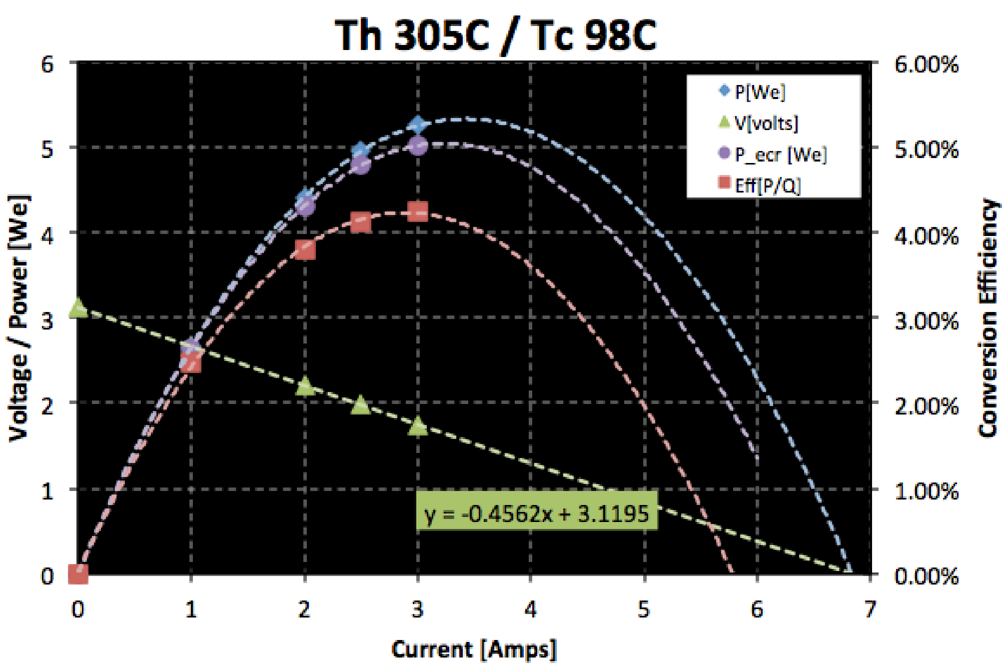



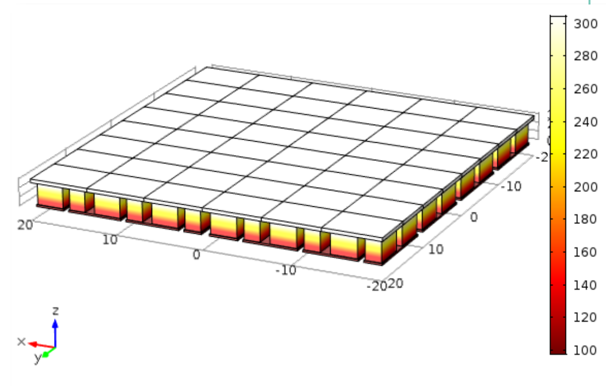
## The Power Curve

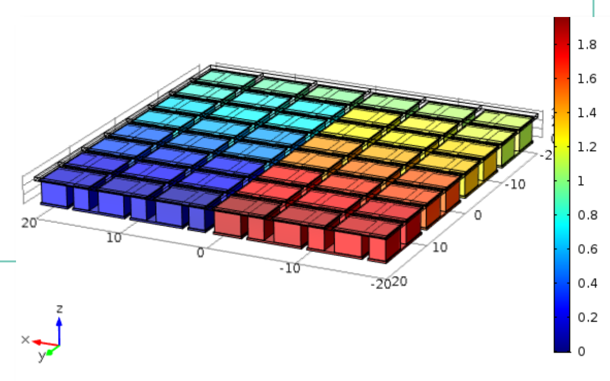
A parametric study of the current density mimics the test load applied by a power electronics system.

**The model then yields:**

- internal resistance of the device
- Peak Power Conversion
- Thermoelectric Efficiency



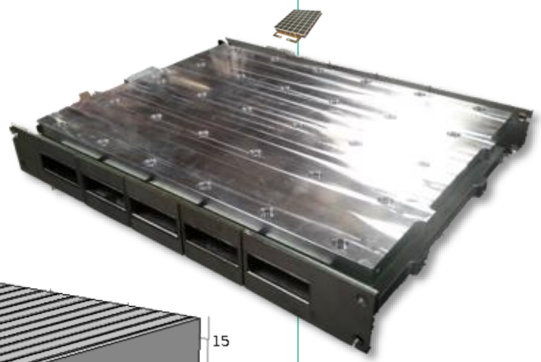


# Unit Cell Performance

of a PowerModule™ ($10^2$-$10^3$ $W_e$)

## General Methodology

In addition to the previous method, parameterize the geometries of the hot gas heat exchanger and cold sink heat exchanger:



## Boundary Conditions

**Hot heat exchanger:**

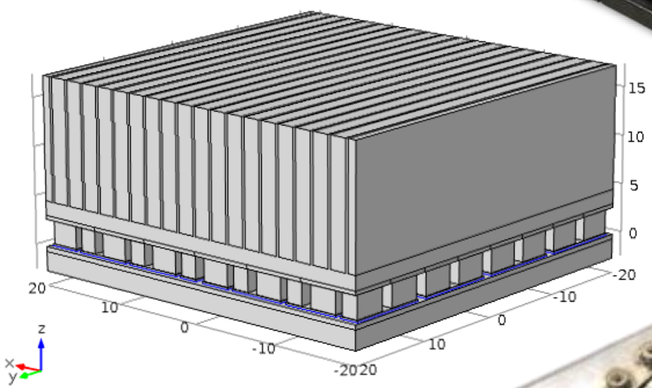
- Inlet mass flow
- Inlet Temperature
- Cold side heat transfer coefficient

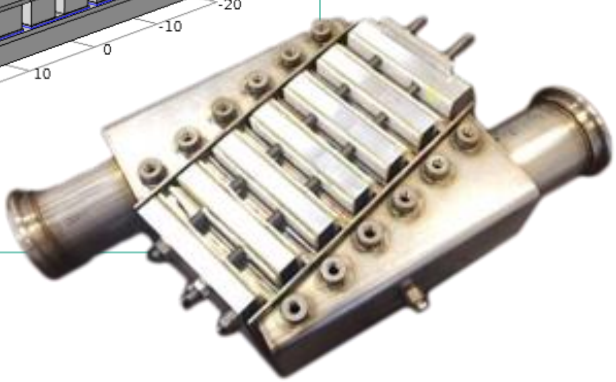
**Thermoelectric PowerCard™**

- Ground
- Current Density

**Cold Heat Exchanger**

- External temperature
- Heat Transfer Coefficient



# Model Output

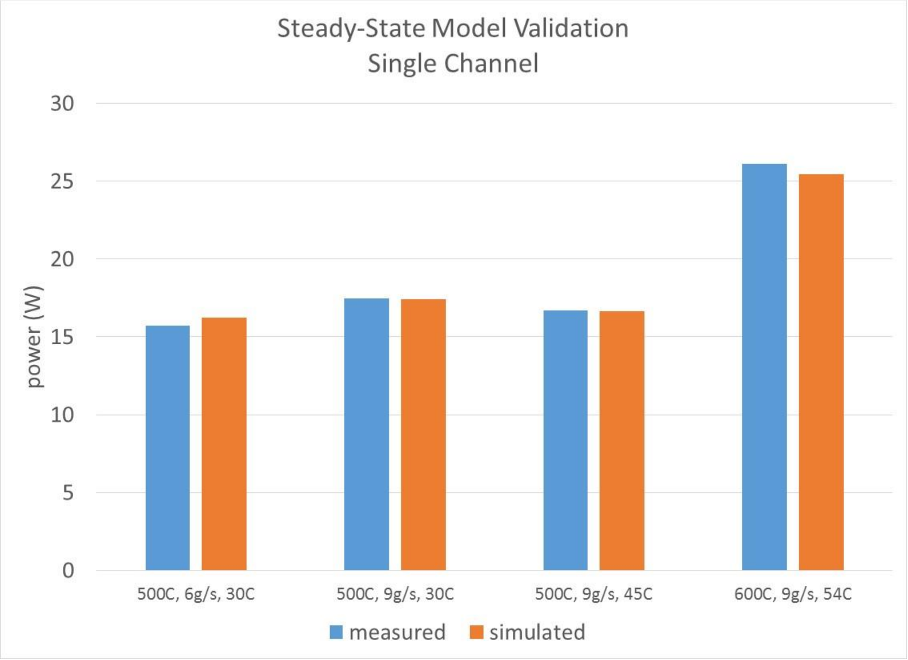
3D heat transfer in solids & fluids + non-isothermal flow + thermoelectric effect

## Motivation

Modeling the coupled system of heat source + thermoelectric device + cold sink incorporates 3D and non-linear effects in contrast to a typical, 1D, empirical model.

Producing electrical characteristics of the complete system provides design inputs for the power electronics system that renders the system practical and economical, and is non-trivial to build beyond 98% efficiency.

- Electrical contact resistivity (Ohmic contacts vs. Schotkey barrier)
- Proper wetting and bonding between metallic surfaces
- Delamination of metallization layers
- Presence and prevalence of micro-cracks



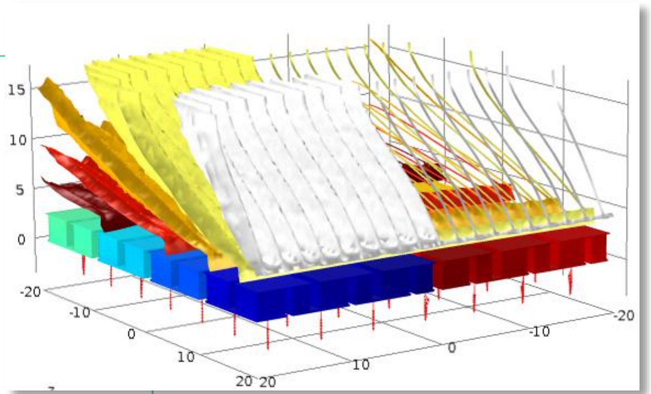
# Results

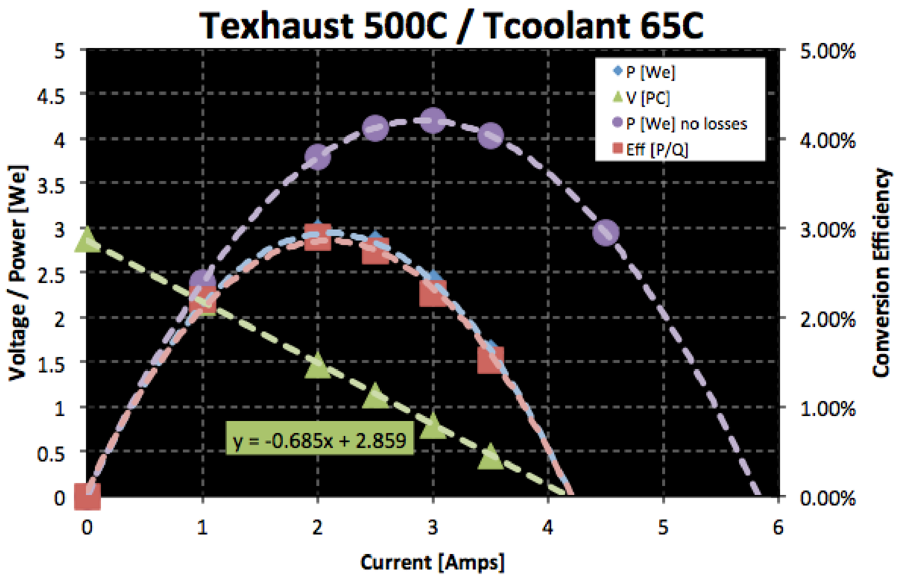
3D heat transfer in solids & fluids + non-isothermal flow + thermoelectric effect

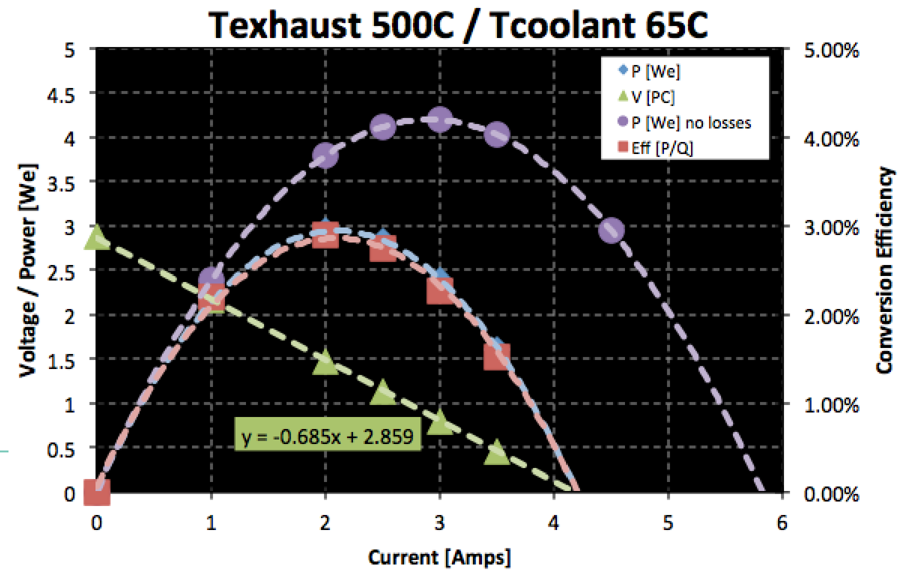
## Power Curves as a function of flow

This model produces the same outputs as the previous. Additional effects come into play that account for:

- 2D, in-plane temperature gradients
- Thermal interface resistances





# Ongoing Work

the usual suspects

## Material Properties

- There is currently no ANSI / NIST protocol for measuring and reporting thermoelectric material properties... honor system
- Intrinsic behavior of TE materials is mechanically brittle, electronically conductive, thermally insulating… proposes unique issues with respect to modeling plastic deformation and critical stress failures
- Simulating interfacial layers of thicknesses between 10 nm & 10μm… begs questions around how these materials (e.g. metals) behave with respect to bulk properties

# Rewind + Q/A

## COMSOL multiphysics at Alphabet Energy

The use of COMSOL builds confidence in:

- The mechanical reliability of our PowerCard$^{TM}$ and educates the design process based on material, geometric, and manufacturing constraints.
- Verifiable transport properties of custom-made thermoelectric materials and devices.
- Our ability to design, model, and construct large thermoelectric systems capable of producing kilowatts of electrical power derived from a core device and/or sub-system that produces hundreds of watts.

Each step in the development of a thermoelectric system combines multiphysics phenomena that are not easily considered in a homogenous modeling tool.

Manufacturing steps of hot-pressing, metallizing, dicing, soldering, bonding, firing, coating, and testing act to bake in a high-cost of development. Any chance to remove iterations of the fabrication process through simulation creates opportunities to start the research at the system level, ultimately allowing us to deliver practical systems to our customers.

The entire Alphabet Energy teams is behind this work & they’re best family of nerds I’ve ever known.

Thank you!

jordan@alphabetenergy.com

www.alphabetenergy.com